Calculated coordinates, energies and vibrational frequencies for the computational chemistry in:

**A comprehensive understanding of carbon-carbon bond formation through alkyne migratory insertion into manganacycles.**

L. Anders Hammarback,[a] Jonathan B. Eastwood,[a] Thomas J. Burden,[a] Callum J. Pearce,[a] Ian P. Clark,[b] Michael Towrie,[b] Alan Robinson,[c] Ian J. S. Fairlamb*[a] and Jason M. Lynam*[a]

[a] Department of Chemistry, University of York, Heslington, York, YO10 5DD, UK ian.fairlamb@york.ac.uk, jason.lynam@york.ac.uk

[b] Central Laser Facility, STFC Rutherford Appleton Laboratory, Harwell Science and Innovation Campus, Didcot, Oxfordshire, OX11 0QX, UK.

[c] Syngenta Crop Protection AG, Münchwilen, Breitenloh 5, 433, Switzerland.
### 2aa

SCF Energy (au) BP86/SV(P)  \(-2427.867667755\)
SCF Energy (au) PBE0/def2-TZVPP  \(-2427.429781153\)
SCF Energy (au) PBE0/def2-TZVPP  \(-2427.4405898830\) (Toluene Correction)
Zero Point Energy (au) 0.2962891
Chemical Potential (kJ mol\(^{-1}\)) 622.29
Dispersion Correction (au) PBE0/def2-TZVPP 0.06324694

xyz coordinates
43

- Mn 1.4645116 0.2343712 0.5909323
- C 1.7816619 0.4425193 2.3507023
- C 3.1502517 -0.3752202 0.3332030
- C 1.9986404 1.9297007 0.2215559
- O 2.3604200 3.0246807 0.0388304
- O 4.2519496 -0.6744970 0.1185508
- O 1.9860597 0.5565279 3.4908732
- C 1.3688135 -0.1875101 1.3527343
- C -0.731050 1.9759850 0.4993644
- C -2.4254157 2.2929513 0.6800968
- C -3.2774363 1.3187041 1.2262739
- C -2.7416292 0.0711722 1.5626743
- C -0.6964351 -1.4521885 1.6603519
- C 0.6639318 -1.4851738 1.6139593
- C 0.6707753 -3.7894906 2.2061021
- C -0.6513101 -3.7241982 2.4956329
- C -1.3727373 -2.5906643 2.2321973
- H -0.3769659 2.7177069 0.0793093
- H -2.7928098 3.2910274 0.3962989
- H -4.3469456 1.5296005 1.3888023
- H -3.3841721 -0.7119417 1.9907119
- O 2.5769801 -2.9477696 1.3720105
- C 1.1727391 -4.9866275 3.1068736
- H -2.446006 -2.5726096 2.4751610
- N -0.5455730 0.7755408 0.8231995
- C 0.8586201 1.2727425 -2.6141879
- C 1.9732273 2.0182441 -3.0776447
- C 1.8089943 2.9990900 -4.0649810
- C 0.5359603 3.2632459 -4.6022414
- C -0.5765511 2.5332325 -4.1481913
- C -0.4219365 1.5470344 -3.1628167
- H 2.9715633 1.8130324 -2.6613145
- H 2.6864145 3.5651591 -4.4186222
- H 0.4115198 4.0380631 -5.3765206
- H -1.5768983 2.7310968 -4.5679957
- H -1.2907383 0.9686119 -2.8108704
- C 1.0036831 0.2255046 -1.6318907
- C 0.9714273 -0.9282526 -1.1151016
- H 0.8955204 -2.0110916 -1.2178750
- H -1.0093753 -5.8521617 2.4222750
- H -2.2559519 -4.9078343 3.3298297
- H -0.6283127 -5.2198957 4.0505213

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number cm\(^{-1}\) | IR intensity km/mol | selection rules |
|---|------|----------|--------------------------|--------------------|-----------------|
| 1 |      |          | 0.00                     | 0.00000            | -               |
| 2 |      |          | 0.00                     | 0.00000            | -               |
| 3 |      |          | 0.00                     | 0.00000            | -               |
| 4 |      |          | 0.00                     | 0.00000            | -               |
| 5 |      |          | 0.00                     | 0.00000            | -               |
|    | a     |     |      | 0.00000 | -     | -     |
|----|-------|-----|------|---------|-------|-------|
| 7  | a     | 12.83 | 0.33682 | YES     | YES   |
| 8  | a     | 28.85 | 0.53951 | YES     | YES   |
| 9  | a     | 32.31 | 0.18001 | YES     | YES   |
| 10 | a     | 37.53 | 1.95531 | YES     | YES   |
| 11 | a     | 60.15 | 0.05712 | YES     | YES   |
| 12 | a     | 69.85 | 0.11556 | YES     | YES   |
| 13 | a     | 75.55 | 0.07607 | YES     | YES   |
| 14 | a     | 81.69 | 0.39008 | YES     | YES   |
| 15 | a     | 91.73 | 1.64917 | YES     | YES   |
| 16 | a     | 99.05 | 0.97666 | YES     | YES   |
| 17 | a     | 109.88 | 0.12991 | YES     | YES   |
| 18 | a     | 119.87 | 0.10005 | YES     | YES   |
| 19 | a     | 123.49 | 1.49253 | YES     | YES   |
| 20 | a     | 137.69 | 0.14153 | YES     | YES   |
| 21 | a     | 148.69 | 1.92865 | YES     | YES   |
| 22 | a     | 153.79 | 1.84421 | YES     | YES   |
| 23 | a     | 159.65 | 1.34880 | YES     | YES   |
| 24 | a     | 163.44 | 2.66553 | YES     | YES   |
| 25 | a     | 192.46 | 1.04417 | YES     | YES   |
| 26 | a     | 219.28 | 0.63073 | YES     | YES   |
| 27 | a     | 249.36 | 0.36492 | YES     | YES   |
| 28 | a     | 257.61 | 1.89803 | YES     | YES   |
| 29 | a     | 294.76 | 2.37808 | YES     | YES   |
| 30 | a     | 302.79 | 4.27708 | YES     | YES   |
| 31 | a     | 322.17 | 10.76010 | YES     | YES   |
| 32 | a     | 330.22 | 13.32318 | YES     | YES   |
| 33 | a     | 398.32 | 4.09474 | YES     | YES   |
| 34 | a     | 401.54 | 0.07874 | YES     | YES   |
| 35 | a     | 414.56 | 12.49803 | YES     | YES   |
| 36 | a     | 428.96 | 1.22830 | YES     | YES   |
| 37 | a     | 455.65 | 0.76864 | YES     | YES   |
| 38 | a     | 457.06 | 9.03126 | YES     | YES   |
| 39 | a     | 467.19 | 5.31735 | YES     | YES   |
| 40 | a     | 479.14 | 10.45341 | YES     | YES   |
| 41 | a     | 486.43 | 4.00283 | YES     | YES   |
| 42 | a     | 493.29 | 15.20698 | YES     | YES   |
| 43 | a     | 500.80 | 11.90031 | YES     | YES   |
| 44 | a     | 521.26 | 39.87505 | YES     | YES   |
| 45 | a     | 532.31 | 6.17382 | YES     | YES   |
| 46 | a     | 537.42 | 1.03599 | YES     | YES   |
| 47 | a     | 544.56 | 5.83322 | YES     | YES   |
| 48 | a     | 561.68 | 1.89963 | YES     | YES   |
| 49 | a     | 581.56 | 3.53684 | YES     | YES   |
| 50 | a     | 590.09 | 1.38142 | YES     | YES   |
2aa'

SCF Energy (au) BP86/SV(P)  -2427.867511092
SCF Energy (au) PBE0/def2-TZVPP  -2427.429306722
SCF Energy (au) PBE0/def2-TZVPP  -2427.4398029146 (Toluene Correction)
Zero Point Energy (au)  0.2965857
Chemical Potential (kJ mol⁻¹)  627.02
Dispersion Correction (au) PBE0/def2-TZVPP  -0.06502154

xyz coordinates
43

Mn   1.5147523  1.8031815  0.1393490
C    1.7127939  2.1387468  1.9018085
C    3.2493306  1.2886291 -0.0008400
C    1.9281023  3.5153518  0.2748048
O    2.1937308  4.6255178  0.5219659
O    4.3733880  1.0453489  0.1588772
O    1.8492529  2.358813  3.0367268

H     0.3079859  1.1705764  0.7982681
C    -1.1705494  3.2587826 -0.2561876
C    -2.5571983  3.4451580  0.1964264
C    -3.3444393  2.4413384  0.3921436
C    -2.7119508  1.2979551  0.8908193
C    -1.3079859  1.1705764  0.7982681
C    -1.1705494  3.2587826 -0.2561876
C    -2.5571983  3.4451580  0.1964264
C    -3.3444393  2.4413384  0.3921436
C    -2.7119508  1.2979551  0.8908193
O     2.1937308  4.6255178  0.5219659
O    4.3733880  1.0453489  0.1588772
O    1.8492529  2.358813  3.0367268

\$vibrational spectrum

| # | mode | symmetry | wave number cm⁻¹ | IR intensity km/mol | selection rules |
|---|------|----------|------------------|---------------------|-----------------|
| 1 |      |          | 0.00             | 0.00000             | -                |
| 2 |      |          | 0.00             | 0.00000             | -                |
| 3 |      |          | 0.00             | 0.00000             | -                |
| 4 |      |          | 0.00             | 0.00000             | -                |
| 5 |      |          | 0.00             | 0.00000             | -                |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 6 | a | 0.00 | 0.00000 | - | - |
| 7 | a | 24.31 | 0.19772 | YES | YES |
| 8 | a | 26.79 | 0.77570 | YES | YES |
| 9 | a | 44.61 | 0.64194 | YES | YES |
| 10 | a | 50.58 | 0.51026 | YES | YES |
| 11 | a | 66.00 | 0.33144 | YES | YES |
| 12 | a | 72.98 | 0.69452 | YES | YES |
| 13 | a | 77.43 | 0.43971 | YES | YES |
| 14 | a | 83.41 | 0.66789 | YES | YES |
| 15 | a | 95.16 | 0.95452 | YES | YES |
| 16 | a | 100.70 | 0.38104 | YES | YES |
| 17 | a | 106.25 | 0.32277 | YES | YES |
| 18 | a | 124.35 | 0.25320 | YES | YES |
| 19 | a | 127.92 | 0.85768 | YES | YES |
| 20 | a | 138.50 | 0.05127 | YES | YES |
| 21 | a | 150.94 | 0.32827 | YES | YES |
| 22 | a | 158.78 | 1.28351 | YES | YES |
| 23 | a | 166.59 | 0.35274 | YES | YES |
| 24 | a | 180.24 | 1.66707 | YES | YES |
| 25 | a | 188.29 | 2.27493 | YES | YES |
| 26 | a | 212.55 | 0.37909 | YES | YES |
| 27 | a | 247.14 | 0.72321 | YES | YES |
| 28 | a | 260.96 | 0.15337 | YES | YES |
| 29 | a | 294.50 | 3.08395 | YES | YES |
| 30 | a | 308.25 | 8.36217 | YES | YES |
| 31 | a | 326.79 | 2.69630 | YES | YES |
| 32 | a | 337.65 | 8.35710 | YES | YES |
| 33 | a | 398.14 | 3.36635 | YES | YES |
| 34 | a | 403.18 | 2.34038 | YES | YES |
| 35 | a | 408.53 | 10.62109 | YES | YES |
| 36 | a | 428.45 | 10.50586 | YES | YES |
| 37 | a | 457.68 | 0.58035 | YES | YES |
| 38 | a | 460.91 | 0.98099 | YES | YES |
| 39 | a | 468.88 | 4.53489 | YES | YES |
| 40 | a | 479.50 | 3.90853 | YES | YES |
| 41 | a | 484.74 | 7.08867 | YES | YES |
| 42 | a | 493.18 | 4.58799 | YES | YES |
| 43 | a | 506.36 | 23.83062 | YES | YES |
| 44 | a | 525.23 | 14.38684 | YES | YES |
| 45 | a | 535.01 | 3.26780 | YES | YES |
| 46 | a | 541.18 | 0.57910 | YES | YES |
| 47 | a | 559.77 | 3.82363 | YES | YES |
| 48 | a | 564.37 | 1.56700 | YES | YES |
| 49 | a | 583.10 | 1.77315 | YES | YES |
| 50 | a | 593.14 | 1.93748 | YES | YES |
2ba

SCF Energy (au) BP86/SV(P) -2277.516190056
SCF Energy (au) PBE0/def2-TZVPP -2277.070640511
SCF Energy (au) PBE0/def2-TZVPP -2277.0778650907 (Toluene Correction)
Zero Point Energy (au) 0.2897773
Chemical Potential (kJ mol⁻¹) 615.66
Dispersion Correction (au) PBE0/def2-TZVPP -0.06110662

xyz coordinates

|   |     |       |      |
|---|-----|-------|------|
|   |     |       |      |
| Mn | 1.3218603 | 0.2161020 | 0.6121444 |
| C  | 1.7788652 | 0.6991612 | 2.2861199 |
| C  | 3.0068573 | -0.2730204 | 0.2487755 |
| C  | 1.5913757 | 1.8997864 | -0.0160227 |
| O  | 2.0830196 | 0.0031429 | 3.3682155 |
| C  | -1.3180498 | -0.4492854 | 1.7886866 |
| C  | -1.8747206 | 1.7644718 | 0.9428058 |
| C  | -3.4261769 | 0.7711469 | 1.7027561 |
| C  | -2.6879074 | -0.3376577 | 2.1237114 |
| C  | -0.4465177 | -1.5624103 | 2.1751019 |
| O  | 0.9072958 | -1.4767290 | 1.7297269 |
| C  | 1.7860999 | -2.5181323 | 2.0955425 |
| C  | 1.3438020 | -3.6150948 | 2.8558307 |
| O  | 2.0029626 | -3.6950653 | 3.2795373 |
| C  | -0.8868254 | -2.6697164 | 2.9404323 |
| H  | -0.8883399 | 2.3555919 | 0.0531607 |
| H  | -3.3179336 | 2.6588013 | 0.5861152 |
| H  | -4.4929401 | 0.8621691 | 1.9652861 |
| H  | -3.1679721 | -1.1282940 | 2.7185786 |
| H  | 2.8433831 | -2.4844404 | 1.7833064 |
| H  | 2.0545812 | -4.4155643 | 3.1237603 |
| H  | -0.3442870 | -4.5537096 | 3.8769362 |
| H  | -1.9343081 | -2.7352412 | 3.2784777 |
| N  | -0.7068340 | 0.5308017 | 1.0490580 |
| C  | 0.4186177 | 0.7604854 | -2.6526220 |
| C  | 1.4639894 | 1.4883082 | -3.2758567 |
| C  | 1.2035674 | 2.2810818 | -4.4019640 |
| C  | -0.1001745 | 2.3746674 | -4.9216796 |
| C  | -1.1459588 | 1.6622080 | -4.3088994 |
| C  | -0.8936096 | 0.8615517 | -3.1851924 |
| H  | 2.4862082 | 1.4183505 | -2.8726273 |
| H  | 2.0294261 | 2.8347075 | -4.8783822 |
| H  | -0.3040426 | 3.0034950 | -5.8047658 |
| H  | -2.1704367 | 1.7271619 | -4.7118877 |
| H  | -1.7103084 | 0.2966645 | -2.7081434 |
| C  | 0.661091 | -0.1065099 | -1.5221846 |
| C  | 0.6813710 | -1.1757627 | -0.8449443 |
| H  | 0.5791166 | -2.2589761 | -0.7729843 |

$vibrational spectrum$

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|-----------------|
| 1 |     |          | 0.00        | 0.00000      | -               |
| 2 |     |          | 0.00        | 0.00000      | -               |
| 3 |     |          | 0.00        | 0.00000      | -               |
| 4 |     |          | 0.00        | 0.00000      | -               |
| 5 |     |          | 0.00        | 0.00000      | -               |
| 6 |     |          | 0.00        | 0.00000      | -               |
| 7 | a    |          | 18.14       | 0.20009      | YES             |
|    |   a |      |     |       |       |  YES |  YES |
|----|-----|------|-----|-------|-------|------|------|
|  8 | a   | 29.04| 0.15401 | YES | YES |
|  9 | a   | 39.82| 0.05836 | YES | YES |
| 10 | a   | 57.15| 0.31155 | YES | YES |
| 11 | a   | 69.46| 0.07269 | YES | YES |
| 12 | a   | 74.18| 0.09666 | YES | YES |
| 13 | a   | 86.23| 1.28775 | YES | YES |
| 14 | a   | 90.54| 0.26084 | YES | YES |
| 15 | a   | 99.10| 0.43721 | YES | YES |
| 16 | a   | 109.57| 0.13096 | YES | YES |
| 17 | a   | 113.25| 0.10437 | YES | YES |
| 18 | a   | 117.38| 0.59846 | YES | YES |
| 19 | a   | 130.55| 0.29161 | YES | YES |
| 20 | a   | 162.17| 1.81464 | YES | YES |
| 21 | a   | 165.28| 5.13092 | YES | YES |
| 22 | a   | 188.98| 1.29120 | YES | YES |
| 23 | a   | 222.35| 0.64998 | YES | YES |
| 24 | a   | 242.82| 2.12591 | YES | YES |
| 25 | a   | 262.80| 0.48548 | YES | YES |
| 26 | a   | 282.79| 1.96336 | YES | YES |
| 27 | a   | 319.03| 24.25280 | YES | YES |
| 28 | a   | 358.43| 1.93112 | YES | YES |
| 29 | a   | 400.88| 0.01385 | YES | YES |
| 30 | a   | 410.80| 1.69648 | YES | YES |
| 31 | a   | 420.57| 10.80509 | YES | YES |
| 32 | a   | 437.44| 2.27242 | YES | YES |
| 33 | a   | 454.64| 16.81944 | YES | YES |
| 34 | a   | 456.28| 1.42207 | YES | YES |
| 35 | a   | 472.05| 4.20216 | YES | YES |
| 36 | a   | 480.46| 6.23593 | YES | YES |
| 37 | a   | 486.64| 1.87109 | YES | YES |
| 38 | a   | 492.13| 5.61083 | YES | YES |
| 39 | a   | 502.05| 7.64352 | YES | YES |
| 40 | a   | 508.50| 13.02943 | YES | YES |
| 41 | a   | 524.55| 36.11294 | YES | YES |
| 42 | a   | 539.45| 10.10604 | YES | YES |
| 43 | a   | 551.07| 5.77890 | YES | YES |
| 44 | a   | 557.04| 1.74908 | YES | YES |
| 45 | a   | 609.09| 21.17504 | YES | YES |
| 46 | a   | 614.47| 7.83987 | YES | YES |
| 47 | a   | 623.39| 7.80591 | YES | YES |
| 48 | a   | 625.85| 11.54609 | YES | YES |
| 49 | a   | 643.05| 9.93463 | YES | YES |
| 50 | a   | 653.95| 72.74795 | YES | YES |
SCF Energy (au) BP86/SV(P) -2277.513915506
SCF Energy (au) PBE0/def2-TZVPP -2277.068149867
SCF Energy (au) PBE0/def2-TZVPP -2277.0753739100 (Toluene Correction)
Zero Point Energy (au) 0.2897472
Chemical Potential (kJ mol$^{-1}$) 615.97
Dispersion Correction (au) PBE0/def2-TZVPP 0.06339944

xyz coordinates

| Atoms | X      | Y      | Z      |
|-------|--------|--------|--------|
| Mn    | 1.2258585 | 1.7959458 | 0.2361359 |
| C     | 1.3726238 | 2.2084123 | 1.9870298 |
| C     | 2.9819188 | 1.4607606 | 0.1062994 |
| C     | 1.4143764 | 3.5362389 | -0.2348193 |
| O     | 1.5584791 | 4.6599386 | -0.5184893 |
| O     | 4.1193272 | 1.2134699 | 0.0247307 |
| O     | 1.4762395 | 2.4873278 | 3.1120387 |
| C     | -1.4586829 | 0.7709355 | 0.9713587 |
| C     | -1.6429054 | 2.8509145 | -0.1047515 |
| C     | -3.0388337 | 2.8435896 | -0.0183476 |
| C     | -3.6627762 | 1.7421360 | 0.5941326 |
| C     | -2.8677031 | 0.7049515 | 1.0873249 |
| O     | -0.5234072 | -0.2504435 | 1.4522467 |
| O     | 0.8585732 | 0.0090274 | 1.2153396 |
| C     | 1.7918361 | -0.9298249 | 1.7020787 |
| C     | 1.3783681 | -2.0989935 | 2.3648978 |
| C     | 0.0097808 | -2.3548680 | 2.5709695 |
| C     | -0.9371225 | -1.4300543 | 2.1171572 |
| H     | -1.1144621 | 3.6948098 | -0.5748638 |
| H     | -3.6178365 | 3.6834080 | -0.4221460 |
| H     | -4.7602400 | 1.6941301 | 0.6854248 |
| H     | -3.3329288 | -0.1690477 | 1.5661469 |
| H     | 2.8730423 | -0.7571295 | 1.5698616 |
| H     | 2.1337988 | -2.8169591 | 2.7274855 |
| H     | -0.3163077 | -3.2707270 | 3.0901531 |
| H     | -2.0076939 | -1.6308725 | 2.2885396 |
| N     | -0.8676015 | 1.8541483 | 0.3737200 |
| H     | 1.0761801 | 2.5805694 | -2.6558619 |
| C     | 0.9964970 | 1.8046790 | -1.8925299 |
| C     | 0.8866792 | 0.5828388 | -1.5683411 |
| C     | 0.6452584 | -0.8197349 | -1.8227326 |
| C     | 0.1610902 | -3.5448254 | -2.4166148 |
| C     | 1.4167314 | -3.1382082 | -1.9305350 |
| C     | 1.6585020 | -1.7912392 | -1.6274982 |
| C     | -0.6176938 | -1.2392218 | -2.3130126 |
| C     | -0.8537739 | -2.5064222 | -2.6051716 |
| H     | -0.0258660 | -4.6064105 | -2.6487203 |
| H     | 2.2185010 | -3.8805090 | -1.7827013 |
| H     | 2.6422624 | -1.4735862 | -1.2495178 |
| H     | -1.4095959 | -0.4891813 | -2.4676116 |
| H     | -1.8404977 | -2.9006858 | -2.9879057 |

$\text{vibrational spectrum}$

| #  | mode | symmetry | wave number (cm$^{-1}$) | IR intensity (km/mol) | selection rules |
|----|------|----------|-------------------------|----------------------|-----------------|
| 1  |      |          | 0.00                    | 0.00000              | -               |
| 2  |      |          | 0.00                    | 0.00000              | -               |
| 3  |      |          | 0.00                    | 0.00000              | -               |
| 4  |      |          | 0.00                    | 0.00000              | -               |
| 5  |      |          | 0.00                    | 0.00000              | -               |
| 6  |      |          | 0.00                    | 0.00000              | -               |
| 7  | a    |          | 17.53                   | 0.21377              | YES             | YES             |
|   |   | 27.79 | 0.28921 | YES | YES |
|---|---|-------|---------|-----|-----|
| 9 | a | 45.99 | 0.13612 | YES | YES |
| 10| a | 51.80 | 0.05357 | YES | YES |
| 11| a | 64.59 | 0.06234 | YES | YES |
| 12| a | 74.37 | 0.68844 | YES | YES |
| 13| a | 87.29 | 0.50886 | YES | YES |
| 14| a | 95.39 | 0.82393 | YES | YES |
| 15| a | 97.32 | 0.37309 | YES | YES |
| 16| a | 105.55| 0.26004 | YES | YES |
| 17| a | 113.04| 0.17732 | YES | YES |
| 18| a | 118.41| 0.31008 | YES | YES |
| 19| a | 133.64| 0.12211 | YES | YES |
| 20| a | 171.70| 2.18610 | YES | YES |
| 21| a | 174.78| 1.43021 | YES | YES |
| 22| a | 190.88| 0.74865 | YES | YES |
| 23| a | 218.04| 0.51180 | YES | YES |
| 24| a | 233.98| 1.36411 | YES | YES |
| 25| a | 264.26| 0.52714 | YES | YES |
| 26| a | 284.82| 0.40484 | YES | YES |
| 27| a | 325.68| 12.47841| YES | YES |
| 28| a | 358.71| 2.00023 | YES | YES |
| 29| a | 399.66| 1.03863 | YES | YES |
| 30| a | 405.23| 14.09467| YES | YES |
| 31| a | 418.07| 2.17454 | YES | YES |
| 32| a | 435.09| 3.43305 | YES | YES |
| 33| a | 457.07| 1.70795 | YES | YES |
| 34| a | 461.68| 1.61109 | YES | YES |
| 35| a | 469.82| 4.73183 | YES | YES |
| 36| a | 483.44| 7.46993 | YES | YES |
| 37| a | 488.14| 0.26797 | YES | YES |
| 38| a | 493.44| 2.16853 | YES | YES |
| 39| a | 502.03| 3.50546 | YES | YES |
| 40| a | 504.26| 20.34088| YES | YES |
| 41| a | 528.28| 12.34652| YES | YES |
| 42| a | 537.56| 7.68174 | YES | YES |
| 43| a | 556.97| 2.32393 | YES | YES |
| 44| a | 567.16| 3.05453 | YES | YES |
| 45| a | 612.23| 15.52465| YES | YES |
| 46| a | 614.71| 25.81800| YES | YES |
| 47| a | 623.17| 8.97027 | YES | YES |
| 48| a | 626.79| 23.25932| YES | YES |
| 49| a | 642.59| 20.75191| YES | YES |
| 50| a | 649.69| 29.46792| YES | YES |
**2bb**

SCF Energy (au) BP86/SV(P) -2505.23795427
SCF Energy (au) PBE0/def2-TZVPP -2504.790885075
SCF Energy (au) PBE0/def2-TZVPP -2504.7995679455 (Toluene Correction)
Zero Point Energy (au) 0.3320389
Chemical Potential (kJ mol\(^{-1}\)) 708.87
Dispersion Correction (au) PBE0/def2-TZVPP -0.06626996

xyz coordinates

47

Mn 1.6180000 0.5959888 1.9890749
C 1.6037650 1.0178592 3.7432338
C 3.3429124 0.1140385 2.0743823
C 2.0168363 2.3041750 1.5309996
O 2.2898686 3.4104105 1.2738312
O 4.4599601 -0.2173966 2.1300973
O 1.6041205 1.2900572 4.8745535
C -1.2314929 -0.1224433 2.4276854
C -1.0754915 1.9328046 1.3034667
C -2.4658745 2.0706299 1.2336300
C -3.2650505 1.0631172 1.7984665
C -2.6424082 -0.0364777 2.3952798
C -0.4700380 -1.2378566 3.0025114
C 0.9489658 -1.1392561 2.9070916
C 1.7198929 -2.1869073 3.4518553
C 1.1128659 -3.3042942 4.0519685
C -0.2897640 -3.3964114 4.1319232
C -1.0772339 -2.3642047 3.6093205
H -0.4188630 2.7004377 0.8690315
H -2.9019077 2.9514510 0.7386382
H -4.3648766 1.1315375 1.7692289
H -3.2468539 -0.8421105 2.8369312
H 2.8210083 -2.1434225 3.4119037
H 1.7424419 -4.1107013 4.4656753
H -0.7662818 -4.2702563 4.6055253
H -2.1750040 -2.4390751 3.6791968
N -0.4669697 0.8778050 1.8856129
C 1.9148815 1.3242364 -1.3107508
C 1.6162769 0.4110700 -0.1848834
C 1.3516612 -0.7098415 0.3370742
H 1.1006053 -1.7696478 0.3014017
H 3.0138820 1.3998505 -1.4583892
O 1.4025969 0.8166996 -2.5617656
H 1.5066926 2.3409297 -1.1390848
C 0.1106493 1.1518490 -2.8526820
O -0.5779918 1.8559542 -2.1311994
C -0.3415613 0.5661932 -4.1515026
C -1.2980410 -0.4808569 -6.5823375
C -2.1297592 0.3353950 -5.7937381
C -1.6539717 0.8572538 -4.5829244
C 0.4903588 -0.2538503 -4.9450346
C 0.0102220 -0.7740441 -6.1565301
H -1.6719762 -0.8915143 -7.5350248
H -3.1552568 0.5653103 -6.1266224
H -2.2846628 1.4989506 -3.9479393
H 1.5114632 -0.4793423 -4.6037506
H 0.6614034 -1.4140937 -6.7744048
| # | mode | symmetry | wave number cm^{-1} | IR intensity km/mol | selection rules |
|---|------|---------|---------------------|---------------------|-----------------|
| 1 |      |         | 0.00                | 0.00000             | -                |
| 2 |      |         | 0.00                | 0.00000             | -                |
| 3 |      |         | 0.00                | 0.00000             | -                |
| 4 |      |         | 0.00                | 0.00000             | -                |
| 5 |      |         | 0.00                | 0.00000             | -                |
| 6 |      |         | 0.00                | 0.00000             | -                |
| 7 | a    |         | 13.78              | 0.63109             | YES             |
| 8 | a    |         | 16.17              | 0.06385             | YES             |
| 9 | a    |         | 26.51              | 0.94380             | YES             |
| 10| a    |         | 40.83              | 0.11857             | YES             |
| 11| a    |         | 44.50              | 0.14099             | YES             |
| 12| a    |         | 60.04              | 0.64516             | YES             |
| 13| a    |         | 69.03              | 0.21975             | YES             |
| 14| a    |         | 72.21              | 0.85703             | YES             |
| 15| a    |         | 84.34              | 1.45753             | YES             |
| 16| a    |         | 90.90              | 0.52749             | YES             |
| 17| a    |         | 96.39              | 0.34389             | YES             |
| 18| a    |         | 97.44              | 0.34176             | YES             |
| 19| a    |         | 108.60             | 0.17659             | YES             |
| 20| a    |         | 112.21             | 0.23145             | YES             |
| 21| a    |         | 134.87             | 0.21442             | YES             |
| 22| a    |         | 147.43             | 0.82215             | YES             |
| 23| a    |         | 158.85             | 0.08209             | YES             |
| 24| a    |         | 184.11             | 0.56099             | YES             |
| 25| a    |         | 192.44             | 2.38537             | YES             |
| 26| a    |         | 210.96             | 1.77207             | YES             |
| 27| a    |         | 233.43             | 1.65430             | YES             |
| 28| a    |         | 247.96             | 0.63882             | YES             |
| 29| a    |         | 261.35             | 0.30126             | YES             |
| 30| a    |         | 284.47             | 0.09530             | YES             |
| 31| a    |         | 304.39             | 0.64005             | YES             |
| 32| a    |         | 335.44             | 25.56220            | YES             |
| 33| a    |         | 352.01             | 10.82510            | YES             |
| 34| a    |         | 358.09             | 2.98049             | YES             |
| 35| a    |         | 403.84             | 0.00135             | YES             |
| 36| a    |         | 404.89             | 3.35779             | YES             |
| 37| a    |         | 418.21             | 9.17855             | YES             |
| 38| a    |         | 437.11             | 1.26946             | YES             |
| 39| a    |         | 443.49             | 0.54007             | YES             |
| 40| a    |         | 456.37             | 13.63186            | YES             |
| 41| a    |         | 456.91             | 1.18641             | YES             |
| 42| a    |         | 470.12             | 3.60864             | YES             |
| 43| a    |         | 474.64             | 4.67313             | YES             |
| 44| a    |         | 485.86             | 2.37910             | YES             |
| 45| a    |         | 492.24             | 4.47263             | YES             |
| 46| a    |         | 503.55             | 2.17480             | YES             |
| 47| a    |         | 534.83             | 27.57216            | YES             |
| 48| a    |         | 551.35             | 6.93128             | YES             |
| 49| a    |         | 555.83             | 2.85141             | YES             |
| 50| a    |         | 586.75             | 24.75587            | YES             |
**2bb’**

| SCF Energy (au) BP86/SV(P) | -2505.236933617 |
|---------------------------|------------------|
| SCF Energy (au) PBE0/def2-TZVPP | -2504.790820918 |
| SCF Energy (au) PBE0/def2-TZVPP (Toluene Correction) | -2504.804063460 |
| Zero Point Energy (au) | 0.3315667 |
| Chemical Potential (kJ mol\(^{-1}\)) | 706.66 |
| Dispersion Correction (au) PBE0/def2-TZVPP | -0.06608119 |

**xyz coordinates**

| 47 |
| Mn | 1.2071453 | 2.0845764 | 1.5175484 |
| C  | 1.5188067 | 2.4327129 | 3.2632450 |
| C  | 2.9535568 | 1.8067143 | 1.2210547 |
| C  | 1.3109007 | 3.8417076 | 1.0832671 |
| O  | 1.3966017 | 4.9769109 | 0.8238098 |
| O  | 4.0859643 | 1.6046888 | 1.0311148 |
| O  | 1.7333257 | 2.6615735 | 4.3833466 |
| C  | -1.3840104 | 1.0164804 | 2.5067439 |
| C  | -1.6943190 | 3.1234148 | 1.5175162 |
| C  | -3.0701762 | 3.1092395 | 1.7689236 |
| C  | -3.6146244 | 1.9914272 | 2.4235040 |
| C  | -2.7682459 | 0.9435312 | 2.7903655 |
| C  | -0.4006485 | -0.0225468 | 2.8330711 |
| C  | 0.9456160 | 0.2488490 | 2.4458893 |
| C  | 1.9236663 | -0.7190291 | 2.7573426 |
| C  | 1.5843701 | -1.9224081 | 3.4016184 |
| C  | 0.2501914 | -2.1840534 | 3.7654303 |
| C  | -0.7378730 | -1.2338403 | 3.4845280 |
| H  | -1.2264610 | 3.9816417 | 1.0106712 |
| H  | -3.6935940 | 3.9614037 | 1.4575101 |
| H  | -4.6949615 | 1.9379273 | 2.6444659 |
| H  | -3.1737855 | 0.0566284 | 3.2988505 |
| H  | 2.9806457 | -0.5440618 | 2.4946808 |
| H  | 2.3709950 | -2.6637524 | 3.6227759 |
| H  | -0.0168191 | -3.1263013 | 4.2706177 |
| H  | -1.7801840 | -1.4411310 | 3.7777907 |
| N  | -0.8674528 | 2.1174004 | 1.8745210 |
| H  | 0.7237230 | 2.9428306 | -1.3284374 |
| C  | 0.7759412 | 2.1447418 | -0.5880217 |
| C  | 0.7649805 | 0.9334115 | -0.2159492 |
| C  | 0.6374431 | -0.5091082 | -0.4762539 |
| H  | 1.5424555 | -1.0611915 | -0.1361967 |
| O  | 0.4464628 | -0.7112175 | -1.8951661 |
| H  | -0.2152662 | -0.9533645 | 0.0840899 |
| C  | 0.3120342 | -2.0094032 | -2.2835204 |
| C  | 0.1420535 | -2.1399345 | -3.7650974 |
| O  | 0.3329019 | -2.9454306 | -1.5003728 |
| C  | -0.1749361 | -2.5062572 | -6.5373558 |
| C  | -0.0310494 | -1.2097279 | -6.0112969 |
| C  | 0.1273187 | -1.0236341 | -4.6295330 |
| C  | -0.0029913 | -3.4390717 | -4.2974052 |
| C  | -0.1608425 | -3.6207548 | -5.6784601 |
| H  | -0.2979793 | -2.6493881 | -7.6239929 |
| H  | -0.0414665 | -0.3366498 | -6.6845058 |
| H  | 0.2423172 | -0.0138216 | -4.2085190 |
| H  | 0.0128639 | -4.2944664 | -3.6037226 |
| H  | -0.2728045 | -4.6372664 | -6.0904863 |
| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|-----|---------|-------------|--------------|-----------------|
| 1 |     |         | 0.00        | 0.00000      | -               |
| 2 |     |         | 0.00        | 0.00000      | -               |
| 3 |     |         | 0.00        | 0.00000      | -               |
| 4 |     |         | 0.00        | 0.00000      | -               |
| 5 |     |         | 0.00        | 0.00000      | -               |
| 6 |     |         | 0.00        | 0.00000      | -               |
| 7 | a   |         | 12.69       | 0.77150      | YES             |
| 8 | a   |         | 14.31       | 0.44876      | YES             |
| 9 | a   |         | 27.98       | 0.18749      | YES             |
| 10| a   |         | 41.43       | 0.34307      | YES             |
| 11| a   |         | 51.94       | 0.21434      | YES             |
| 12| a   |         | 56.54       | 0.08029      | YES             |
| 13| a   |         | 68.27       | 0.37237      | YES             |
| 14| a   |         | 70.82       | 0.45542      | YES             |
| 15| a   |         | 83.57       | 0.05551      | YES             |
| 16| a   |         | 85.91       | 0.91697      | YES             |
| 17| a   |         | 96.63       | 0.69206      | YES             |
| 18| a   |         | 101.41      | 0.21988      | YES             |
| 19| a   |         | 107.13      | 0.45072      | YES             |
| 20| a   |         | 111.31      | 0.30546      | YES             |
| 21| a   |         | 128.18      | 0.55150      | YES             |
| 22| a   |         | 135.51      | 0.37011      | YES             |
| 23| a   |         | 157.84      | 0.40895      | YES             |
| 24| a   |         | 186.62      | 0.71237      | YES             |
| 25| a   |         | 188.13      | 0.18813      | YES             |
| 26| a   |         | 206.37      | 1.05808      | YES             |
| 27| a   |         | 220.77      | 1.27731      | YES             |
| 28| a   |         | 235.13      | 0.37823      | YES             |
| 29| a   |         | 265.42      | 0.69843      | YES             |
| 30| a   |         | 281.00      | 2.87185      | YES             |
| 31| a   |         | 293.67      | 13.05060     | YES             |
| 32| a   |         | 322.49      | 3.95365      | YES             |
| 33| a   |         | 354.65      | 5.38279      | YES             |
| 34| a   |         | 358.97      | 1.99179      | YES             |
| 35| a   |         | 396.54      | 16.64607     | YES             |
| 36| a   |         | 403.91      | 0.00075      | YES             |
| 37| a   |         | 418.13      | 3.11457      | YES             |
| 38| a   |         | 436.08      | 2.26241      | YES             |
| 39| a   |         | 445.18      | 0.20183      | YES             |
| 40| a   |         | 454.14      | 2.00641      | YES             |
| 41| a   |         | 458.13      | 1.36604      | YES             |
| 42| a   |         | 469.31      | 2.75263      | YES             |
| 43| a   |         | 473.59      | 6.60098      | YES             |
| 44| a   |         | 487.20      | 4.16042      | YES             |
| 45| a   |         | 491.46      | 3.65311      | YES             |
| 46| a   |         | 504.47      | 3.40863      | YES             |
| 47| a   |         | 529.10      | 20.02646     | YES             |
| 48| a   |         | 547.18      | 6.22080      | YES             |
| 49| a   |         | 557.27      | 2.47483      | YES             |
| 50| a   |         | 585.62      | 8.21677      | YES             |
2bc

SCF Energy (au) BP86/SV(P) -2281.120982087
SCF Energy (au) PBE0/def2-TZVPP -2280.691348894
SCF Energy (au) PBE0/def2-TZVPP -2280.6975966102 (Toluene Correction)
Zero Point Energy (au) 0.3575200
Chemical Potential (kJ mol$^{-1}$) 791.47
Dispersion Correction (au) PBE0/def2-TZVPP -0.06509361

xyz coordinates
47

Mn 1.2025069 0.1620360 1.0932740
C  1.9568143 0.6239857 2.6631145
C  2.7626127 -0.4707803 0.4834922
C  1.4816754 1.8042180 0.3880616
O  1.6872442 2.8755222 -0.0350056
O  3.7740952 -0.08988125 0.0895477
O  2.4567165 0.9146208 3.6736798
C -1.2674439 -0.3023652 2.6745928
C -1.3912158 1.7610984 1.5612277
C -2.6659539 2.0309656 2.0698859
C -3.2584096 1.0819363 2.9213569
C -2.5540902 -0.0861767 3.2217314
C -0.4365673 -1.4859299 2.915833
C  0.8303787 -1.5029309 2.9195833
C  0.8426867 -2.5634264 3.7452354
H -0.8890702 2.4838705 0.8994692
H -3.1751348 2.9700773 1.8036640
H -4.2600129 1.2541116 3.3483852
H -2.9958712 -0.8431618 3.8858832
H  2.6655322 -2.6671882 2.0133031
H  1.9364916 -4.5450173 3.4598796
H -0.3169334 -4.4982914 4.5831522
H -1.8256840 -2.5481467 4.2443786
N -0.7037795 0.6342783 1.8461413
C  0.1497651 0.7721964 -2.1486257
C  0.2718754 -0.0683968 -0.9320319
C  0.1891642 -1.1366730 -0.2631221
H -0.0993771 -2.1746493 -0.1043557
C  1.4730397 0.8028500 -2.9612945
C -1.0183065 0.2671813 -3.0382063
H -0.0792297 1.8227280 -1.8535928
C -1.1565103 1.1132381 -4.3163661
H -1.9654677 0.2801394 -2.4548417
H -0.8234627 -0.7970045 -3.3086006
H  2.2961270 1.1998921 -2.3286030
C  1.3263403 1.6449803 -4.2404805
H  1.7477958 -0.2449558 -3.2238571
H  1.1602417 2.7121905 -3.9595975
H  2.2790566 1.6176752 -4.8155415
C  0.1575487 1.1588161 -5.1149762
H -1.4552353 2.1520586 -4.0381253
H -1.9808817 0.7083946 -4.9460352
H  0.0445918 1.8137098 -6.0082216
H  0.3872873 0.1367419 -5.4999742
| #  | mode | symmetry | wave number (cm\(^{-1}\)) | IR intensity (km/mol) | IR intensity | selection rules |
|----|------|----------|---------------------------|-----------------------|--------------|-----------------|
| 1  | 0    | 0.00     | 0.00000                   | -                     | -            |                 |
| 2  | 0    | 0.00     | 0.00000                   | -                     | -            |                 |
| 3  | 0    | 0.00     | 0.00000                   | -                     | -            |                 |
| 4  | 0    | 0.00     | 0.00000                   | -                     | -            |                 |
| 5  | 0    | 0.00     | 0.00000                   | -                     | -            |                 |
| 6  | 0    | 0.00     | 0.00000                   | -                     | -            |                 |
| 7  | a    | 21.31    | 0.24853                   | YES                   | YES          |                 |
| 8  | a    | 34.94    | 0.01906                   | YES                   | YES          |                 |
| 9  | a    | 38.46    | 0.04270                   | YES                   | YES          |                 |
| 10 | a    | 56.12    | 0.16270                   | YES                   | YES          |                 |
| 11 | a    | 66.63    | 0.03245                   | YES                   | YES          |                 |
| 12 | a    | 77.27    | 0.13836                   | YES                   | YES          |                 |
| 13 | a    | 83.57    | 0.79291                   | YES                   | YES          |                 |
| 14 | a    | 91.64    | 0.35616                   | YES                   | YES          |                 |
| 15 | a    | 98.95    | 0.67833                   | YES                   | YES          |                 |
| 16 | a    | 107.88   | 0.25597                   | YES                   | YES          |                 |
| 17 | a    | 112.19   | 0.26611                   | YES                   | YES          |                 |
| 18 | a    | 116.96   | 0.11094                   | YES                   | YES          |                 |
| 19 | a    | 125.21   | 0.31890                   | YES                   | YES          |                 |
| 20 | a    | 144.42   | 2.49941                   | YES                   | YES          |                 |
| 21 | a    | 170.19   | 2.12557                   | YES                   | YES          |                 |
| 22 | a    | 188.62   | 1.02686                   | YES                   | YES          |                 |
| 23 | a    | 213.81   | 0.39124                   | YES                   | YES          |                 |
| 24 | a    | 230.38   | 0.08836                   | YES                   | YES          |                 |
| 25 | a    | 242.25   | 1.38666                   | YES                   | YES          |                 |
| 26 | a    | 245.53   | 2.60861                   | YES                   | YES          |                 |
| 27 | a    | 264.09   | 0.25243                   | YES                   | YES          |                 |
| 28 | a    | 284.24   | 0.01913                   | YES                   | YES          |                 |
| 29 | a    | 348.77   | 2.37378                   | YES                   | YES          |                 |
| 30 | a    | 358.13   | 2.17632                   | YES                   | YES          |                 |
| 31 | a    | 381.93   | 9.42387                   | YES                   | YES          |                 |
| 32 | a    | 409.55   | 0.56836                   | YES                   | YES          |                 |
| 33 | a    | 417.09   | 5.99506                   | YES                   | YES          |                 |
| 34 | a    | 425.66   | 0.41850                   | YES                   | YES          |                 |
| 35 | a    | 436.05   | 0.68267                   | YES                   | YES          |                 |
| 36 | a    | 454.69   | 13.16624                  | YES                   | YES          |                 |
| 37 | a    | 457.31   | 1.49122                   | YES                   | YES          |                 |
| 38 | a    | 473.52   | 2.84621                   | YES                   | YES          |                 |
| 39 | a    | 483.72   | 3.74094                   | YES                   | YES          |                 |
| 40 | a    | 493.07   | 1.51086                   | YES                   | YES          |                 |
| 41 | a    | 495.13   | 1.75850                   | YES                   | YES          |                 |
| 42 | a    | 497.07   | 5.09040                   | YES                   | YES          |                 |
| 43 | a    | 505.51   | 2.43664                   | YES                   | YES          |                 |
| 44 | a    | 535.73   | 28.50850                  | YES                   | YES          |                 |
| 45 | a    | 548.84   | 10.33325                  | YES                   | YES          |                 |
| 46 | a    | 557.11   | 1.46236                   | YES                   | YES          |                 |
| 47 | a    | 563.44   | 9.53427                   | YES                   | YES          |                 |
| 48 | a    | 615.81   | 12.89888                  | YES                   | YES          |                 |
| 49 | a    | 624.34   | 4.08364                   | YES                   | YES          |                 |
| 50 | a    | 627.92   | 29.19440                  | YES                   | YES          |                 |
xyz coordinates

Mn  1.0348289  2.0037251  0.7072396
C   1.3546343  2.3648770  2.4445458
C   2.7685807  1.6679846  0.4096337
C   1.1942521  3.7522246  0.2578736
O   1.3200183  4.8827259 -0.0095936
O   3.8951655  1.4302241  0.2189937
O   1.5757112  2.6034661  3.5623050
C   1.1942521  3.7522246  0.4096337
C   1.1942521  3.7522246  0.2578736
O   1.3200183  4.8827259 -0.0095936
O   3.8951655  1.4302241  0.2189937
O   1.5757112  2.6034661  3.5623050
C   1.1942521  3.7522246  0.2578736
C   1.1942521  3.7522246  0.2578736
O   1.3200183  4.8827259 -0.0095936
O   3.8951655  1.4302241  0.2189937
O   1.5757112  2.6034661  3.5623050
C   1.1942521  3.7522246  0.2578736
C   1.1942521  3.7522246  0.2578736
O   1.3200183  4.8827259 -0.0095936
O   3.8951655  1.4302241  0.2189937
O   1.5757112  2.6034661  3.5623050
| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|----------------|
| 1 | 0.00 | 0.00000  | -           | -            | YES            |
| 2 | 0.00 | 0.00000  | -           | -            | YES            |
| 3 | 0.00 | 0.00000  | -           | -            | YES            |
| 4 | 0.00 | 0.00000  | -           | -            | YES            |
| 5 | 0.00 | 0.00000  | -           | -            | YES            |
| 6 | 0.00 | 0.00000  | -           | -            | YES            |
| 7 | 24.72| 0.36389  | YES         | YES          |
| 8 | 41.59| 0.07488  | YES         | YES          |
| 9 | 45.25| 0.06575  | YES         | YES          |
| 10| 52.15| 0.11210  | YES         | YES          |
| 11| 63.64| 0.04811  | YES         | YES          |
| 12| 76.29| 0.28325  | YES         | YES          |
| 13| 87.06| 0.59299  | YES         | YES          |
| 14| 94.90| 0.57956  | YES         | YES          |
| 15| 96.08| 0.16813  | YES         | YES          |
| 16| 104.24| 0.55311  | YES         | YES          |
| 17| 111.89| 0.16725  | YES         | YES          |
| 18| 117.23| 0.10103  | YES         | YES          |
| 19| 125.86| 0.20698  | YES         | YES          |
| 20| 155.34| 0.95071  | YES         | YES          |
| 21| 176.64| 2.31596  | YES         | YES          |
| 22| 189.40| 0.72962  | YES         | YES          |
| 23| 217.68| 0.38679  | YES         | YES          |
| 24| 228.82| 1.35028  | YES         | YES          |
| 25| 239.91| 0.04320  | YES         | YES          |
| 26| 252.70| 0.27808  | YES         | YES          |
| 27| 267.89| 0.60585  | YES         | YES          |
| 28| 285.93| 0.07364  | YES         | YES          |
| 29| 357.82| 1.81800  | YES         | YES          |
| 30| 359.68| 1.20955  | YES         | YES          |
| 31| 379.42| 12.58201 | YES         | YES          |
| 32| 413.80| 2.47893  | YES         | YES          |
| 33| 421.06| 2.16931  | YES         | YES          |
| 34| 425.08| 1.18950  | YES         | YES          |
| 35| 436.27| 1.59759  | YES         | YES          |
| 36| 457.23| 1.43469  | YES         | YES          |
| 37| 460.02| 1.13592  | YES         | YES          |
| 38| 472.28| 2.42811  | YES         | YES          |
| 39| 485.41| 5.28717  | YES         | YES          |
| 40| 489.47| 2.52597  | YES         | YES          |
| 41| 494.19| 9.12418  | YES         | YES          |
| 42| 498.54| 0.71289  | YES         | YES          |
| 43| 508.60| 2.78867  | YES         | YES          |
| 44| 529.06| 16.45843 | YES         | YES          |
| 45| 554.23| 2.74309  | YES         | YES          |
| 46| 558.08| 2.78602  | YES         | YES          |
| 47| 580.21| 5.14682  | YES         | YES          |
| 48| 615.69| 26.75293 | YES         | YES          |
| 49| 623.84| 7.32930  | YES         | YES          |
| 50| 627.13| 24.83024 | YES         | YES          |
| Element | x       | y       | z       |
|---------|---------|---------|---------|
| Mn      | 1.3925957 | -0.2876905 | 1.7876510 |
| C       | 1.8013007  | 0.3501230   | 3.4179483 |
| C       | 3.0913075  | -0.7763907  | 1.5034861 |
| C       | 1.6475177  | 1.3305527   | 1.0040488 |
| O       | 1.8535412  | 2.3906773   | 0.5573821 |
| O       | 4.1949478  | -1.118628   | 1.3195940 |
| O       | 2.0741051  | 0.7505419   | 4.4776491 |
| C       | -1.2733784 | -0.9329752  | 2.9018538 |
| C       | -1.3729850 | 1.0364967   | 1.6250640 |
| C       | -2.7435242 | 1.1929112   | 1.8591491 |
| C       | -3.3985417 | 0.2359856   | 2.6539271 |
| O       | -0.9719780 | -1.9081982  | 2.989035 |
| O       | 1.8536763  | -2.9048410  | 3.4696009 |
| C       | 1.4022611  | -3.9601422  | 4.2816231 |
| C       | 0.0462868  | -4.0446748  | 4.6538200 |
| C       | -0.8488814 | -3.0647430  | 4.2109765 |
| H       | -0.8228403 | 1.7657238   | 1.0107653 |
| H       | -3.2774785 | 2.0527496   | 1.4261788 |
| H       | -4.4767091 | 0.3212295   | 2.8676273 |
| H       | -3.1472115 | -1.5898039  | 3.7984506 |
| H       | 2.9227283  | -2.8677717  | 3.1999172 |
| H       | 2.1173776  | -4.7245731  | 4.6315816 |
| H       | -0.3082608 | -4.8711275  | 5.2912563 |
| H       | -1.9088144 | -3.1333749  | 4.5079584 |
| N       | -0.6495121 | 0.0106224   | 2.1251006 |
| C       | 0.5362402  | 0.0227771   | -1.5621652 |
| C       | 1.5876226  | 0.6627500   | -2.2691490 |
| C       | 1.3426892  | 1.4197705   | -3.4145819 |
| C       | 0.0190698  | 1.5921664   | -3.9213900 |
| C       | -1.0380191 | 0.9549214   | -3.2052885 |
| O       | -0.7817999 | 0.1962930   | -2.0610430 |
| H       | 2.6225990  | 0.5547868   | -1.9084296 |
| H       | 2.1984547  | 1.8871607   | -3.9215151 |
| N       | -0.2266218 | 2.3434817   | -5.0577128 |
| H       | -2.0784857 | 1.0466807   | -3.5477473 |
| H       | -1.6206983 | -0.2895092  | -1.5372084 |
| C       | 0.7777766  | -0.8031245  | -0.4136716 |
| C       | 0.8486570  | -1.7866419  | 0.3766648 |
| H       | 0.8017729  | -2.8648223  | 0.5341916 |
| C       | -1.5867253 | 2.5044316   | -5.5419388 |
| C       | 0.8740447  | 2.9812261   | -5.7608789 |
| H       | -1.5795323 | 3.1316451   | -6.4551821 |
| H       | -2.2440036 | 3.0052468   | -4.7904017 |
| H       | -2.0562801 | 1.5261755   | -5.8054631 |
| H       | 1.4160308  | 3.7142408   | -5.1163019 |
| H       | 0.4790910  | 3.5301722   | -6.6385994 |
| H       | 1.6201958  | 2.2383414   | -6.1318513 |
| #  | mode | symmetry | wave number (cm\(^{-1}\)) | IR intensity (km/mol) | IR | RAMAN |
|----|------|----------|-----------------------------|-----------------------|----|-------|
| 1  |      |          | 0.00                        | 0.00000               | -  | -     |
| 2  |      |          | 0.00                        | 0.00000               | -  | -     |
| 3  |      |          | 0.00                        | 0.00000               | -  | -     |
| 4  |      |          | 0.00                        | 0.00000               | -  | -     |
| 5  |      |          | 0.00                        | 0.00000               | -  | -     |
| 6  |      |          | 0.00                        | 0.00000               | -  | -     |
| 7  | a    |          | 9.77                        | 0.32390               | YES| YES   |
| 8  | a    |          | 19.49                       | 0.47829               | YES| YES   |
| 9  | a    |          | 27.15                       | 0.84414               | YES| YES   |
| 10 | a    |          | 46.55                       | 0.42645               | YES| YES   |
| 11 | a    |          | 59.63                       | 0.00369               | YES| YES   |
| 12 | a    |          | 65.68                       | 0.40984               | YES| YES   |
| 13 | a    |          | 73.58                       | 0.27310               | YES| YES   |
| 14 | a    |          | 77.07                       | 1.07304               | YES| YES   |
| 15 | a    |          | 85.22                       | 1.87030               | YES| YES   |
| 16 | a    |          | 86.06                       | 0.62738               | YES| YES   |
| 17 | a    |          | 93.48                       | 0.56900               | YES| YES   |
| 18 | a    |          | 101.53                      | 1.07347               | YES| YES   |
| 19 | a    |          | 105.80                      | 0.14299               | YES| YES   |
| 20 | a    |          | 110.21                      | 0.77764               | YES| YES   |
| 21 | a    |          | 113.50                      | 1.28888               | YES| YES   |
| 22 | a    |          | 119.50                      | 10.86627              | YES| YES   |
| 23 | a    |          | 145.24                      | 8.95151               | YES| YES   |
| 24 | a    |          | 176.05                      | 12.15749              | YES| YES   |
| 25 | a    |          | 189.53                      | 2.39487               | YES| YES   |
| 26 | a    |          | 211.64                      | 0.15863               | YES| YES   |
| 27 | a    |          | 222.89                      | 0.47711               | YES| YES   |
| 28 | a    |          | 238.63                      | 2.17760               | YES| YES   |
| 29 | a    |          | 247.84                      | 5.48849               | YES| YES   |
| 30 | a    |          | 261.30                      | 2.39248               | YES| YES   |
| 31 | a    |          | 271.68                      | 15.76820              | YES| YES   |
| 32 | a    |          | 287.07                      | 1.13771               | YES| YES   |
| 33 | a    |          | 340.00                      | 40.93114              | YES| YES   |
| 34 | a    |          | 358.73                      | 1.91607               | YES| YES   |
| 35 | a    |          | 380.91                      | 7.35874               | YES| YES   |
| 36 | a    |          | 416.00                      | 11.15977              | YES| YES   |
| 37 | a    |          | 416.77                      | 1.74031               | YES| YES   |
| 38 | a    |          | 430.09                      | 6.89579               | YES| YES   |
| 39 | a    |          | 444.10                      | 19.38440              | YES| YES   |
| 40 | a    |          | 454.05                      | 5.54465               | YES| YES   |
| 41 | a    |          | 456.73                      | 3.22540               | YES| YES   |
| 42 | a    |          | 463.11                      | 1.77583               | YES| YES   |
| 43 | a    |          | 477.34                      | 6.19032               | YES| YES   |
| 44 | a    |          | 488.73                      | 3.79858               | YES| YES   |
| 45 | a    |          | 490.92                      | 32.76320              | YES| YES   |
| 46 | a    |          | 493.72                      | 5.07364               | YES| YES   |
| 47 | a    |          | 503.77                      | 0.62555               | YES| YES   |
| 48 | a    |          | 515.82                      | 15.69978              | YES| YES   |
| 49 | a    |          | 530.05                      | 43.15597              | YES| YES   |
| 50 | a    |          | 541.11                      | 9.60241               | YES| YES   |
SCF Energy (au) BP86/SV(P) -2411.383229723
SCF Energy (au) PBE0/def2-TZVPP -2410.926493690
SCF Energy (au) PBE0/def2-TZVPP -2410.9348447962 (Toluene Correction)

Zero Point Energy (au) 0.3602809
Chemical Potential (kJ mol\(^{-1}\)) 784.73
Dispersion Correction (au) PBE0/def2-TZVPP 0.07187072

xyz coordinates

| Atom | x      | y      | z      |
|------|--------|--------|--------|
| Mn   | 1.2663945 | 2.7708307 | 0.7416893 |
| C    | 1.4115506  | 3.1773508   | 2.4898686  |
| C    | 3.0235475  | 2.4470980   | 0.6081276  |
| C    | 1.4377476  | 4.5142685   | 0.2781122  |
| O    | 1.5718707  | 5.6406263   | -0.0035219 |
| O    | 4.1629481  | 2.2064819   | 0.5236885  |
| O    | 1.5137044  | 3.4534435   | 3.616834   |
| C    | -1.4098168 | 1.6986085   | 1.4244989  |
| C    | -1.6060832 | 3.7981651   | 0.3895549  |
| C    | -3.0028394 | 3.7713887   | 0.4556699  |
| C    | -3.6212881 | 2.6491378   | 1.0354332  |
| C    | -2.8195531 | 1.6122698   | 1.5180890  |
| C    | -0.4678684 | 0.6812651   | 1.8996707  |
| O    | 0.9129646  | 0.9617008   | 1.6764839  |
| C    | 1.8511667  | 0.0264272   | 2.1633669  |
| C    | 1.4456810  | -1.1538910  | 2.8107245  |
| C    | 0.0782650  | -1.4282234  | 3.0020761  |
| C    | -0.8747426 | -0.5094966  | 2.5486916  |
| H    | -1.0820154 | 4.6583592   | -0.0550827 |
| H    | -3.5867634 | 4.6172874   | 0.0613717  |
| H    | -4.7193202 | 2.5851346   | 1.1094389  |
| H    | -3.2796616 | 0.7219630   | 1.9712661  |
| H    | 2.9317907  | 0.2123774   | 2.0422032  |
| H    | 2.2063352  | -1.8663679  | 3.1738634  |
| H    | -0.2418906 | -2.3522389  | 3.5107730  |
| H    | -1.946100  | -0.7226850  | 2.7103168  |
| N    | -0.8239537 | 2.8016353   | 0.8578603  |
| H    | 1.1464438  | 3.5642565   | -2.1452500 |
| H    | 1.0506260  | 2.7722205   | -1.4007081 |
| C    | 0.9395331  | 1.5400747   | -1.1284499 |
| C    | 0.6900209  | 0.1433434   | -1.3608377 |
| C    | 0.1781382  | -2.6299613  | -1.9369723 |
| C    | 1.4415419  | -2.1922956  | -1.4386935 |
| C    | 1.6820764  | -0.8477882  | -1.1527721 |
| C    | -0.5672552 | -0.2881822  | -1.8552967 |
| C    | -0.8214450 | -1.6326957  | -2.1363533 |
| N    | -0.0659869 | -3.9654548  | -2.2155184 |
| H    | 2.2525575  | -2.9136067  | -1.2664274 |
| H    | 2.6699657  | -0.5470040  | -0.7712270 |
| H    | -1.3609945 | 0.4573031   | -2.0274221 |
| H    | -1.8144344 | -1.9063088  | -2.5204744 |
| C    | -1.3609442 | -4.3745029  | -2.7290627 |
| C    | 0.9772797  | -4.9540055  | -2.0061756 |
| H    | -1.6005157 | -3.8869288  | -3.7054739 |
| H    | -2.1894685 | -4.1344632  | -2.0195169 |
| H    | -1.3624895 | -5.4706853  | -2.8908988 |
| H    | 1.3071293  | -4.9967255  | -0.9402114 |
| H    | 1.8802211  | -4.7528585  | 2.6321530  |
| H    | 0.5935398  | -5.9566532  | -2.2810229 |
| # | mode | symmetry | wave number (cm^-1) | IR intensity (km/mol) | IR | RAMAN |
|---|------|----------|---------------------|-----------------------|----|-------|
| 1 |      |          | 0.00                | 0.00000               | -  | -     |
| 2 |      |          | 0.00                | 0.00000               | -  | -     |
| 3 |      |          | 0.00                | 0.00000               | -  | -     |
| 4 |      |          | 0.00                | 0.00000               | -  | -     |
| 5 |      |          | 0.00                | 0.00000               | -  | -     |
| 6 |      |          | 0.00                | 0.00000               | -  | -     |
| 7 | a    |          | 11.44               | 0.42500               | YES| YES   |
| 8 | a    |          | 22.17               | 0.05493               | YES| YES   |
| 9 | a    |          | 36.74               | 0.87475               | YES| YES   |
| 10| a    |          | 48.62               | 0.05701               | YES| YES   |
| 11| a    |          | 58.52               | 1.12493               | YES| YES   |
| 12| a    |          | 66.92               | 0.69761               | YES| YES   |
| 13| a    |          | 74.69               | 0.34991               | YES| YES   |
| 14| a    |          | 78.56               | 0.56269               | YES| YES   |
| 15| a    |          | 84.94               | 0.59614               | YES| YES   |
| 16| a    |          | 92.36               | 1.30066               | YES| YES   |
| 17| a    |          | 94.03               | 0.15738               | YES| YES   |
| 18| a    |          | 97.12               | 1.58291               | YES| YES   |
| 19| a    |          | 104.13              | 0.18552               | YES| YES   |
| 20| a    |          | 109.18              | 0.28495               | YES| YES   |
| 21| a    |          | 117.19              | 0.83929               | YES| YES   |
| 22| a    |          | 128.57              | 2.09589               | YES| YES   |
| 23| a    |          | 149.49              | 6.73147               | YES| YES   |
| 24| a    |          | 184.48              | 5.05036               | YES| YES   |
| 25| a    |          | 194.26              | 4.53220               | YES| YES   |
| 26| a    |          | 214.95              | 0.25485               | YES| YES   |
| 27| a    |          | 216.70              | 1.13080               | YES| YES   |
| 28| a    |          | 232.49              | 1.84431               | YES| YES   |
| 29| a    |          | 250.02              | 1.07986               | YES| YES   |
| 30| a    |          | 263.54              | 0.20893               | YES| YES   |
| 31| a    |          | 279.47              | 8.73793               | YES| YES   |
| 32| a    |          | 286.00              | 0.78289               | YES| YES   |
| 33| a    |          | 338.56              | 29.90249              | YES| YES   |
| 34| a    |          | 359.12              | 2.14220               | YES| YES   |
| 35| a    |          | 389.80              | 11.97136              | YES| YES   |
| 36| a    |          | 414.66              | 1.31078               | YES| YES   |
| 37| a    |          | 416.05              | 1.78230               | YES| YES   |
| 38| a    |          | 428.09              | 10.10769              | YES| YES   |
| 39| a    |          | 441.38              | 4.97791               | YES| YES   |
| 40| a    |          | 453.54              | 0.48186               | YES| YES   |
| 41| a    |          | 458.02              | 1.92772               | YES| YES   |
| 42| a    |          | 467.96              | 3.93729               | YES| YES   |
| 43| a    |          | 475.17              | 0.36120               | YES| YES   |
| 44| a    |          | 488.63              | 5.04201               | YES| YES   |
| 45| a    |          | 491.82              | 6.89705               | YES| YES   |
| 46| a    |          | 494.74              | 10.14941              | YES| YES   |
| 47| a    |          | 503.51              | 1.69264               | YES| YES   |
| 48| a    |          | 515.44              | 19.65428              | YES| YES   |
| 49| a    |          | 532.86              | 21.08297              | YES| YES   |
| 50| a    |          | 537.10              | 6.36060               | YES| YES   |
2be

SCF Energy (au) BP86/SV( P  -2391.960168240  
SCF Energy (au) PBE0/def2-TZVPP -2391.515765535  
SCF Energy (au) PBE0/def2-TZVPP -2391.5241006317 (Toluene Correction)  
Zero Point Energy (au) 0.3213065  
Chemical Potential (kJ mol$^{-1}$) 689.58  
Dispersion Correction (au) PBE0/def2-TZVPP -0.06471746  

xyz coordinates  
45

Mn  1.2454519  -0.1636177  1.2461568  
C   1.6903274   0.3277975  2.9190853  
C   2.9289665  -0.6687297  0.9011828  
C   1.5333880   1.5091092  0.6006049  
O   1.7617757   2.5966867  0.2410407  
O   4.0223501  -1.0121397  0.6782891  
O   1.9851445   0.6352659  4.0029599  
C   -1.4166805  -0.8122930  2.3802386  
C   -1.4917666   1.2371547  1.2347438  
C   -2.8522728   1.4111914  1.5105874  
C   -3.5136263   0.4212793  2.2581960  
C   -2.7895105  -0.6922078  2.6912325  
C   -0.5548900  -1.9308340  2.7806847  
C    0.8047510   2.9000083  2.7373162  
C    1.2087281  -3.9945510  3.4897093  
C   -0.1393528  -4.0664895  3.8914818  
C   -1.0169583  -3.0354668  3.5381285  
H   -0.9371454   1.9909849  0.6548643  
H   -3.3738921   2.3091286  1.1452779  
H   -4.5843606   0.5185292  2.5017612  
H   -3.2847640  -1.4804512  3.2767930  
H    2.7327403  -2.8730782  2.4426186  
H    1.9100487  -4.7995708  3.7698543  
H   -0.5016334   4.9231798  4.4828214  
H   -2.0703379  -3.0946166  3.8588525  
N   -0.7844127   0.1642747  1.6516163  
C    0.3793082   0.3930496  -2.0429389  
C    1.4345356   1.0980323  -2.6697050  
C    1.2055671   1.9129660  -3.7871178  
C   -0.1023718   2.0528749  -4.3032530  
C   -1.1681430   1.3593666  -3.6828095  
C   -0.9317977   0.5456915  -2.5743106  
H    2.4585896   0.9989824  -2.2773574  
H    2.0563759   2.4375977  -4.2458196  
O   -0.4334359   2.8199435  -5.3773085  
H   -2.1811248   1.4757238  -4.0991596  
H   -1.7678363   0.0040392  -2.1041006  
C    0.6035550  -0.4910616  -0.9271151  
C    0.6165874  -1.5478216  -0.2322546  
C    0.5125044  -2.6303703  -0.1533227  
C    0.5904440   3.5378490  -6.0467717  
H    0.0933132   4.0802171  -6.8759145  
H    1.3640469   2.8545614  -6.4703852  
H    1.0856745   4.2764476  -5.3727552  

$vibrational spectrum$

| # | mode | symmetry | wave number cm$^{-1}$ | IR intensity km/mol | selection rules |
|---|------|----------|-----------------------|---------------------|-----------------|
| 1 |      |          | 0.00                  | 0.00000             | -               |
| 2 |      |          | 0.00                  | 0.00000             | -               |
| 3 |      |          | 0.00                  | 0.00000             | -               |

S22
|   |   |   |   |   |
|---|---|---|---|---|
| 4 | 0.00 | 0.00 | - | - |
| 5 | 0.00 | 0.00 | - | - |
| 6 | 0.00 | 0.00 | - | - |
| 7 | a | 14.73 | 0.48528 | YES | YES |
| 8 | a | 27.54 | 0.12557 | YES | YES |
| 9 | a | 33.83 | 1.31325 | YES | YES |
| 10 | a | 49.40 | 0.41729 | YES | YES |
| 11 | a | 63.10 | 0.05113 | YES | YES |
| 12 | a | 68.82 | 0.12965 | YES | YES |
| 13 | a | 84.84 | 1.50868 | YES | YES |
| 14 | a | 87.60 | 0.96268 | YES | YES |
| 15 | a | 94.72 | 0.65057 | YES | YES |
| 16 | a | 98.26 | 0.23069 | YES | YES |
| 17 | a | 107.68 | 0.58782 | YES | YES |
| 18 | a | 111.22 | 0.26776 | YES | YES |
| 19 | a | 113.72 | 0.43342 | YES | YES |
| 20 | a | 124.37 | 0.81217 | YES | YES |
| 21 | a | 142.73 | 7.98195 | YES | YES |
| 22 | a | 152.38 | 4.16835 | YES | YES |
| 23 | a | 188.93 | 1.98886 | YES | YES |
| 24 | a | 208.51 | 4.11258 | YES | YES |
| 25 | a | 232.84 | 2.10901 | YES | YES |
| 26 | a | 242.91 | 6.62047 | YES | YES |
| 27 | a | 251.98 | 0.82755 | YES | YES |
| 28 | a | 262.32 | 0.48982 | YES | YES |
| 29 | a | 275.23 | 8.01602 | YES | YES |
| 30 | a | 286.09 | 0.47693 | YES | YES |
| 31 | a | 357.60 | 4.93075 | YES | YES |
| 32 | a | 371.46 | 41.59569 | YES | YES |
| 33 | a | 401.58 | 1.57177 | YES | YES |
| 34 | a | 410.70 | 0.87504 | YES | YES |
| 35 | a | 417.33 | 7.84680 | YES | YES |
| 36 | a | 431.89 | 5.36836 | YES | YES |
| 37 | a | 447.02 | 9.62630 | YES | YES |
| 38 | a | 456.52 | 1.15156 | YES | YES |
| 39 | a | 461.81 | 2.74505 | YES | YES |
| 40 | a | 475.05 | 13.77999 | YES | YES |
| 41 | a | 477.54 | 10.19568 | YES | YES |
| 42 | a | 488.10 | 3.35668 | YES | YES |
| 43 | a | 493.60 | 4.70623 | YES | YES |
| 44 | a | 503.81 | 2.30819 | YES | YES |
| 45 | a | 521.30 | 53.32399 | YES | YES |
| 46 | a | 530.71 | 22.79117 | YES | YES |
| 47 | a | 541.23 | 7.10764 | YES | YES |
| 48 | a | 551.30 | 6.72379 | YES | YES |
| 49 | a | 557.16 | 1.63201 | YES | YES |
| 50 | a | 610.92 | 29.31754 | YES | YES |
2be'

SCF Energy (au) BP86/SV(P) -2391.957322776
SCF Energy (au) PBE0/def2-TZVPP -2391.512741707
SCF Energy (au) PBE0/def2-TZVPP -2391.5210557956 (Toluene Correction)
Zero Point Energy (au) 0.3212850
Chemical Potential (kJ mol\(^{-1}\)) 689.45
Dispersion Correction (au) PBE0/def2-TZVPP -0.06706478

xyz coordinates

|  |  |  |  |
|---|---|---|---|
| Mn | 1.2018114 | 2.3230176 | 0.7548611 |
| C | 1.1966094 | 2.6674406 | 2.5251254 |
| C | 2.9759053 | 2.0685991 | 0.7475998 |
| C | 1.3417653 | 4.0885188 | 0.3717193 |
| O | 1.4525414 | 5.2294814 | 0.1461870 |
| O | 4.1263842 | 1.8728426 | 0.7439207 |
| O | 1.2027896 | 2.9051979 | 3.6646116 |
| C | 1.4774602 | 1.1365428 | 1.2069601 |
| C | 1.6775184 | 3.2640542 | 0.2317406 |
| C | 3.0735233 | 3.1863285 | 0.1953522 |
| C | 3.6891506 | 2.0223060 | 0.6893591 |
| C | 2.8858991 | 0.9971163 | 1.1939489 |
| C | 0.5349590 | 0.1369759 | 1.7179660 |
| C | 0.8469663 | 0.4745153 | 1.6144229 |
| O | 1.3738901 | -1.5295390 | 2.7139420 |
| C | 0.0794585 | -1.991637 | 2.7849735 |
| C | -0.9429351 | -0.559629 | 2.2907844 |
| H | -1.1555815 | 4.1579091 | -0.138556 |
| H | -3.6592854 | 4.0254717 | -0.204464 |
| H | -4.7846733 | 1.9171727 | 0.6805989 |
| H | -3.3436826 | 0.0755080 | 1.5820225 |
| H | 2.8596110 | -0.2012367 | 2.1153004 |
| H | 2.1318358 | -2.3568796 | 3.110001 |
| H | -0.314988 | 2.9523274 | 3.2342524 |
| H | -2.0125979 | -1.3508374 | 2.3596834 |
| N | -0.8945810 | 2.2786934 | 0.7214380 |
| H | 1.2437389 | 3.2338625 | -2.1008219 |
| C | 1.1369187 | 2.4156359 | -1.3866901 |
| C | 1.0657742 | 1.1735248 | -1.1394614 |
| C | 0.9027471 | -0.2214474 | -1.4706394 |
| C | 0.5774429 | -2.9145021 | -2.2325676 |
| C | 1.7520298 | -2.5162861 | -1.5678323 |
| C | 1.9080735 | -1.1843100 | -1.1866765 |
| C | -0.2675862 | -0.658157 | -2.1352765 |
| C | -0.4362164 | -1.9999745 | -2.5139696 |
| O | 0.5206688 | -4.2637539 | -2.5571430 |
| H | 2.5333940 | -3.2634943 | -1.3587178 |
| H | 2.8282443 | -0.8685552 | -0.6735143 |
| H | -1.0597815 | 0.0716795 | -2.3632990 |
| H | -1.3607870 | -2.2966877 | -3.0307668 |
| C | -0.6259038 | -4.7517284 | -3.2312324 |
| H | -2.7672266 | -4.2549073 | -4.2209286 |
| H | -1.5520862 | -4.6194973 | -2.6224653 |
| H | -0.4512763 | -5.8346902 | -3.3925732 |

$vibrational spectrum$

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|---|
| 1 | 0.00 | 0.00000 | - | - |
| 2 | 0.00 | 0.00000 | - | - |
| 3 | 0.00 | 0.00000 | - | - |
|   |   |   |   |   |
|---|---|---|---|---|
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | a | 13.39 | 0.19688 | YES | YES |
| 8 | a | 19.98 | 0.14787 | YES | YES |
| 9 | a | 44.37 | 0.00775 | YES | YES |
| 10 | a | 48.89 | 0.01718 | YES | YES |
| 11 | a | 61.20 | 0.59746 | YES | YES |
| 12 | a | 68.25 | 0.68447 | YES | YES |
| 13 | a | 81.88 | 0.18327 | YES | YES |
| 14 | a | 87.08 | 1.58370 | YES | YES |
| 15 | a | 95.70 | 0.24980 | YES | YES |
| 16 | a | 97.57 | 0.86361 | YES | YES |
| 17 | a | 102.60 | 0.63889 | YES | YES |
| 18 | a | 110.71 | 0.22605 | YES | YES |
| 19 | a | 117.52 | 0.87571 | YES | YES |
| 20 | a | 122.30 | 0.55115 | YES | YES |
| 21 | a | 150.40 | 5.39288 | YES | YES |
| 22 | a | 161.61 | 1.44765 | YES | YES |
| 23 | a | 190.00 | 0.15297 | YES | YES |
| 24 | a | 216.68 | 1.37135 | YES | YES |
| 25 | a | 225.75 | 4.27679 | YES | YES |
| 26 | a | 237.39 | 0.07127 | YES | YES |
| 27 | a | 253.95 | 0.92664 | YES | YES |
| 28 | a | 264.92 | 0.43227 | YES | YES |
| 29 | a | 278.53 | 4.50877 | YES | YES |
| 30 | a | 285.83 | 0.30984 | YES | YES |
| 31 | a | 358.53 | 2.62385 | YES | YES |
| 32 | a | 375.40 | 30.36449 | YES | YES |
| 33 | a | 396.79 | 5.19120 | YES | YES |
| 34 | a | 411.11 | 1.55916 | YES | YES |
| 35 | a | 417.35 | 3.54155 | YES | YES |
| 36 | a | 431.69 | 7.33705 | YES | YES |
| 37 | a | 441.25 | 3.09284 | YES | YES |
| 38 | a | 457.69 | 1.41522 | YES | YES |
| 39 | a | 467.45 | 2.67182 | YES | YES |
| 40 | a | 473.68 | 0.88691 | YES | YES |
| 41 | a | 487.20 | 13.32081 | YES | YES |
| 42 | a | 489.99 | 5.98088 | YES | YES |
| 43 | a | 492.50 | 15.77534 | YES | YES |
| 44 | a | 502.67 | 4.65991 | YES | YES |
| 45 | a | 517.38 | 1.53708 | YES | YES |
| 46 | a | 531.20 | 25.42967 | YES | YES |
| 47 | a | 538.74 | 7.43532 | YES | YES |
| 48 | a | 556.96 | 2.89561 | YES | YES |
| 49 | a | 566.53 | 2.71462 | YES | YES |
| 50 | a | 614.64 | 47.84106 | YES | YES |
bf
SCF Energy (au) BP86/SV(P) -2376.686035034
SCF Energy (au) PBE0/def2-TZVPP -2376.263171392
SCF Energy (au) PBE0/def2-TZVPP -2376.2704120363 (Toluene Correction)
Zero Point Energy (au) 0.2818722
Chemical Potential (kJ mol\(^{-1}\)) 591.01
Dispersion Correction (au) PBE0/def2-TZVPP -0.06135801

xyz coordinates
41

Mn  1.3698504  0.2105297  0.6366223
C   1.8030365  0.6855900  2.3195994
C   3.0564347 -0.2930315  0.2993493
C   1.6658100  1.8905940  0.0127788
O   1.8958418  2.9812785 -0.3345833
O   4.1506892 -0.6357557  0.0829671
O   2.0890447  0.9837826  3.4077538
C   -1.3001451 -0.4349008  1.7536845
C   -1.3619793  1.6277135  0.6309972
C   -2.7232705  1.8043899  2.0565742
C   -3.3934818  0.8079514  1.6314084
C   -2.6767037 -0.3132861  2.1509347
C   -0.4461613 -1.5590405  1.7399506
C   -1.7783799 -2.5325499  2.1201434
C   -1.3081757 -3.6313270  2.8607364
C   -0.0437438 -3.7037738  3.2492435
C   -0.9163816 -2.6685955  2.8960569
H   -0.8006641  2.3863890  0.0640316
H   -3.2386840  2.7090901  0.5432493
H   -4.4654821  0.9065288  1.8686038
H   -3.1790790 -1.1058875  2.6299977
H   -2.8433144 -2.5053590  1.8343217
H   -2.0055263 -4.4394494  3.1405788
H   -0.4129731 -4.5643381  3.8304449
H   -1.9766005 -2.7281497  3.2068953
N  -0.6620770  0.5465688  1.0391254
C   0.4232149  0.7503603 -2.6191902
C   1.4166841  1.5477296 -3.2432736
C   1.1096203  2.3325225 -4.3616439
C   -0.2022105  2.3320446 -4.8574375
C   -1.2107086  1.5617863 -4.2621677
C   -0.8952720  0.7751300 -3.1468047
H   2.4446425  1.5412858 -2.8500957
H   1.8755802  2.9494154 -4.8565640
F  -0.5016656  3.0885787 -5.9302302
H  -2.2287345  1.5845994 -4.6811698
H  -1.6753528  0.1596039 -2.6721317
C   0.7167115 -0.1111110 -1.4981636
C   0.7573191 -1.1846136 -0.8280762
H   0.6802769 -2.2704970 -0.7650598

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number (cm$^{-1}$) | IR intensity (km/mol) | selection rules |
|---|------|----------|-------------------------|-----------------------|-----------------|
| 1 |      |          | 0.00                    | 0.00000               | -               |
| 2 |      |          | 0.00                    | 0.00000               | -               |
| 3 |      |          | 0.00                    | 0.00000               | -               |
| 4 |      |          | 0.00                    | 0.00000               | -               |
| 5 |      |          | 0.00                    | 0.00000               | -               |
| 6 |      |          | 0.00                    | 0.00000               | -               |
| 7 |      | a        | 15.26                   | 0.30305               | YES             | YES             |
| #  | Value 1 | Value 2   | Value 3   | Value 4 | Value 5 | Value 6 | Value 7 | Value 8 |
|----|---------|-----------|-----------|---------|---------|---------|---------|---------|
| 8  | a       | 22.55     | 0.21713   | YES     | YES     |
| 9  | a       | 36.75     | 0.03404   | YES     | YES     |
| 10 | a       | 54.19     | 0.12635   | YES     | YES     |
| 11 | a       | 68.66     | 0.12992   | YES     | YES     |
| 12 | a       | 69.04     | 0.03680   | YES     | YES     |
| 13 | a       | 85.76     | 1.19921   | YES     | YES     |
| 14 | a       | 89.39     | 0.32021   | YES     | YES     |
| 15 | a       | 98.28     | 0.65821   | YES     | YES     |
| 16 | a       | 108.74    | 0.22748   | YES     | YES     |
| 17 | a       | 111.52    | 0.15179   | YES     | YES     |
| 18 | a       | 112.93    | 0.28324   | YES     | YES     |
| 19 | a       | 121.44    | 0.12117   | YES     | YES     |
| 20 | a       | 139.59    | 2.64905   | YES     | YES     |
| 21 | a       | 158.76    | 3.46708   | YES     | YES     |
| 22 | a       | 189.00    | 1.22604   | YES     | YES     |
| 23 | a       | 214.26    | 1.85074   | YES     | YES     |
| 24 | a       | 239.50    | 0.51428   | YES     | YES     |
| 25 | a       | 259.39    | 6.47716   | YES     | YES     |
| 26 | a       | 264.27    | 3.68135   | YES     | YES     |
| 27 | a       | 284.68    | 0.09891   | YES     | YES     |
| 28 | a       | 357.70    | 3.02508   | YES     | YES     |
| 29 | a       | 378.20    | 28.05821  | YES     | YES     |
| 30 | a       | 391.70    | 11.00793  | YES     | YES     |
| 31 | a       | 409.93    | 0.75986   | YES     | YES     |
| 32 | a       | 415.89    | 1.48373   | YES     | YES     |
| 33 | a       | 419.65    | 11.81778  | YES     | YES     |
| 34 | a       | 435.47    | 6.80079   | YES     | YES     |
| 35 | a       | 451.76    | 20.06276  | YES     | YES     |
| 36 | a       | 456.40    | 2.32529   | YES     | YES     |
| 37 | a       | 461.08    | 1.55757   | YES     | YES     |
| 38 | a       | 477.37    | 5.21520   | YES     | YES     |
| 39 | a       | 486.93    | 2.06431   | YES     | YES     |
| 40 | a       | 493.26    | 5.14778   | YES     | YES     |
| 41 | a       | 502.04    | 11.11529  | YES     | YES     |
| 42 | a       | 503.59    | 1.08353   | YES     | YES     |
| 43 | a       | 526.90    | 38.61188  | YES     | YES     |
| 44 | a       | 538.69    | 9.57228   | YES     | YES     |
| 45 | a       | 550.87    | 7.09999   | YES     | YES     |
| 46 | a       | 556.89    | 1.66527   | YES     | YES     |
| 47 | a       | 609.50    | 33.01311  | YES     | YES     |
| 48 | a       | 622.64    | 9.01751   | YES     | YES     |
| 49 | a       | 625.26    | 5.49474   | YES     | YES     |
| 50 | a       | 630.58    | 8.65305   | YES     | YES     |
2bf'

SCF Energy (au) BP86/SV(P) -2376.684012464
SCF Energy (au) PBE0/def2-TZVPP -2376.261119915
SCF Energy (au) PBE0/def2-TZVPP -2376.2683674155 (Toluene Correction)
Zero Point Energy (au) 0.2819030
Chemical Potential (kJ mol$^{-1}$) 591.74
Dispersion Correction (au) PBE0/def2-TZVPP 0.06372121

xyz coordinates

41

Mn   1.2369841    1.8112428    0.2458945
C    1.3710057    2.2239260    1.9979497
C    2.9973830    1.4946875    0.1231140
C    1.4070378    3.5547432    0.2208095
O    1.5385251    4.6804844    0.5020000
O    4.1374258    1.2590269    0.0458268
O    1.4653967    2.5035421    3.1234923
C    1.4385143    0.7493141    0.9600496
C    1.6425046    2.8281922    0.1147058
C    3.0389787    2.7999555    0.0423265
C    3.6527406    1.6883888    0.5621785
C    2.8474098    0.6622517    1.0618302
C    0.4931389    0.2595865    1.4480186
C    0.8870150    0.0197608    1.2230263
C    1.8292920    0.9052704    1.7195257
C    1.4278866    0.8614105    2.3776020
C    0.0601603    2.3574599    0.5696724
C    0.8958064    0.1447124    2.1080509
H    1.1218721    3.6804176    0.5784063
H    3.6263729    3.636933     0.4506317
H    4.7502280    1.6239560    0.6421708
H    3.0344980    0.2195121    1.5341995
H    2.9092528    0.7158254    1.5984144
H    2.1890698    2.7877433    2.7481177
H    0.2575013    3.2783122    3.0851389
H    1.9677731    1.6620028    2.2701512
N    0.8574199    1.8421104    0.3700461
H    1.1178314    2.5991783    2.6467347
C    1.0251692    1.8237949    1.8842664
C    0.9074673    0.6019790    1.5617475
C    0.6359327    0.7934439    1.8185723
C    0.0850213    3.4861763    2.3095169
C    1.3372732    3.1407576    1.8718695
C    1.6054862    1.7987903    1.5754972
C    0.6198875    1.1771431    2.3554369
C    0.8990480    2.5194103    2.6455898
F    0.1785803    4.7781744    2.6779051
H    2.0861359    3.9282089    1.6949677
H    2.5847550    1.5154101    1.1615720
H    1.3812274    0.4052900    2.5485932
H    1.8699069    2.8282538    3.0633400

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|-----------------|
| 1 | 0.00 | 0.00000  | -           | -            |
| 2 | 0.00 | 0.00000  | -           | -            |
| 3 | 0.00 | 0.00000  | -           | -            |
| 4 | 0.00 | 0.00000  | -           | -            |
| 5 | 0.00 | 0.00000  | -           | -            |
| 6 | 0.00 | 0.00000  | -           | -            |
| 7 | a   | 15.39    | 0.27467     | YES          | YES             |
|    |   |        |        |   |   |
|----|---|--------|--------|---|---|
|  8 | a | 21.55  | 0.51847| YES | YES|
|  9 | a | 44.50  | 0.11890| YES | YES|
| 10 | a | 50.19  | 0.06929| YES | YES|
| 11 | a | 63.50  | 0.12389| YES | YES|
| 12 | a | 70.81  | 0.39479| YES | YES|
| 13 | a | 86.26  | 0.60158| YES | YES|
| 14 | a | 93.80  | 0.51872| YES | YES|
| 15 | a | 96.25  | 0.54080| YES | YES|
| 16 | a |103.98  | 0.46765| YES | YES|
| 17 | a |111.32  | 0.04869| YES | YES|
| 18 | a |112.85  | 0.20982| YES | YES|
| 19 | a |127.43  | 0.18839| YES | YES|
| 20 | a |148.93  | 1.14170| YES | YES|
| 21 | a |165.79  | 2.17073| YES | YES|
| 22 | a |189.15  | 0.17288| YES | YES|
| 23 | a |218.42  | 0.44821| YES | YES|
| 24 | a |231.41  | 2.55714| YES | YES|
| 25 | a |255.37  | 1.15210| YES | YES|
| 26 | a |271.20  | 1.74803| YES | YES|
| 27 | a |284.92  | 0.21224| YES | YES|
| 28 | a |358.46  | 2.27539| YES | YES|
| 29 | a |382.81  |26.61717| YES | YES|
| 30 | a |389.11  | 7.98426| YES | YES|
| 31 | a |409.08  | 0.41539| YES | YES|
| 32 | a |411.80  | 2.83525| YES | YES|
| 33 | a |420.64  | 1.59546| YES | YES|
| 34 | a |434.52  | 4.52181| YES | YES|
| 35 | a |448.98  | 7.51490| YES | YES|
| 36 | a |457.87  | 1.61266| YES | YES|
| 37 | a |468.81  | 5.63922| YES | YES|
| 38 | a |476.20  | 2.44933| YES | YES|
| 39 | a |488.08  | 1.56393| YES | YES|
| 40 | a |490.83  | 1.81398| YES | YES|
| 41 | a |499.72  | 3.43406| YES | YES|
| 42 | a |505.68  |14.63655| YES | YES|
| 43 | a |529.19  |23.69735| YES | YES|
| 44 | a |535.60  | 4.82454| YES | YES|
| 45 | a |557.17  | 2.54145| YES | YES|
| 46 | a |565.67  | 3.11213| YES | YES|
| 47 | a |613.82  |45.67900| YES | YES|
| 48 | a |622.84  |13.82057| YES | YES|
| 49 | a |625.83  |15.93175| YES | YES|
| 50 | a |629.85  | 3.56307| YES | YES|
2bg

SCF Energy (au) BP86/SV(P) -2614.328819566
SCF Energy (au) PBE0/def2-TZVPP -2613.948640333
SCF Energy (au) PBE0/def2-TZVPP -2613.955675194 (Toluene Correction)
Zero Point Energy (au) 0.2944290
Chemical Potential (kJ mol⁻¹) 612.46
Dispersion Correction (au) PBE0/def2-TZVPP -0.06476787

xyz coordinates
44

Mn  1.37660622 -0.0299156 1.0645268
C   1.8229581 0.4356415 2.7480525
C   3.0622173 -0.5265104 0.7094753
C   1.6638503 1.6585459 0.4552845
O   1.8874604 2.7516652 0.1141967
O   4.1554677 -0.8631109 0.4807096
O   2.1184501 0.7296068 3.8343661
C  -1.2766004 -0.6795420 2.2218831
C  -1.3620294 1.3794322 1.0940160
C  -2.7193760 1.5530719 1.3849393
C  -3.3748007 0.5573279 2.1295807
C  -2.6482706 -0.5605927 2.5468182
C  -0.4139833 -1.8012923 2.6080498
O   1.8120399 -2.7718873 2.5409442
O  -1.3560960 -3.8700920 3.2912667
C   0.0112576 -3.9433639 3.7031411
C  -0.8691605 -2.9102356 3.3632339
H  -0.8122469 2.1383073 0.5159744
H  -3.2432126 2.4549779 1.0324646
H  -4.4429880 0.6539621 2.3839604
H  -3.1391444 -1.3524911 3.1310133
H   2.8717417 -2.7431955 2.2367681
H   2.0593057 -4.6767524 3.5601350
H  -0.3465864 -4.8032959 4.2922161
H  -1.9166367 -2.9708702 3.6924543
N  -0.6527397 0.3016419 1.4946763
C   0.4549691 0.5132800 -2.1782245
C   1.4807382 1.2754454 -2.7931028
C   1.2051413 2.0684467 -3.9116446
C  -0.1007871 2.1280631 -4.4368587
C  -1.1299957 1.3826546 -3.8324164
C  -0.8568091 0.5831906 -2.7158327
H   2.5032306 1.2358872 -2.3876885
H   2.0116705 2.6551033 -4.3782887
C  -0.3766414 2.9532026 -5.6723436
H  -2.1527451 1.4310007 -4.2369787
H  -1.6623480 -0.0018611 -2.2452578
C   0.7144502 -0.3458806 -1.0471444
C   0.7396745 -1.4246914 -0.3831151
H   0.6447374 -2.5096058 -0.3253393
F   0.3742405 4.0809757 -5.7000792
F  -1.6778870 3.3258943 -5.7536733
F  -0.0904370 2.2616444 -6.8066550

$vibrational spectrum

| # | mode | symmetry | wave number (cm⁻¹) | IR intensity (km/mol) | selection rules |
|---|------|---------|-------------------|----------------------|-----------------|
| 1 |      |         | 0.00              | 0.00000              | -               |
| 2 |      |         | 0.00              | 0.00000              | -               |
| 3 |      |         | 0.00              | 0.00000              | -               |
| 4 |      |         | 0.00              | 0.00000              | -               |
| Row | Value 1 | Value 2 | Value 3 | Value 4 | Value 5 | Value 6 |
|-----|---------|---------|---------|---------|---------|---------|
| 5   | 0.00    | 0.0000  | -       | -       |         |         |
| 6   | 0.00    | 0.0000  | -       | -       |         |         |
| 7   | a       | 12.17   | 0.41522 | YES     | YES     |         |
| 8   | a       | 20.39   | 0.15130 | YES     | YES     |         |
| 9   | a       | 35.27   | 0.10531 | YES     | YES     |         |
| 10  | a       | 37.43   | 0.03820 | YES     | YES     |         |
| 11  | a       | 49.21   | 0.09937 | YES     | YES     |         |
| 12  | a       | 62.82   | 0.21459 | YES     | YES     |         |
| 13  | a       | 69.00   | 0.07337 | YES     | YES     |         |
| 14  | a       | 83.96   | 0.19366 | YES     | YES     |         |
| 15  | a       | 85.66   | 1.32995 | YES     | YES     |         |
| 16  | a       | 92.84   | 0.36282 | YES     | YES     |         |
| 17  | a       | 95.29   | 0.95302 | YES     | YES     |         |
| 18  | a       | 106.47  | 0.10456 | YES     | YES     |         |
| 19  | a       | 109.91  | 0.10488 | YES     | YES     |         |
| 20  | a       | 113.97  | 0.26757 | YES     | YES     |         |
| 21  | a       | 122.89  | 0.94308 | YES     | YES     |         |
| 22  | a       | 152.58  | 1.00454 | YES     | YES     |         |
| 23  | a       | 178.29  | 2.11843 | YES     | YES     |         |
| 24  | a       | 187.68  | 2.07863 | YES     | YES     |         |
| 25  | a       | 204.44  | 0.65822 | YES     | YES     |         |
| 26  | a       | 223.75  | 0.27808 | YES     | YES     |         |
| 27  | a       | 240.54  | 0.77371 | YES     | YES     |         |
| 28  | a       | 260.93  | 0.55345 | YES     | YES     |         |
| 29  | a       | 280.59  | 0.60115 | YES     | YES     |         |
| 30  | a       | 291.71  | 0.57093 | YES     | YES     |         |
| 31  | a       | 320.94  | 39.44566| YES     | YES     |         |
| 32  | a       | 358.15  | 1.90390 | YES     | YES     |         |
| 33  | a       | 382.50  | 3.39938 | YES     | YES     |         |
| 34  | a       | 397.47  | 9.23041 | YES     | YES     |         |
| 35  | a       | 403.54  | 6.39425 | YES     | YES     |         |
| 36  | a       | 417.84  | 10.02122| YES     | YES     |         |
| 37  | a       | 429.45  | 1.95527 | YES     | YES     |         |
| 38  | a       | 446.92  | 4.61272 | YES     | YES     |         |
| 39  | a       | 456.06  | 1.37970 | YES     | YES     |         |
| 40  | a       | 456.24  | 8.85877 | YES     | YES     |         |
| 41  | a       | 473.87  | 3.19751 | YES     | YES     |         |
| 42  | a       | 485.82  | 2.00936 | YES     | YES     |         |
| 43  | a       | 491.78  | 5.65688 | YES     | YES     |         |
| 44  | a       | 496.06  | 1.61189 | YES     | YES     |         |
| 45  | a       | 501.48  | 5.88190 | YES     | YES     |         |
| 46  | a       | 515.47  | 9.01132 | YES     | YES     |         |
| 47  | a       | 535.60  | 26.33736| YES     | YES     |         |
| 48  | a       | 548.45  | 5.41518 | YES     | YES     |         |
| 49  | a       | 556.91  | 3.03587 | YES     | YES     |         |
| 50  | a       | 561.76  | 8.27135 | YES     | YES     |         |
SCF Energy (au) BP86/SV(P)  -2614.327168892
SCF Energy (au) PBE0/def2-TZVPP  -2613.947026262
SCF Energy (au) PBE0/def2-TZVPP  -2613.9542738044 (Toluene Correction)
Zero Point Energy (au)  0.2946089
Chemical Potential (kJ mol⁻¹)  615.65
Dispersion Correction (au) PBE0/def2-TZVPP  -0.06779443

xyz coordinates
44

Mn    1.2573837    2.1963969    0.4486841
C     1.3531009    2.5665551    2.2135486
C     3.0245241    1.9082488    0.3486739
C     1.4107084    3.9540834    0.0305177
O     1.5310693    5.0887235 -0.2159537
O     4.1686241    1.6910536    0.2840612
O     1.4228473    2.8195984    3.3467836
C     1.4121583    1.0754608    1.0929445
C     1.6333439    3.1754795    0.0628049
C     3.0302405    3.1192127    0.1047146
C     3.6349183    1.9818055    0.6689859
C     2.8208450    0.9593536    1.1620807
C     0.4584825    0.0722705    1.5772752
C     1.8703617    0.3822284    1.3919805
C     1.4759048    0.3822284    1.3919805
C     0.1110156    0.3822284    1.3919805
C     0.9207441    0.3822284    1.3919805
C     1.8703617 -0.10754608    2.4966351
C     1.4228473 -0.30457681    2.4966351
C     0.1110156 -0.30457681    2.4966351
C     -0.8522662 -0.1404826    2.1924812
H     -1.1195922    4.0480721 -0.3696454
H     -3.6251749    3.9540940    0.2963112
H     -4.7323954    1.8944362    0.7229211
H     -3.2707823    0.0580324    1.6033314
H     2.9487511 -0.3250674    1.7901990
H     2.2430310 -2.4437773    2.8624149
H     -0.2003424 -2.9907485    3.1256045
H     -1.9199092 -1.3831785    2.3217010
N     -0.8401231    2.1925027    0.5405406
H     1.1982519    3.0457681 -2.4312254
H     1.0905043    2.2587945 -1.6825979
H     0.9622207    1.0325429 -1.3807726
H     0.6868258 -0.3602690 -1.6397991
H     0.0939562 -3.0769722 -2.1473174
H     1.3701303 -2.7079213 -1.6823147
H     1.6628496 -1.3646825 -1.4238984
H     -0.5884926 -0.7447573 -2.1270631
H     -0.8805765 -2.0905795 -2.3769088
H     -0.2506350 -4.5380390 -2.3353709
H     2.1393655 -3.4781489 -1.5177800
H     2.6599586 -1.0783748 -1.0571861
H     -1.3505437    0.2888712 -2.3095423
H     -1.8735156 -2.3768497 -2.7570294
F     0.8329323 -5.2770393 -2.6769699
F     -1.1879230 -4.7182721 -3.2986776
F     -0.7528007 -5.0803084 -1.1934013

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number (cm⁻¹) | IR intensity (km/mol) | selection rules |
|---|------|----------|-------------------|----------------------|-----------------|
| 1 |      |          | 0.00              | 0.00000              | -               |
| 2 |      |          | 0.00              | 0.00000              | -               |
| 3 |      |          | 0.00              | 0.00000              | -               |
| 4 |      |          | 0.00              | 0.00000              | -               |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | a | 14.98 | 0.63488 | YES | YES |
| 8 | a | 24.73 | 0.22465 | YES | YES |
| 9 | a | 43.41 | 0.03090 | YES | YES |
| 10 | a | 47.63 | 0.31629 | YES | YES |
| 11 | a | 49.76 | 0.06600 | YES | YES |
| 12 | a | 61.87 | 0.26106 | YES | YES |
| 13 | a | 67.06 | 0.16659 | YES | YES |
| 14 | a | 82.71 | 0.48376 | YES | YES |
| 15 | a | 89.55 | 0.21796 | YES | YES |
| 16 | a | 94.33 | 0.63058 | YES | YES |
| 17 | a | 98.47 | 0.91191 | YES | YES |
| 18 | a | 103.09 | 0.30264 | YES | YES |
| 19 | a | 109.36 | 0.12101 | YES | YES |
| 20 | a | 118.51 | 0.23764 | YES | YES |
| 21 | a | 126.63 | 0.43690 | YES | YES |
| 22 | a | 159.54 | 0.91062 | YES | YES |
| 23 | a | 184.02 | 0.14154 | YES | YES |
| 24 | a | 193.52 | 0.22917 | YES | YES |
| 25 | a | 210.22 | 0.93389 | YES | YES |
| 26 | a | 217.04 | 0.33259 | YES | YES |
| 27 | a | 235.08 | 1.62107 | YES | YES |
| 28 | a | 264.01 | 0.57022 | YES | YES |
| 29 | a | 282.63 | 0.22548 | YES | YES |
| 30 | a | 298.91 | 0.34890 | YES | YES |
| 31 | a | 316.84 | 22.44646 | YES | YES |
| 32 | a | 358.59 | 1.90104 | YES | YES |
| 33 | a | 384.74 | 1.73648 | YES | YES |
| 34 | a | 399.82 | 0.67506 | YES | YES |
| 35 | a | 402.85 | 10.35245 | YES | YES |
| 36 | a | 417.48 | 3.87632 | YES | YES |
| 37 | a | 430.27 | 2.50205 | YES | YES |
| 38 | a | 438.67 | 2.11925 | YES | YES |
| 39 | a | 457.39 | 1.48654 | YES | YES |
| 40 | a | 465.98 | 1.18742 | YES | YES |
| 41 | a | 470.47 | 2.76870 | YES | YES |
| 42 | a | 485.67 | 6.06921 | YES | YES |
| 43 | a | 489.03 | 1.53234 | YES | YES |
| 44 | a | 497.56 | 4.15803 | YES | YES |
| 45 | a | 502.00 | 11.68884 | YES | YES |
| 46 | a | 521.01 | 4.96104 | YES | YES |
| 47 | a | 528.15 | 14.73262 | YES | YES |
| 48 | a | 556.28 | 1.44075 | YES | YES |
| 49 | a | 558.45 | 2.58503 | YES | YES |
| 50 | a | 566.31 | 2.08477 | YES | YES |
2bh

SCF Energy (au) BP86/SV(P) -2505.243220756
SCF Energy (au) PBE0/def2-TZVPP -2504.795978988
SCF Energy (au) PBE0/def2-TZVPP -2504.8052396137 (Toluene Correction)
Zero Point Energy (au) 0.3311844
Chemical Potential (kJ mol\(^{-1}\)) 706.41
Dispersion Correction (au) PBE0/def2-TZVPP -0.06732812

xyz coordinates
47

Mn  1.3037687 -0.3393686  1.5642927
C   1.7730387  0.1344454  3.2386633
C   2.9894863 -0.8119268  1.1812376
C   1.5546961  1.3527175  0.9477769
O   1.7573715  2.4484425  0.6023689
O   4.0837222 -1.1330871  0.9345719
O   2.0847189  0.4335773  4.3194731
C   -1.3138688 -1.0269365  2.7797729
C   -1.4593333  1.0217737  1.6394196
C   -2.8103401  1.1770946  1.9618594
C   -3.4317669  0.1781784  2.7313711
C   -2.6784524 -0.9257404  3.1383201
C   -0.4265261 -2.1349737  3.1495659
C    0.9175908 -2.0393267  2.6841830
C    1.8101083 -3.0749629  3.0315404
C    1.3873740 -4.177526  3.7946080
C    0.0540064 -4.2683357  4.2389227
C   -0.8483498 -3.2481047  3.9178066
H   -0.9341412  1.7839641  1.0418882
H   -3.3566609  2.0677959  1.6155462
H   -4.4945293  0.2610368  3.0119807
H   -3.1425832 -1.7205382  3.7401988
H    2.8618655 -3.0326314  2.7023972
H    2.1077454 -4.9742865  4.0480141
H   -0.2779135 -5.1315735  4.8383119
H   -1.8898483 -3.3223666  4.2718269
N   -0.7224954 -0.0414370  2.0314249
C    0.3817212  0.2025585 -1.6825569
C    1.4305623  0.9225264 -2.3113210
C    1.1772920  1.7120587 -3.4373745
C   -0.1314288  1.8162960 -3.9587425
C   -1.1811545  1.1092983 -3.3339399
C   -0.9323909  0.3121893 -2.2126835
H    2.4533471  0.8470271 -1.9109724
H    1.9984106  2.2594003 -3.9235976
H   -0.4621050  2.6479676 -5.1560877
H   -2.1956412  1.1981318 -3.7536394
H   -1.7525776 -0.2447689 -1.7327883
C    0.6246510 -0.6587717 -0.5500646
C    0.6522165 -1.7324185  0.1221244
H    0.5521967 -2.8167169  0.1840923
O    0.6347577  3.2637250 -5.6739877
O   -1.5811101  2.7704014 -5.6290021
C    0.3952956  4.0772873 -6.8291640
H    1.3816802  4.4905983 -7.1168170
H   -0.3167022  4.8971929 -6.5931624
H   -0.0291043  3.4703400 -7.6578580

$vibrational spectrum

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|----------------|
| 1 |      |          | 0.00        | 0.00000      | -              | -              |

S34
|   |   |   |   |   |
|---|---|---|---|---|
| 2 | 0.00 | 0.00000 | - | - |
| 3 | 0.00 | 0.00000 | - | - |
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | a | 12.57 | 0.40934 | YES | YES |
| 8 | a | 21.74 | 0.40464 | YES | YES |
| 9 | a | 27.08 | 1.41359 | YES | YES |
| 10 | a | 46.22 | 0.15075 | YES | YES |
| 11 | a | 59.22 | 0.08189 | YES | YES |
| 12 | a | 65.99 | 0.43548 | YES | YES |
| 13 | a | 72.96 | 0.34214 | YES | YES |
| 14 | a | 81.48 | 0.30844 | YES | YES |
| 15 | a | 84.43 | 1.94921 | YES | YES |
| 16 | a | 90.25 | 0.19612 | YES | YES |
| 17 | a | 93.42 | 0.21922 | YES | YES |
| 18 | a | 103.84 | 0.38580 | YES | YES |
| 19 | a | 109.74 | 0.07931 | YES | YES |
| 20 | a | 113.53 | 0.35221 | YES | YES |
| 21 | a | 120.73 | 0.30032 | YES | YES |
| 22 | a | 125.90 | 0.91882 | YES | YES |
| 23 | a | 147.48 | 1.71613 | YES | YES |
| 24 | a | 152.66 | 4.50491 | YES | YES |
| 25 | a | 177.22 | 1.29846 | YES | YES |
| 26 | a | 188.89 | 1.54772 | YES | YES |
| 27 | a | 209.11 | 1.48568 | YES | YES |
| 28 | a | 234.98 | 0.55588 | YES | YES |
| 29 | a | 245.53 | 4.50037 | YES | YES |
| 30 | a | 262.35 | 0.79599 | YES | YES |
| 31 | a | 283.14 | 0.95130 | YES | YES |
| 32 | a | 311.13 | 27.87040 | YES | YES |
| 33 | a | 327.93 | 11.67023 | YES | YES |
| 34 | a | 350.73 | 23.39475 | YES | YES |
| 35 | a | 359.49 | 5.82019 | YES | YES |
| 36 | a | 404.30 | 0.02491 | YES | YES |
| 37 | a | 416.19 | 3.06781 | YES | YES |
| 38 | a | 426.53 | 2.24478 | YES | YES |
| 39 | a | 440.49 | 1.77115 | YES | YES |
| 40 | a | 449.10 | 1.71625 | YES | YES |
| 41 | a | 455.95 | 1.03867 | YES | YES |
| 42 | a | 457.74 | 24.14923 | YES | YES |
| 43 | a | 473.30 | 2.85469 | YES | YES |
| 44 | a | 485.96 | 1.78627 | YES | YES |
| 45 | a | 491.68 | 6.24711 | YES | YES |
| 46 | a | 501.47 | 4.97107 | YES | YES |
| 47 | a | 514.16 | 12.33024 | YES | YES |
| 48 | a | 525.09 | 28.57055 | YES | YES |
| 49 | a | 538.51 | 13.49851 | YES | YES |
| 50 | a | 549.73 | 5.41364 | YES | YES |
2hh'

SCF Energy (au) BP86/SV(P)  -2505.241127470
SCF Energy (au) PBE0/def2-TZVPP -2504.793700599
SCF Energy (au) PBE0/def2-TZVPP -2504.803126288 (Toluene Correction)
Zero Point Energy (au) 0.3312181
Chemical Potential (kJ mol\(^{-1}\)) 706.73
Dispersion Correction (au) PBE0/def2-TZVPP -0.06985329

xyz coordinates
47

Mn  1.3525788  2.6404515  0.6752257
C  1.4623236  3.0505351  2.4306510
C  3.1180559  2.3426824  0.5704972
C  1.5125479  4.3868787  0.2159357
O  1.6366598  5.5146486 -0.0592851
O  4.2612268  2.1210474  0.5048932
O  1.5409259  3.3295203  3.5572676
C  1.3186215  1.5605827  1.3798475
C  1.5332292  3.6333060  0.2947321
C  2.9296576  3.5961481  0.3631720
C  3.5376511  2.4833359  0.9711769
C  2.7271811  1.4647459  1.4779097
C  0.3682498  0.5597142  1.8746643
C  1.0111152  0.8482912  1.6580389
C  1.9583656 -0.0697541  2.1565151
C  1.5609619 -1.2495664  2.8106551
C  0.1954744 -1.5350771  2.9666555
C  2.7271811  1.4647459  1.4779097
H  1.0168526  4.4866881 -0.1716124
H  3.5214392  4.4269324 -0.0508772
H  4.639005  2.4121097  1.0484499
H  3.1798632  0.5823249  1.9532209
H  0.3073138  0.1269373  2.0393990
H  2.3263312 -1.9524765  3.1813687
H  0.1177088 -2.4595193  3.5083338
H  1.8332349 -0.8548593  2.6874203
N  0.7433560  2.6546985  0.7866600
H  1.2544836  3.4323463 -2.2177885
C  1.1606076  2.6610036 -1.4510573
C  1.0487005  1.4375808 -1.1274324
C  0.8093861  0.0385225 -1.3890164
C  0.3167967 -2.6897427 -1.936557
C  1.5686989 -2.2825122 -1.4724613
C  1.8129129 -0.9403944 -1.1709397
C  0.4473827 -0.3759304 -1.9026725
C  0.6896091 -1.7225133 -2.1952754
C  0.1185604 -4.1403013 -2.2799951
H  2.3449415 -3.0478617 -1.3160285
H  2.7914949 -0.6294426 -0.7751307
H  1.2314324  0.3781846 -2.0747522
H  1.6651795 -2.0356814 -2.5961769
O  1.1267215 -4.4022476 -2.7663730
O  0.9619567 -5.0071900 -2.1138995
C  1.3865221 -5.7761092 -3.0780381
H  0.6831782 -6.1448367 -3.8557727
H  -2.4287497 -5.8093542 -3.4516302
H  -1.2765696 -6.4141971 -2.1747089
### Vibrational Spectrum

| #  | Mode | Symmetry | Wave Number (cm\(^{-1}\)) | IR Intensity (km/mol) | Selection Rules |
|----|------|----------|-----------------------------|-----------------------|----------------|
| 1  |      |          | 0.00                        | 0.00000               | -              |
| 2  |      |          | 0.00                        | 0.00000               | -              |
| 3  |      |          | 0.00                        | 0.00000               | -              |
| 4  |      |          | 0.00                        | 0.00000               | -              |
| 5  |      |          | 0.00                        | 0.00000               | -              |
| 6  |      |          | 0.00                        | 0.00000               | -              |
| 7  | a    |          | 12.77                       | 0.48046               | YES            |
| 8  | a    |          | 16.49                       | 0.07359               | YES            |
| 9  | a    |          | 34.31                       | 0.26905               | YES            |
| 10 | a    |          | 48.86                       | 0.02328               | YES            |
| 11 | a    |          | 55.73                       | 1.09007               | YES            |
| 12 | a    |          | 63.10                       | 0.70619               | YES            |
| 13 | a    |          | 67.93                       | 0.07690               | YES            |
| 14 | a    |          | 82.43                       | 0.35489               | YES            |
| 15 | a    |          | 88.48                       | 0.45152               | YES            |
| 16 | a    |          | 90.74                       | 0.41964               | YES            |
| 17 | a    |          | 96.71                       | 0.40586               | YES            |
| 18 | a    |          | 99.94                       | 0.43111               | YES            |
| 19 | a    |          | 107.38                      | 0.34149               | YES            |
| 20 | a    |          | 114.78                      | 0.64331               | YES            |
| 21 | a    |          | 116.87                      | 0.28711               | YES            |
| 22 | a    |          | 123.33                      | 0.47748               | YES            |
| 23 | a    |          | 151.43                      | 2.54072               | YES            |
| 24 | a    |          | 158.10                      | 1.69009               | YES            |
| 25 | a    |          | 184.44                      | 0.56521               | YES            |
| 26 | a    |          | 191.79                      | 0.56599               | YES            |
| 27 | a    |          | 216.79                      | 0.56283               | YES            |
| 28 | a    |          | 226.23                      | 2.33570               | YES            |
| 29 | a    |          | 241.58                      | 0.48368               | YES            |
| 30 | a    |          | 265.96                      | 0.88216               | YES            |
| 31 | a    |          | 283.59                      | 0.15454               | YES            |
| 32 | a    |          | 310.54                      | 23.14858              | YES            |
| 33 | a    |          | 326.65                      | 1.88924               | YES            |
| 34 | a    |          | 357.04                      | 8.70207               | YES            |
| 35 | a    |          | 361.20                      | 13.57125              | YES            |
| 36 | a    |          | 403.29                      | 0.05072               | YES            |
| 37 | a    |          | 416.59                      | 9.13494               | YES            |
| 38 | a    |          | 422.54                      | 1.21557               | YES            |
| 39 | a    |          | 434.43                      | 5.46699               | YES            |
| 40 | a    |          | 457.11                      | 2.85989               | YES            |
| 41 | a    |          | 458.87                      | 3.97714               | YES            |
| 42 | a    |          | 466.11                      | 1.90131               | YES            |
| 43 | a    |          | 470.44                      | 2.27312               | YES            |
| 44 | a    |          | 486.24                      | 6.29781               | YES            |
| 45 | a    |          | 489.75                      | 3.99537               | YES            |
| 46 | a    |          | 500.49                      | 2.36214               | YES            |
| 47 | a    |          | 508.50                      | 10.92025              | YES            |
| 48 | a    |          | 526.16                      | 19.44830              | YES            |
| 49 | a    |          | 534.84                      | 2.05306               | YES            |
| 50 | a    |          | 556.88                      | 1.91812               | YES            |
2bi

SCF Energy (au) BP86/SV(P) -2508.412127961
SCF Energy (au) PBE0/def2-TZVPP -2507.929859714
SCF Energy (au) PBE0/def2-TZVPP -2507.9381342801 (Toluene Correction)
Zero Point Energy (au) 0.3689319
Chemical Potential (kJ mol\(^{-1}\)) 802.70
Dispersion Correction (au) PBE0/def2-TZVPP -0.08008127

xyz coordinates

Mn  1.2130299  1.1283460  0.7677901
C  1.7035251  1.6930919  2.4075242
C  2.9060224  0.7196004  0.3489977
C  1.3402844  2.8290054  0.1489828
O  1.4529387  3.9427431  0.1788935
O  2.0398828  0.4309846  0.0798274
C  1.3170678  0.3238844  2.0891977
C  1.6520221  2.2439038  0.7770437
C  3.0119197  2.3031509  1.0993219
C  3.5366106  1.3238318  1.9611220
C  2.6842758  0.3326735  2.4536215
C  0.3319129  0.6649198  2.5369774
O  0.9908736  3.9427431  0.1788935
C  1.9782768  1.4050739  2.4707026
C  1.6657888  3.4558032
O  4.0048144  0.4309846  0.0798274
O  2.0398828  2.0723864  3.4558032
C  1.5366106  0.3238844  2.0891977
C  1.6520221  2.2439038  0.7770437
C  3.0119197  2.3031509  1.0993219
C  3.5366106  1.3238318  1.9611220
C  2.6842758  0.3326735  2.4536215
C  0.3319129  0.6649198  2.5369774
O  0.9908736  3.9427431  0.1788935
C  1.9782768  1.4050739  2.4707026
C  1.6657888  3.4558032
C  1.3170678  0.3238844  2.0891977
C  1.6520221  2.2439038  0.7770437
C  2.6842758  0.3326735  2.4536215
C  0.3319129  0.6649198  2.5369774
C  0.9908736  3.9427431  0.1788935

| # | mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules |
|---|------|----------|----------------------|---------------------|-----------------|
| 1 |      |          | 0.00                 | 0.00000             | -               |
| 2 |      |          | 0.00                 | 0.00000             | -               |
| 3 |      |          | 0.00                 | 0.00000             | -               |
| 4 |      |          | 0.00                 | 0.00000             | -               |
| 5 |      |          | 0.00                 | 0.00000             | -               |
| 6 |      |          | 0.00                 | 0.00000             | -               |
| 7 | a    |          | 11.30                | 0.22300             | YES             |
| 8 | a    |          | 22.06                | 0.05960             | YES             |
| 9 | a    |          | 26.37                | 0.05122             | YES             |
| 10| a    |          | 29.53                | 0.26518             | YES             |
| 11| a    |          | 42.86                | 0.19185             | YES             |
| 12| a    |          | 47.27                | 0.19769             | YES             |
| 13| a    |          | 58.61                | 0.22167             | YES             |
| 14| a    |          | 69.78                | 0.25509             | YES             |
| 15| a    |          | 77.43                | 0.33119             | YES             |
| 16| a    |          | 86.68                | 0.52791             | YES             |
| 17| a    |          | 93.21                | 0.55682             | YES             |
| 18| a    |          | 99.48                | 0.43536             | YES             |
| 19| a    |          | 110.27               | 0.03955             | YES             |
| 20| a    |          | 112.40               | 0.07220             | YES             |
| 21| a    |          | 118.74               | 0.41670             | YES             |
| 22| a    |          | 128.61               | 0.09602             | YES             |
| 23| a    |          | 155.09               | 0.23330             | YES             |
| 24| a    |          | 172.92               | 0.64525             | YES             |
| 25| a    |          | 184.50               | 2.96286             | YES             |
| 26| a    |          | 190.36               | 1.46917             | YES             |
| 27| a    |          | 217.37               | 2.47697             | YES             |
| 28| a    |          | 227.91               | 3.62925             | YES             |
| 29| a    |          | 246.59               | 2.66370             | YES             |
| 30| a    |          | 263.96               | 0.15492             | YES             |
| 31| a    |          | 285.78               | 0.04935             | YES             |
| 32| a    |          | 357.97               | 2.19617             | YES             |
| 33| a    |          | 380.42               | 15.73501            | YES             |
| 34| a    |          | 396.16               | 3.45386             | YES             |
| 35| a    |          | 400.56               | 0.70936             | YES             |
| 36| a    |          | 402.72               | 0.46689             | YES             |
| 37| a    |          | 419.58               | 7.53622             | YES             |
| 38| a    |          | 434.67               | 7.51619             | YES             |
| 39| a    |          | 447.78               | 18.79443            | YES             |
| 40| a    |          | 455.69               | 1.81735             | YES             |
| 41| a    |          | 466.54               | 3.39152             | YES             |
| 42| a    |          | 473.94               | 4.02064             | YES             |
| 43| a    |          | 487.42               | 1.59525             | YES             |
| 44| a    |          | 494.62               | 8.89332             | YES             |
| 45| a    |          | 500.57               | 40.66585            | YES             |
| 46| a    |          | 510.17               | 18.38623            | YES             |
| 47| a    |          | 532.27               | 6.91702             | YES             |
| 48| a    |          | 541.86               | 10.49425            | YES             |
| 49| a    |          | 546.65               | 14.41346            | YES             |
| 50| a    |          | 556.32               | 1.85781             | YES             |
**2bj**

SCF Energy (au) BP86/SV(P) -2360.882425609
SCF Energy (au) PBE0/def2-TZVPP -2360.449384567
SCF Energy (au) PBE0/def2-TZVPP -2360.455550952 (Toluene Correction)
Zero Point Energy (au) 0.4312242
Chemical Potential (kJ mol⁻¹) 961.18
Dispersion Correction (au) PBE0/def2-TZVPP -0.07158498

xyz coordinates

55

Mn    0.9063604    1.1654989    1.2513929
C     1.4579883    1.7774516    2.8523784
C     2.5778462    0.7095393    0.8022817
C     1.0471178    2.8159490    0.5310960
O     1.1618663    3.9010142    0.1081574
O     3.6639685    0.3933969    0.512264
O     1.8356109    2.1749044    3.8800338
C     1.6068028    0.4517863    2.6622762
C     1.9209358    2.3794980    1.3603483
C     3.2626150    0.7095393    2.654461
C     2.9554606    0.514195    3.0851400
C     0.6429715   -0.5760285    3.0695296
O     0.6614645   -0.4621593    2.5021412
O     1.6210372   -1.4248806    2.8842198
O     1.3013794   -2.4730750    3.7653559
C     0.0050144   -2.5810691    4.3047530
C    -0.9629187   -1.6313920    3.9585385
H    -1.4682090    3.1144091    0.6768561
H    -3.8740846    3.3216238    1.347960
H    -4.8395069    1.5912199    2.9550566
H    -3.3440641   -0.2459782    3.7769777
H     2.6490455   -1.3666327    2.4885330
H     2.0741428   -3.2123366    4.0379284
H    -0.2459702   -3.396086    4.9989108
H    -1.9742205   -1.7143196    4.3901050
N    -1.1078899    1.3957218    1.8015117
C     0.1463747    1.6673289   -2.0651955
C     0.2249000    0.8325196   -0.8403622
C     0.1834660   -0.2677396   -0.2129122
C    -0.0838458   -1.7237446   -0.1591217
H     0.8271177   -2.2503474    0.2092813
C    -0.5210201   -2.3071547   -1.5199947
H    -0.8611075   -1.9334766    0.6115887
C    -0.7974492   -3.8183739   -1.4622855
H    -0.2702275   -2.0995950   -2.2773694
H    -1.4349885   -1.7730181   -1.8707999
C    -1.2269150   -4.4107003   -2.8113143
H    -1.5858337   -4.0181631   -0.987829
H     0.1167171   -4.3439965   -1.0984921
H    -1.4183266   -5.5036238   -2.7325177
H    -0.4421516   -4.2618467   -3.5870862
H    -2.1600508   -3.9322296   -3.1856164
C     1.5045309    1.8713812   -2.7748815
H    -0.5587833    1.1609294   -2.7667554
H    -0.2988621    2.6637806   -1.8441008
H     2.2194946    2.3506684   -2.0687930
C     1.3891197    2.7256069   -4.0470473
H     1.9342444    0.8736357   -3.0233639
C     2.7307898    2.9294680   -4.7625803
H     0.9547438    3.7182795   -3.7817327
H     0.6615254    2.2502414   -4.7469750
| #  | mode | symmetry | wave number | IR intensity | selection rules |
|----|------|----------|-------------|--------------|-----------------|
| 1  |      |          | 0.00        | 0.00000      | -               |
| 2  |      |          | 0.00        | 0.00000      | -               |
| 3  |      |          | 0.00        | 0.00000      | -               |
| 4  |      |          | 0.00        | 0.00000      | -               |
| 5  |      |          | 0.00        | 0.00000      | -               |
| 6  |      |          | 0.00        | 0.00000      | -               |
| 7  | a    |          | 11.02       | 0.17245      | YES, YES        |
| 8  | a    |          | 25.23       | 0.14043      | YES, YES        |
| 9  | a    |          | 27.66       | 0.17493      | YES, YES        |
| 10 | a    |          | 40.79       | 0.02801      | YES, YES        |
| 11 | a    |          | 48.69       | 0.22577      | YES, YES        |
| 12 | a    |          | 55.13       | 0.08372      | YES, YES        |
| 13 | a    |          | 61.84       | 0.07792      | YES, YES        |
| 14 | a    |          | 63.89       | 0.05944      | YES, YES        |
| 15 | a    |          | 73.91       | 0.05961      | YES, YES        |
| 16 | a    |          | 84.70       | 0.87413      | YES, YES        |
| 17 | a    |          | 86.28       | 0.56138      | YES, YES        |
| 18 | a    |          | 91.79       | 0.23567      | YES, YES        |
| 19 | a    |          | 101.15      | 0.08415      | YES, YES        |
| 20 | a    |          | 105.03      | 0.28350      | YES, YES        |
| 21 | a    |          | 105.92      | 0.16061      | YES, YES        |
| 22 | a    |          | 115.10      | 0.13407      | YES, YES        |
| 23 | a    |          | 123.42      | 0.37657      | YES, YES        |
| 24 | a    |          | 127.51      | 0.13969      | YES, YES        |
| 25 | a    |          | 134.65      | 0.14269      | YES, YES        |
| 26 | a    |          | 167.09      | 1.19662      | YES, YES        |
| 27 | a    |          | 185.09      | 1.62408      | YES, YES        |
| 28 | a    |          | 192.02      | 1.72794      | YES, YES        |
| 29 | a    |          | 207.29      | 0.25131      | YES, YES        |
| 30 | a    |          | 212.04      | 0.94338      | YES, YES        |
| 31 | a    |          | 230.67      | 0.44577      | YES, YES        |
| 32 | a    |          | 245.13      | 0.09361      | YES, YES        |
| 33 | a    |          | 251.99      | 0.09030      | YES, YES        |
| 34 | a    |          | 257.44      | 0.71190      | YES, YES        |
| 35 | a    |          | 284.92      | 0.04044      | YES, YES        |
| 36 | a    |          | 287.84      | 1.99290      | YES, YES        |
| 37 | a    |          | 342.65      | 1.35575      | YES, YES        |
| 38 | a    |          | 351.28      | 10.47142     | YES, YES        |
| 39 | a    |          | 358.57      | 2.50273      | YES, YES        |
| 40 | a    |          | 377.52      | 7.71193      | YES, YES        |
| 41 | a    |          | 413.42      | 0.40739      | YES, YES        |
| 42 | a    |          | 417.98      | 3.93799      | YES, YES        |
| 43 | a    |          | 436.39      | 0.17315      | YES, YES        |
| 44 | a    |          | 456.70      | 1.43676      | YES, YES        |
| 45 | a    |          | 459.24      | 3.11548      | YES, YES        |
| 46 | a    |          | 472.34      | 2.92312      | YES, YES        |
| 47 | a    |          | 487.20      | 4.26455      | YES, YES        |
| 48 | a    |          | 493.34      | 0.83376      | YES, YES        |
| 49 | a    |          | 504.92      | 1.30037      | YES, YES        |
| 50 | a    |          | 511.34      | 0.08654      | YES, YES        |
2ca

SCF Energy (au) BP86/SV(P) -2678.190493143
SCF Energy (au) PBE0/def2-TZVPP -2677.706850638
SCF Energy (au) PBE0/def2-TZVPP -2677.7183769724 (Toluene Correction)
Zero Point Energy (au) 0.4157036
Chemical Potential (kJ mol\(^{-1}\)) 911.24
Dispersion Correction (au) PBE0/def2-TZVPP -0.08425883

xyz coordinates

| Element | x (Å) | y (Å) | z (Å) |
|---------|-------|-------|-------|
| Mn      | 0.7905336 | 1.5285988 | -0.7423591 |
| C       | 1.3273161 | 1.7047316 | 0.9650669 |
| C       | 2.4456986 | 0.9692036 | -1.2253026 |
| C       | 1.2218679 | 3.2420649 | -1.1491495 |
| O       | 1.5213430 | 4.3518560 | -1.3572636 |
| O       | 3.5159990 | 0.7182341 | -1.6022172 |
| C       | 1.6847253 | 1.7901848 | 2.0709940 |
| C       | -1.9172557 | 1.0193716 | 0.3528721 |
| C       | -1.7957953 | 3.1873913 | -0.5318246 |
| C       | -3.1303600 | 3.4572049 | -0.2048991 |
| C       | -3.8817482 | 2.4552653 | 0.4318321 |
| C       | -2.6787464 | 1.2300441 | 0.7097169 |
| O       | -1.1664315 | -0.2164499 | 0.5942100 |
| C       | -0.1556688 | -0.2054871 | 0.1489748 |
| C       | -3.0219888 | -1.3733598 | 0.3826172 |
| N       | 0.3757456 | -2.4857002 | 1.0476719 |
| C       | -0.9849693 | -2.4820290 | 1.4670707 |
| C       | -1.7248080 | -1.3636875 | 1.2467454 |
| H       | -1.1767336 | 3.9503746 | -1.0275713 |
| H       | -3.5624970 | 4.4401795 | -0.476092 |
| H       | -4.9345600 | 2.6281933 | 0.7088086 |
| H       | -3.8313851 | 0.4263969 | 1.2057034 |
| O       | 2.1917129 | -1.4589280 | 0.0571630 |
| C       | -1.4998894 | -3.7096034 | 2.1450369 |
| H       | -2.7692106 | -1.3801603 | 1.5893197 |
| N       | -1.1933158 | 2.0084472 | -0.2649113 |
| C       | -0.2026858 | 2.5515868 | -3.8505661 |
| C       | 0.8330593 | 3.3351690 | -4.4204606 |
| C       | 0.5392223 | 4.3032118 | -5.3907774 |
| O       | -0.7879149 | 4.5174378 | -5.8053061 |
| C       | -1.8237181 | 3.7496072 | -5.2446583 |
| C       | -1.5387683 | 2.7755920 | -4.2763370 |
| H       | 1.8734261 | 3.1710737 | -4.099638 |
| H       | 1.3574875 | 4.8993708 | -5.8272260 |
| H       | -1.0141382 | 5.2828874 | -6.5658297 |
| H       | -2.8665484 | 3.9080653 | -5.5667153 |
| H       | -2.3482659 | 2.1684774 | -3.8410303 |
| C       | 0.0717449 | 1.5172662 | -2.8807799 |
| C       | 0.0979632 | 0.3619270 | -2.3637414 |
| H       | -0.0035840 | -0.7198586 | -2.4531376 |
| H       | -1.5173194 | -4.5908682 | 1.4635559 |
| H       | -2.5420262 | -3.5195711 | 2.4730421 |
| H       | -0.9011095 | -3.9959174 | 3.0374664 |
| C       | 1.2519414 | -3.6507605 | 1.2827453 |
| C       | 1.8231970 | -3.7377665 | 2.6904001 |
| H       | 2.0819419 | -3.5235044 | 0.5560890 |
| H       | 0.7002069 | -4.5790914 | 1.0321895 |
| C       | 2.9472178 | -3.9354974 | 5.2820534 |
| C       | 2.3163704 | -5.0476178 | 4.7009390 |
| C       | 1.7566335 | -4.9455809 | 3.4153647 |
| C       | 2.4693801 | -2.6285701 | 3.2789892 |
| C       | 3.0218256 | -2.7272481 | 4.5658847 |
| #  | mode | symmetry | wave number | IR intensity | selection rules |
|----|------|----------|-------------|--------------|-----------------|
| 1  |      |          | 0.00        | 0.00000      | -               |
| 2  |      |          | 0.00        | 0.00000      | -               |
| 3  |      |          | 0.00        | 0.00000      | -               |
| 4  |      |          | 0.00        | 0.00000      | -               |
| 5  |      |          | 0.00        | 0.00000      | -               |
| 6  |      |          | 0.00        | 0.00000      | -               |
| 7  | a    | a        | 11.75       | 0.05816      | YES             |
| 8  | a    | a        | 14.17       | 0.44665      | YES             |
| 9  | a    | a        | 18.27       | 0.27503      | YES             |
| 10 | a    | a        | 25.24       | 0.43345      | YES             |
| 11 | a    | a        | 28.41       | 0.17720      | YES             |
| 12 | a    | a        | 33.39       | 0.16288      | YES             |
| 13 | a    | a        | 52.56       | 2.02624      | YES             |
| 14 | a    | a        | 61.46       | 0.06639      | YES             |
| 15 | a    | a        | 70.66       | 0.31006      | YES             |
| 16 | a    | a        | 77.87       | 0.45878      | YES             |
| 17 | a    | a        | 82.82       | 0.65931      | YES             |
| 18 | a    | a        | 91.77       | 2.72653      | YES             |
| 19 | a    | a        | 98.13       | 0.53621      | YES             |
| 20 | a    | a        | 101.45      | 0.06260      | YES             |
| 21 | a    | a        | 111.21      | 0.12231      | YES             |
| 22 | a    | a        | 118.61      | 0.89381      | YES             |
| 23 | a    | a        | 121.91      | 1.04289      | YES             |
| 24 | a    | a        | 152.08      | 0.91687      | YES             |
| 25 | a    | a        | 152.54      | 0.72509      | YES             |
| 26 | a    | a        | 160.88      | 4.90822      | YES             |
| 27 | a    | a        | 183.22      | 0.71152      | YES             |
| 28 | a    | a        | 194.04      | 1.37194      | YES             |
| 29 | a    | a        | 208.22      | 1.82511      | YES             |
| 30 | a    | a        | 222.93      | 0.28827      | YES             |
| 31 | a    | a        | 244.70      | 1.18420      | YES             |
| 32 | a    | a        | 247.38      | 0.73847      | YES             |
| 33 | a    | a        | 261.67      | 1.67246      | YES             |
| 34 | a    | a        | 279.46      | 0.50349      | YES             |
| 35 | a    | a        | 311.39      | 3.41575      | YES             |
| 36 | a    | a        | 323.37      | 15.15492     | YES             |
| 37 | a    | a        | 333.50      | 13.91151     | YES             |
| 38 | a    | a        | 369.01      | 6.10197      | YES             |
| 39 | a    | a        | 388.19      | 1.01913      | YES             |
| 40 | a    | a        | 401.34      | 0.06661      | YES             |
| 41 | a    | a        | 402.35      | 0.33753      | YES             |
| 42 | a    | a        | 416.94      | 18.50278     | YES             |
| 43 | a    | a        | 429.83      | 3.80817      | YES             |
| 44 | a    | a        | 439.12      | 14.05357     | YES             |
| 45 | a    | a        | 455.41      | 8.65813      | YES             |
| 46 | a    | a        | 462.46      | 13.72343     | YES             |
| 47 | a    | a        | 465.15      | 2.29291      | YES             |
| 48 | a    | a        | 470.80      | 0.71839      | YES             |
| 49 | a    | a        | 479.01      | 8.66726      | YES             |
| 50 | a    | a        | 486.70      | 6.50033      | YES             |
2ca'

SCF Energy (au) BP86/SV(P) -2678.190378706
SCF Energy (au) PBE0/def2-TZVPP -2677.706376595
SCF Energy (au) PBE0/def2-TZVPP -2677.7174819824 (Toluene Correction)
Zero Point Energy (au) 0.4159746
Chemical Potential (kJ mol\(^{-1}\)) 916.06
Dispersion Correction (au) PBE0/def2-TZVPP -0.08639897

xyz coordinates

Mn  0.7961401  2.5847105  -1.0851902
C  1.2500491  2.7717503   0.6500830
C  2.4813310  2.0544182  -1.5070732
C  1.1939145  4.3117903  -1.4411958
O  1.4534377  5.4315807  -1.6517531
O  3.5663854  1.8259195  -1.8522930
O  1.5603437  2.8875984   1.7671783
C  -1.9187337  1.9701171  -0.0555799
C  -1.8776272  4.1124029  -1.0050859
C  -3.2343521  4.3236173  -0.7320304
C  -3.9555682  3.3029040  -0.0892464
C  -3.2903241  2.1206326   0.2481533
C  -1.1141102  0.7822773   0.2480661
O   0.2167596  0.8397673  -0.1695494
C  -0.8113962  1.4330731  -1.2170725
C  -1.6355385  0.3635921   0.9287325
H  -1.2791530  4.8905777  -1.5034612
H  -3.7078776  5.2752248  -1.0190629
H  -5.0252499  3.4288905   0.1451857
H  -3.8303504  1.3024026   0.7462112
O   2.3204438 -0.3020275  -0.1188913
C  -1.3260705  2.6620627   1.9203533
H  -2.6889701  0.4207582   1.2375034
N  -1.2260492  2.9768015  -0.6777181
H   0.4305322  3.6470920  -3.8642917
C   0.3284714  2.8248482  -3.1539352
C   0.1072887  1.5993603  -2.8967459
C  -0.3320158  0.2701243  -3.266099
H  -1.2831841  3.5629399   1.2663069
H  -2.3851514  2.5114458   2.2126235
H  -0.7412688  2.8920748   2.8379881
C   1.4470592  2.4902952   1.1537664
C   1.9717429  2.4950662   2.5821842
H   2.2958274  2.3481379   0.4523575
H   0.9511891  3.4540546   0.9211390
C   0.0486945  2.5396166   5.2130484
C   2.4738845  3.7060846   4.6516553
C   1.9522292  3.6820239   3.3463164
C   2.5307111  1.3301185   3.1518695
C   3.0488033  1.3531065   4.4581470
H   3.4249358  2.5541871   6.2379724
H   2.4496076  4.6430481   5.2327775
H   1.5253732  4.6016461   2.9121475
H   2.5769806  0.4018958   2.5601036
H   3.4779642  0.4344876   4.8877950
C  -1.1888456  2.2916190  -4.1159708
C  -2.0009716  1.1662434  -4.3406083
C  -1.5782448  0.1047369  -3.9237175
C   0.4736494  0.8723298  -3.0325241
C   0.0486945 -2.1367172  -3.4651808
| mode | symmetry | wave number  | IR intensity | selection rules |
|------|----------|--------------|--------------|-----------------|
|      |          | cm**(-1)     | km/mol       | IR     | RAMAN |
| 1    |          | 0.00         | 0.00000      | -      | -     |
| 2    |          | 0.00         | 0.00000      | -      | -     |
| 3    |          | 0.00         | 0.00000      | -      | -     |
| 4    |          | 0.00         | 0.00000      | -      | -     |
| 5    |          | 0.00         | 0.00000      | -      | -     |
| 6    |          | 0.00         | 0.00000      | -      | -     |
| 7    | a        | 13.98        | 0.16013      | YES    | YES   |
| 8    | a        | 18.45        | 0.16169      | YES    | YES   |
| 9    | a        | 23.39        | 0.91198      | YES    | YES   |
| 10   | a        | 26.84        | 0.00583      | YES    | YES   |
| 11   | a        | 34.42        | 0.15750      | YES    | YES   |
| 12   | a        | 49.10        | 0.02982      | YES    | YES   |
| 13   | a        | 52.96        | 1.01254      | YES    | YES   |
| 14   | a        | 63.51        | 0.73153      | YES    | YES   |
| 15   | a        | 73.89        | 0.63088      | YES    | YES   |
| 16   | a        | 79.38        | 0.96375      | YES    | YES   |
| 17   | a        | 82.15        | 1.07061      | YES    | YES   |
| 18   | a        | 95.65        | 0.70579      | YES    | YES   |
| 19   | a        | 100.84       | 0.36578      | YES    | YES   |
| 20   | a        | 104.48       | 0.08703      | YES    | YES   |
| 21   | a        | 109.67       | 0.84019      | YES    | YES   |
| 22   | a        | 122.89       | 1.57095      | YES    | YES   |
| 23   | a        | 128.37       | 0.61223      | YES    | YES   |
| 24   | a        | 153.86       | 0.54673      | YES    | YES   |
| 25   | a        | 158.56       | 0.16737      | YES    | YES   |
| 26   | a        | 178.88       | 0.53684      | YES    | YES   |
| 27   | a        | 185.41       | 2.14388      | YES    | YES   |
| 28   | a        | 192.23       | 1.63138      | YES    | YES   |
| 29   | a        | 206.72       | 1.76481      | YES    | YES   |
| 30   | a        | 213.42       | 0.34350      | YES    | YES   |
| 31   | a        | 243.95       | 1.05407      | YES    | YES   |
| 32   | a        | 247.83       | 1.08144      | YES    | YES   |
| 33   | a        | 262.98       | 0.36073      | YES    | YES   |
| 34   | a        | 281.31       | 1.23538      | YES    | YES   |
| 35   | a        | 310.09       | 5.88444      | YES    | YES   |
| 36   | a        | 330.66       | 9.26868      | YES    | YES   |
| 37   | a        | 342.45       | 5.75582      | YES    | YES   |
| 38   | a        | 367.77       | 4.50765      | YES    | YES   |
| 39   | a        | 391.01       | 1.25030      | YES    | YES   |
| 40   | a        | 402.56       | 0.10780      | YES    | YES   |
| 41   | a        | 403.68       | 2.37536      | YES    | YES   |
| 42   | a        | 409.01       | 13.17384     | YES    | YES   |
| 43   | a        | 431.49       | 11.95146     | YES    | YES   |
| 44   | a        | 442.41       | 14.97434     | YES    | YES   |
| 45   | a        | 457.92       | 0.40690      | YES    | YES   |
| 46   | a        | 464.95       | 1.20181      | YES    | YES   |
| 47   | a        | 468.56       | 6.69897      | YES    | YES   |
| 48   | a        | 471.25       | 3.35441      | YES    | YES   |
| 49   | a        | 478.00       | 3.89641      | YES    | YES   |
| 50   | a        | 485.52       | 6.40456      | YES    | YES   |
2da

SCF Energy (au) BP86/SV(P) -2409.004534403
SCF Energy (au) PBE0/def2-TZVPP -2408.542817634
SCF Energy (au) PBE0/def2-TZVPP -2408.5510777761 (Toluene Correction)
Zero Point Energy (au) 0.3178444
Chemical Potential (kJ mol\(^{-1}\)) 679.64
Dispersion Correction (au) PBE0/def2-TZVPP 0.06709809

xyz coordinates
45

Mn  1.5197310  0.5470025  0.3436074
C  1.9098030  0.8269867  2.0810763
C  3.1834914 -0.0444268  0.0203656
C  1.9301135  2.2698775 -0.0671300
O  2.237609  3.3814057 -0.2662464
O  4.2544275 -0.4565929 -0.1836553
O  2.161682  1.0008020  3.2032102
C -1.2049045 -0.1258313  1.2768286
C -1.1589754  2.0562942  0.4177521
C -2.5219656  2.2484199  0.6575306
C -3.2447226  1.1885736  1.2332793
C -2.5904925 -0.0046829  1.5445731
N -0.4345005 -1.2439296  1.5412602
C  0.9499691 -1.2028048  1.1921142
C  1.5082306 -2.4082537  1.5598700
C  0.4804587 -3.2427178  2.1402405
C -0.7448065 -2.4960049  2.1266952
H -0.5477021  2.8540095 -0.0310344
H -2.9972974  3.2064907  0.3991233
H -4.3222679  1.2891001  1.4423592
H -3.1456491 -0.8365420  1.9889389
H -2.5624864 -2.6854686  1.4310032
C  0.4951000 -4.5502559  2.6685547
N -0.5072941  0.9101560  0.7131965
C  0.8271748  1.5978722 -2.8620085
C  1.9509091  2.3147130 -3.3463859
C  1.7939842  3.2932883 -4.3372283
C  0.5191695  3.5832855 -4.8561966
C -0.6026395  2.8814165 -4.3811110
C -0.4550859  1.8969480 -3.3931721
H  2.9505721  2.0905373 -2.9429216
H  2.6781598  3.8308295 -4.7070955
H  0.4001929  4.3572543 -5.6321738
H -1.6046992  3.1003949 -4.7859256
H -1.3312893  1.3401530 -3.0245511
C  0.9579810  0.5504308 -1.8770337
C  0.8890639 -0.5923575 -1.3453656
H  0.7411585 -1.6707348 -1.3980957
H  1.4336625 -5.1283198  2.6819725
C -0.6914407 -5.1000768  3.1740729
H -0.6902216 -6.1214082  3.5892289
C -1.8900312 -4.3559507  3.1584690
H -2.8156297 -4.7983334  3.5616334
C -1.9319458 -3.0495780  2.6376779
H -2.8877072 -2.5094957  2.6526528
$
vibrational spectrum

| # | mode | symmetry | wave number (cm⁻¹) | IR intensity (km/mol) | selection rules |
|---|------|----------|-------------------|----------------------|-----------------|
| 1 | 0.00 | 0.00000   | IR                 | -                    | -               |
| 2 | 0.00 | 0.00000   | IR                 | -                    | -               |
| 3 | 0.00 | 0.00000   | IR                 | -                    | -               |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | a | 16.31 | 0.07965 | YES | YES |
| 8 | a | 17.65 | 0.09997 | YES | YES |
| 9 | a | 25.65 | 0.26847 | YES | YES |
| 10 | a | 47.19 | 0.24354 | YES | YES |
| 11 | a | 56.47 | 0.07018 | YES | YES |
| 12 | a | 64.10 | 0.09528 | YES | YES |
| 13 | a | 67.11 | 0.32495 | YES | YES |
| 14 | a | 79.62 | 0.42679 | YES | YES |
| 15 | a | 87.94 | 0.74734 | YES | YES |
| 16 | a | 99.82 | 0.51131 | YES | YES |
| 17 | a | 104.85 | 1.07356 | YES | YES |
| 18 | a | 111.88 | 0.11920 | YES | YES |
| 19 | a | 122.33 | 0.21282 | YES | YES |
| 20 | a | 143.47 | 1.40069 | YES | YES |
| 21 | a | 157.32 | 5.11267 | YES | YES |
| 22 | a | 168.97 | 2.48278 | YES | YES |
| 23 | a | 178.12 | 0.99525 | YES | YES |
| 24 | a | 215.31 | 0.22371 | YES | YES |
| 25 | a | 238.99 | 0.23718 | YES | YES |
| 26 | a | 256.73 | 6.23442 | YES | YES |
| 27 | a | 280.88 | 0.52625 | YES | YES |
| 28 | a | 306.39 | 21.32459 | YES | YES |
| 29 | a | 315.88 | 1.87150 | YES | YES |
| 30 | a | 352.24 | 1.47949 | YES | YES |
| 31 | a | 366.05 | 5.07142 | YES | YES |
| 32 | a | 400.09 | 0.38943 | YES | YES |
| 33 | a | 407.71 | 7.20090 | YES | YES |
| 34 | a | 422.47 | 1.06470 | YES | YES |
| 35 | a | 431.12 | 1.93796 | YES | YES |
| 36 | a | 456.79 | 15.18417 | YES | YES |
| 37 | a | 473.69 | 2.51350 | YES | YES |
| 38 | a | 478.93 | 13.77269 | YES | YES |
| 39 | a | 486.33 | 3.55622 | YES | YES |
| 40 | a | 493.78 | 13.48945 | YES | YES |
| 41 | a | 501.81 | 16.05292 | YES | YES |
| 42 | a | 513.21 | 1.64317 | YES | YES |
| 43 | a | 516.95 | 0.49905 | YES | YES |
| 44 | a | 523.19 | 37.80879 | YES | YES |
| 45 | a | 537.83 | 7.06320 | YES | YES |
| 46 | a | 554.10 | 7.08855 | YES | YES |
| 47 | a | 571.12 | 0.17654 | YES | YES |
| 48 | a | 589.91 | 8.62866 | YES | YES |
| 49 | a | 611.07 | 12.74284 | YES | YES |
| 50 | a | 613.67 | 2.03699 | YES | YES |
2da'
SCF Energy (au) BP86/SV(P) -2409.003236277
SCF Energy (au) PBE0/def2-TZVPP -2408.541068212
SCF Energy (au) PBE0/def2-TZVPP (Toluene Correction) -2408.5491894788
Zero Point Energy (au) 0.3178436
Chemical Potential (kJ mol^{-1}) 680.78
Dispersion Correction (au) PBE0/def2-TZVPP -0.06958346

xyz coordinates
45

Mn 1.6114787 2.0224123 -0.1294482
C 1.9124242 2.3882433 1.6130026
C 3.3069043 1.4797935 -0.3640030
C 1.9537395 3.7493582 -0.5687954
O 2.1911893 4.8621185 -0.8290349
O 4.3951818 1.0868426 -0.5076838
O 2.1133826 2.6348062 2.7313371
C -1.099543 1.1959393 0.7151392
C -1.1734098 3.3233061 -0.2672068
C -2.5598082 3.4139375 -0.1227346
C -3.2331398 2.3243121 0.4589504
C -2.5076960 1.2075558 0.7892940
N 1.1285164 0.1667125 1.0975266
C 1.7639615 -0.8264179 1.2966744
C 0.7824824 -1.6835292 1.9209479
C -0.4947175 -1.0432808 1.7940818
H -0.5986462 4.1430608 -0.7250315
H -3.0927997 4.3144785 -0.4625970
H -4.3280388 2.3403880 0.5843860
H -3.0244406 0.3456729 1.3111972
H 2.8428089 -1.0225844 1.2437251
C 0.8787449 -2.9251389 2.5820625
N -0.4526673 2.2542483 0.1355482
H 1.4252327 2.9305479 -2.9825719
C 1.2749429 2.1317966 -2.2549764
C 1.0302276 0.9214792 -1.9744502
C 0.6010528 -0.4326949 -2.2310418
H 1.8581874 -3.4207374 2.6835846
C -0.2794590 -3.5132887 3.1097021
H -0.2150666 -4.4835600 3.6292674
C -1.5294780 -2.8709534 2.9860483
H -2.4316533 -3.3406685 3.4109535
C -1.6528098 -1.6320255 2.3307129
H -2.6452131 -1.1660218 2.2707994
C -0.2569970 -3.0608890 -2.8308959
H -1.1188276 -1.9713558 -3.0487209
C -0.6974520 -0.6670022 -2.7534160
C 1.4590036 -1.5386594 -2.0074787
C 1.0315616 -2.8379490 -2.3143524
H -0.5904122 -4.0856771 -3.0632895
H -2.1299911 -2.1378258 -3.4561038
H -1.3683259 0.1890256 -2.9296280
H 2.4680464 -1.3648277 -1.6056212
H 1.7124272 -3.6878085 -2.1426469

$vibrational$ spectrum

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|----------------|
| 1 | 0.00 | 0.00000  | -           | -            |
| 2 | 0.00 | 0.00000  | -           | -            |
| 3 | 0.00 | 0.00000  | -           | -            |
2ea
SCF Energy (au) BP86/SV(P) -2583.758694363
SCF Energy (au) PBE0/def2-TZVPP -2583.308834131
SCF Energy (au) PBE0/def2-TZVPP -2583.3186219410 (Toluene Correction)
Zero Point Energy (au) 0.3858375
Chemical Potential (kJ mol\(^{-1}\)) 840.51
Dispersion Correction (au) PBE0/def2-TZVPP -0.07229098

xyz coordinates

Mn  2.2230988  0.6317792  -0.0380673
C  2.6156062  1.1476731  1.6392340
C  3.9387085  0.1811112  -0.3247176
C  2.4125292  2.3193182  -0.6911169
O  2.5413774  3.4196005  -1.0551924
O  5.0506470  -0.1331539  -0.4981009
O  2.8767051  1.4700797  2.7277647
C  -0.4539945  -0.0297274  0.9096872
C  -1.9246317  0.0913870  1.0871830
C  0.3558878  -1.1297064  1.4172808
C  1.7432603  -1.0509487  1.0754004
C  2.0677351  -2.0542027  2.3474416
C  0.7427944  -3.1752783  2.6929163
C  -0.1235398  -2.1864952  2.2356941
H  3.6801806  -2.0058785  1.3091043
O  2.5413774  -4.1224309  2.8426613
H  0.3950079  -4.0008383  3.3326722
H  -1.848113  -2.2197783  2.5316610
C  0.2295362  0.8918881  0.2643551
C  1.2662731  1.0751896  -3.2954025
C  2.2345091  1.8668127  -3.9638754
C  1.8687155  2.6586890  -5.0606656
C  0.5347223  2.6874656  -5.5058725
C  -0.4352712  1.9114622  -4.8473054
C  -0.0776139  1.1120552  -3.7519775
H  3.2792071  1.8489973  -3.6164200
H  2.6348500  3.263171  -5.5724379
H  0.2515102  3.3164568  -6.3659739
H  -1.4830307  1.9265356  -5.1911149
H  -0.8346306  0.4992213  -3.2369763
C  1.6163849  0.2176182  -2.1884952
C  1.7524455  -0.8361841  -1.5029239
H  1.7703661  -1.9228945  -1.4187534
C  -0.7416295  0.3982927  1.3390996
C  -4.1874919  -0.8306805  0.9085777
C  -2.8044347  -0.9812409  0.7916161
C  -2.4915732  1.3143236  1.5082184
C  -3.8796569  1.4757364  1.6412510
O  -6.0976318  0.4422766  1.4283706
H  -4.8744120  -1.6562320  0.6648427
H  -2.3950795  -1.9390571  0.4327292
H  -1.8296331  2.1579555  1.7662896
H  -4.2759343  2.4409076  1.9886844
H  -0.3377541  1.6556536  -0.1300338
C  -6.7187729  1.6476577  1.8463775
H  -6.4076413  1.9356514  2.8783423
H  -7.8093098  1.4493254  1.8391284
H  -6.4964900  2.4895023  1.1487841
C  4.2807820  -4.1239894  2.5719257
H  4.7805171  -3.2159617  2.9829648
H  4.4885289  -4.1896897  1.4784253
| #  | mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules |
|----|------|----------|----------------------|---------------------|-----------------|
| 1  |      |          | 0.00                 | 0.00000             | -               |
| 2  |      |          | 0.00                 | 0.00000             | -               |
| 3  |      |          | 0.00                 | 0.00000             | -               |
| 4  |      |          | 0.00                 | 0.00000             | -               |
| 5  |      |          | 0.00                 | 0.00000             | -               |
| 6  |      |          | 0.00                 | 0.00000             | -               |
| 7  | a    |          | 12.66                | 0.11198             | YES             |
| 8  | a    |          | 23.85                | 0.14135             | YES             |
| 9  | a    |          | 28.24                | 0.19019             | YES             |
| 10 | a    |          | 35.42                | 0.79697             | YES             |
| 11 | a    |          | 38.32                | 0.42459             | YES             |
| 12 | a    |          | 47.51                | 0.69116             | YES             |
| 13 | a    |          | 61.68                | 0.10633             | YES             |
| 14 | a    |          | 65.84                | 0.17130             | YES             |
| 15 | a    |          | 75.47                | 0.44825             | YES             |
| 16 | a    |          | 85.53                | 1.07252             | YES             |
| 17 | a    |          | 87.59                | 0.33363             | YES             |
| 18 | a    |          | 94.62                | 0.20706             | YES             |
| 19 | a    |          | 101.89               | 0.26170             | YES             |
| 20 | a    |          | 103.56               | 2.42543             | YES             |
| 21 | a    |          | 114.60               | 0.52142             | YES             |
| 22 | a    |          | 121.22               | 1.35366             | YES             |
| 23 | a    |          | 146.22               | 0.28143             | YES             |
| 24 | a    |          | 154.04               | 1.68102             | YES             |
| 25 | a    |          | 160.20               | 0.18190             | YES             |
| 26 | a    |          | 168.67               | 8.51326             | YES             |
| 27 | a    |          | 180.21               | 2.01157             | YES             |
| 28 | a    |          | 190.96               | 1.43101             | YES             |
| 29 | a    |          | 204.10               | 0.46082             | YES             |
| 30 | a    |          | 236.74               | 0.90063             | YES             |
| 31 | a    |          | 246.28               | 0.61014             | YES             |
| 32 | a    |          | 256.47               | 2.28427             | YES             |
| 33 | a    |          | 266.71               | 1.10966             | YES             |
| 34 | a    |          | 300.24               | 1.39938             | YES             |
| 35 | a    |          | 316.99               | 24.15601            | YES             |
| 36 | a    |          | 319.55               | 2.82845             | YES             |
| 37 | a    |          | 342.78               | 0.96020             | YES             |
| 38 | a    |          | 361.53               | 5.33052             | YES             |
| 39 | a    |          | 400.11               | 0.10893             | YES             |
| 40 | a    |          | 409.14               | 5.85992             | YES             |
| 41 | a    |          | 415.96               | 2.75722             | YES             |
| 42 | a    |          | 422.26               | 1.54838             | YES             |
| 43 | a    |          | 444.19               | 13.52271            | YES             |
| 44 | a    |          | 454.37               | 1.42207             | YES             |
| 45 | a    |          | 458.56               | 2.83272             | YES             |
| 46 | a    |          | 475.83               | 3.34516             | YES             |
| 47 | a    |          | 478.06               | 8.31028             | YES             |
| 48 | a    |          | 488.23               | 4.80640             | YES             |
| 49 | a    |          | 495.22               | 10.53210            | YES             |
| 50 | a    |          | 502.27               | 14.32391            | YES             |
2ea'  
SCF Energy (au) BP86/SV(P) -2583.755936542  
SCF Energy (au) PBE0/def2-TZVPP -2583.30604497  
SCF Energy (au) PBE0/def2-TZVPP -2583.316494270 (Toluene Correction)  
Zero Point Energy (au) 0.3858163  
Chemical Potential (kJ mol⁻¹) 841.85  
Dispersion Correction (au) PBE0/def2-TZVPP -0.07594655  

xyz coordinates  
53  
Mn 1.9919400 1.9445815 -0.2125446  
C 2.1534808 2.3744254 1.5290994  
C 3.7492214 1.5853193 -0.3113953  
C 2.1488295 3.6785107 -0.7263564  
O 2.2404524 4.7993586 -1.0377011  
O 4.8853661 1.3177075 -0.3697285  
O 2.2698990 2.6577750 2.6525923  
C -0.7159006 1.1112818 0.4928948  
C 0.1043036 0.0054276 0.9687169  
C 1.5091645 1.8524320 2.3511876  
C 1.7682332 0.6340095 2.0105774  
C 1.8077286 2.3511876 2.1790042  
C 1.9200425 3.6011320 2.5779877  
O 2.6454017 -3.0414030 2.2472929  
H 0.1110908 -3.1192603 2.433817  
H -1.4825776 -1.3313196 1.6747097  
N -0.0377682 2.0698256 -0.1025837  
H 1.6963008 2.6226932 -3.1216314  
C 1.7555164 1.8524320 -2.3511876  
C 1.7682332 0.6340095 -2.0105774  
C 1.8077286 -0.8002035 -2.1790042  
H 1.9200425 -3.6011320 -2.5779877  
C 3.0989686 -2.8350822 -2.615416  
C -3.0485007 -1.4479013 -2.4103047  
C 0.6263831 -1.5815302 -2.1436240  
C -0.6047498 -2.9683920 -2.5432424  
H 1.9626934 -4.6916637 -2.7344687  
H 4.0704284 -3.3222218 -2.7994052  
H 3.9712861 -0.8460555 -2.4342545  
H -0.3402928 -1.0879230 -1.9607610  
H -0.2421060 -3.5621325 -2.3141260  
C -2.1920915 1.1993839 0.6436670  
C -5.0083214 1.4914085 0.9169598  
C -4.2119099 1.1238512 2.0274378  
C -2.8306057 0.9750933 1.8900714  
C -2.9975772 1.5734107 -0.4539791  
C -4.3894494 1.7150685 -0.3325568  
O -6.3429842 1.6032685 1.1508950  
H -4.7089911 0.9678227 2.9977093  
H -2.2261438 0.7135808 2.7732747  
H -2.5283966 1.7355727 -1.4391278  
H -4.9787167 1.9923799 -1.2184360  
H -0.6034216 2.8775078 -0.3994740  
C -7.1972825 1.9790936 0.0823794  
H -7.1680455 1.2368679 -0.7501530  
H -6.9375345 2.9876305 -0.3178743  
H -8.2215719 2.0095391 0.5047845  
C 4.0556463 -2.9552201 2.1058369  
H 4.4730160 -2.0857501 2.6654880  
H 4.3560879 -2.8782928 1.0352177  

S52
| # | mode | symmetry | wave number (cm⁻¹) | IR intensity (km/mol) | selection rules |
|---|------|----------|-------------------|----------------------|-----------------|
| 1 |      |          | 0.00              | 0.00000              | -                |
| 2 |      |          | 0.00              | 0.00000              | -                |
| 3 |      |          | 0.00              | 0.00000              | -                |
| 4 |      |          | 0.00              | 0.00000              | -                |
| 5 |      |          | 0.00              | 0.00000              | -                |
| 6 |      |          | 0.00              | 0.00000              | -                |
| 7 | a    |          | 14.75             | 0.06828              | YES             |
| 8 | a    |          | 28.47             | 0.19583              | YES             |
| 9 | a    |          | 33.94             | 0.28112              | YES             |
| 10| a    |          | 36.54             | 0.25294              | YES             |
| 11| a    |          | 38.48             | 0.16597              | YES             |
| 12| a    |          | 49.80             | 1.04111              | YES             |
| 13| a    |          | 54.04             | 0.26221              | YES             |
| 14| a    |          | 64.84             | 0.11492              | YES             |
| 15| a    |          | 76.74             | 0.35850              | YES             |
| 16| a    |          | 84.30             | 1.11652              | YES             |
| 17| a    |          | 89.15             | 0.20915              | YES             |
| 18| a    |          | 93.26             | 0.14079              | YES             |
| 19| a    |          | 96.89             | 1.50910              | YES             |
| 20| a    |          | 107.51            | 0.21592              | YES             |
| 21| a    |          | 113.30            | 0.33480              | YES             |
| 22| a    |          | 120.74            | 2.23271              | YES             |
| 23| a    |          | 149.98            | 1.82201              | YES             |
| 24| a    |          | 158.02            | 1.52750              | YES             |
| 25| a    |          | 163.84            | 1.18213              | YES             |
| 26| a    |          | 175.37            | 3.19118              | YES             |
| 27| a    |          | 176.20            | 2.30265              | YES             |
| 28| a    |          | 183.71            | 0.31709              | YES             |
| 29| a    |          | 192.21            | 0.53953              | YES             |
| 30| a    |          | 242.22            | 0.72845              | YES             |
| 31| a    |          | 249.25            | 0.73961              | YES             |
| 32| a    |          | 255.05            | 0.48763              | YES             |
| 33| a    |          | 268.62            | 1.23736              | YES             |
| 34| a    |          | 296.84            | 2.72505              | YES             |
| 35| a    |          | 305.94            | 17.11122             | YES             |
| 36| a    |          | 317.81            | 1.02634              | YES             |
| 37| a    |          | 340.78            | 0.34148              | YES             |
| 38| a    |          | 362.30            | 4.98498              | YES             |
| 39| a    |          | 398.05            | 10.51671             | YES             |
| 40| a    |          | 399.04            | 1.53104              | YES             |
| 41| a    |          | 415.91            | 3.33119              | YES             |
| 42| a    |          | 420.81            | 0.98381              | YES             |
| 43| a    |          | 444.89            | 0.66886              | YES             |
| 44| a    |          | 454.90            | 1.69616              | YES             |
| 45| a    |          | 461.02            | 2.68253              | YES             |
| 46| a    |          | 479.34            | 5.64347              | YES             |
| 47| a    |          | 484.40            | 10.14586             | YES             |
| 48| a    |          | 486.59            | 7.70917              | YES             |
| 49| a    |          | 495.03            | 1.45340              | YES             |
| 50| a    |          | 507.34            | 4.79824              | YES             |
2fa

SCF Energy (au) BP86/SV(P) -2391.961394095
SCF Energy (au) PBE0/def2-TZVPP -2391.518095263
SCF Energy (au) PBE0/def2-TZVPP -2391.5259797091 (Toluene Correction)
Zero Point Energy (au) 0.3211004
Chemical Potential (kJ mol⁻¹) 689.84
Dispersion Correction (au) PBE0/def2-TZVPP -0.06699866

xyz coordinates
45

Mn 1.4798866 -0.2187247 0.6042757
C 1.9858282 0.1850369 2.2864095
C 3.1078742 0.1850369 2.2864095
C 1.9261647 1.4494384 0.0171510
O 2.3355042 2.4877551 -0.3203568
O 4.1697137 -1.2232451 -0.0717724
O 2.3152063 0.4401459 3.3737385

$vibrational spectrum$

| #  | mode | symmetry | wave number cm⁻¹ | IR intensity km/mol | selection rules IR | selection rules RAMAN |
|----|------|----------|------------------|---------------------|---------------------|-----------------------|
| 1  | 0.00 | 0.00000  | -                 | -                   | -                   | -                     |
| 2  | 0.00 | 0.00000  | -                 | -                   | -                   | -                     |
| 3  | 0.00 | 0.00000  | -                 | -                   | -                   | -                     |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | a | 15.69 | 0.21459 | YES | YES |
| 8 | a | 29.61 | 0.05641 | YES | YES |
| 9 | a | 34.01 | 0.12405 | YES | YES |
| 10 | a | 43.43 | 0.08971 | YES | YES |
| 11 | a | 63.13 | 1.35943 | YES | YES |
| 12 | a | 75.59 | 1.13964 | YES | YES |
| 13 | a | 80.60 | 0.41255 | YES | YES |
| 14 | a | 90.18 | 0.49284 | YES | YES |
| 15 | a | 93.53 | 0.02787 | YES | YES |
| 16 | a | 100.58 | 0.83466 | YES | YES |
| 17 | a | 114.14 | 0.30028 | YES | YES |
| 18 | a | 118.32 | 0.18218 | YES | YES |
| 19 | a | 122.21 | 0.39617 | YES | YES |
| 20 | a | 129.25 | 0.90286 | YES | YES |
| 21 | a | 154.99 | 1.38789 | YES | YES |
| 22 | a | 156.86 | 0.72739 | YES | YES |
| 23 | a | 167.85 | 3.83857 | YES | YES |
| 24 | a | 182.29 | 1.19717 | YES | YES |
| 25 | a | 218.81 | 0.80044 | YES | YES |
| 26 | a | 229.75 | 0.95873 | YES | YES |
| 27 | a | 242.21 | 3.23163 | YES | YES |
| 28 | a | 254.84 | 0.06903 | YES | YES |
| 29 | a | 288.66 | 0.56483 | YES | YES |
| 30 | a | 305.04 | 0.17203 | YES | YES |
| 31 | a | 324.49 | 21.26696 | YES | YES |
| 32 | a | 334.75 | 2.71008 | YES | YES |
| 33 | a | 402.42 | 0.01934 | YES | YES |
| 34 | a | 407.91 | 0.84390 | YES | YES |
| 35 | a | 415.07 | 4.41464 | YES | YES |
| 36 | a | 435.04 | 8.05753 | YES | YES |
| 37 | a | 454.51 | 15.75093 | YES | YES |
| 38 | a | 459.11 | 2.46109 | YES | YES |
| 39 | a | 471.16 | 4.40160 | YES | YES |
| 40 | a | 478.30 | 3.94107 | YES | YES |
| 41 | a | 490.99 | 6.31778 | YES | YES |
| 42 | a | 499.39 | 3.20063 | YES | YES |
| 43 | a | 508.02 | 18.13741 | YES | YES |
| 44 | a | 513.95 | 2.54387 | YES | YES |
| 45 | a | 529.00 | 31.57498 | YES | YES |
| 46 | a | 536.56 | 11.31513 | YES | YES |
| 47 | a | 541.47 | 12.12873 | YES | YES |
| 48 | a | 555.01 | 2.26347 | YES | YES |
| 49 | a | 581.31 | 2.25487 | YES | YES |
| 50 | a | 606.94 | 24.76174 | YES | YES |
**2ej**

SCF Energy (au) BP86/SV(P) -2814.654527730
SCF Energy (au) PBE0/def2-TZVPP -2814.168815490
SCF Energy (au) PBE0/def2-TZVPP -2814.179225655 (Toluene Correction)
Zero Point Energy (au) 0.4650797
Chemical Potential (kJ mol⁻¹) 1029.53
Dispersion Correction (au) PBE0/def2-TZVPP -0.09205668

**xyz coordinates**

63

| Atom | x       | y       | z       | x       | y       | z       |
|------|---------|---------|---------|---------|---------|---------|
| Mn   | 1.9456160 | 1.1548608 | 0.1958505 |
| C    | 2.3174964 | 1.7535376 | 1.8490724 |
| C    | 3.6459403 | 0.6209492 | -0.0252364 |
| C    | 2.2417920 | 2.8057008 | -0.5079093 |
| O    | 2.4490777 | 3.8871159 | -0.8928812 |
| O    | 4.7469566 | 0.2515105 | -0.1584022 |
| O    | 2.5659906 | 2.1407198 | 2.919120 |
| C    | -0.7687233 | 0.6675232 | 1.1429281 |
| C    | -2.2330554 | 0.8694433 | 1.2963279 |
| C    | -0.0099007 | -0.4218190 | 1.7424040 |
| C    | 1.3817626 | -0.4320683 | 1.4019474 |
| C    | 2.1968402 | -1.4323580 | 1.9608592 |
| C    | 1.6568351 | -2.4100915 | 2.8285623 |
| O    | 0.2808277 | -2.3773202 | 3.1737144 |
| O    | -0.5390031 | -1.3877409 | 2.638067 |
| H    | 3.2693013 | -1.4571753 | 1.7161129 |
| O    | 2.3758798 | -3.4141733 | 3.3952372 |
| H    | -0.1049106 | -3.1348798 | 3.8732171 |
| H    | -1.606016 | -1.3485107 | 2.9327252 |
| N    | 0.0394002 | 1.5042181 | 0.4342321 |
| C    | 0.7799226 | 1.6009485 | -2.9389564 |
| C    | 1.6257514 | 2.4310501 | -3.7179503 |
| C    | 1.0916549 | 3.2341651 | -4.7350415 |
| C    | -0.2917779 | 3.2368847 | -4.9889727 |
| C    | -1.141542 | 2.4223127 | -4.2198555 |
| C    | -0.6147849 | 1.6105739 | -3.2041981 |
| H    | 2.7091332 | 2.4347565 | -3.5215034 |
| H    | 1.7642898 | 3.8688724 | -5.3354938 |
| H    | -0.7074816 | 3.8743582 | -5.7867409 |
| H    | -2.2266108 | 2.4146907 | -4.4148064 |
| H    | -1.2773778 | 0.9640588 | -2.6069194 |
| C    | 1.3055038 | 0.7353344 | -1.9069689 |
| C    | 1.5375929 | -0.3836632 | -1.3569005 |
| C    | 1.7895150 | -1.8090780 | -1.4301288 |
| C    | -5.0344965 | 1.3238325 | 1.5025429 |
| C    | -4.5355261 | 0.0372441 | 1.1884665 |
| C    | -3.1605106 | -0.1846951 | 1.0941285 |
| C    | -2.7457344 | 2.1499997 | 1.6003473 |
| C    | -4.1252938 | 2.3847820 | 1.7093693 |
| O    | -6.3870314 | 1.4358920 | 1.5812182 |
| H    | -5.2583003 | -0.7757992 | 1.0176185 |
| H    | -2.7951668 | -1.1888858 | 0.8259732 |
| H    | -2.0473340 | 2.9833999 | 1.7849273 |
| H    | -4.4783142 | 3.3945124 | 1.9645007 |
| H    | -0.5664635 | 2.2572249 | -0.0305651 |
| C    | -6.9544541 | 2.7007651 | 1.8840578 |
| H    | -6.6311035 | 3.0681702 | 2.8864834 |
| H    | -8.0526205 | 2.5505129 | 1.8903394 |
| C    | -6.6950736 | 3.4643635 | 1.1130867 |
| C    | 3.7623117 | -3.5203748 | 3.1025461 |
| H    | 4.3241281 | -2.6193473 | 3.4428990 |
| H    | 3.9408832 | -3.6724222 | 2.0130853 |
$\text{vibrational spectrum}$

| #  | mode | symmetry | wave number cm$^{-1}$ | IR intensity km/mol | IR | RAMAN |
|----|------|----------|-----------------------|---------------------|----|-------|
| 1  |      |          | 0.00                  | 0.00000             | -  | -     |
| 2  |      |          | 0.00                  | 0.00000             | -  | -     |
| 3  |      |          | 0.00                  | 0.00000             | -  | -     |
| 4  |      |          | 0.00                  | 0.00000             | -  | -     |
| 5  |      |          | 0.00                  | 0.00000             | -  | -     |
| 6  |      |          | 0.00                  | 0.00000             | -  | -     |
| 7  | a    |          | 11.41                 | 0.09327             | YES | YES   |
| 8  | a    |          | 16.85                 | 0.05804             | YES | YES   |
| 9  | a    |          | 20.99                 | 0.16957             | YES | YES   |
| 10 | a    |          | 28.16                 | 0.10066             | YES | YES   |
| 11 | a    |          | 36.00                 | 0.86956             | YES | YES   |
| 12 | a    |          | 39.01                 | 0.31055             | YES | YES   |
| 13 | a    |          | 45.19                 | 0.10445             | YES | YES   |
| 14 | a    |          | 48.27                 | 0.84812             | YES | YES   |
| 15 | a    |          | 53.24                 | 0.12915             | YES | YES   |
| 16 | a    |          | 61.97                 | 0.17545             | YES | YES   |
| 17 | a    |          | 70.80                 | 0.30147             | YES | YES   |
| 18 | a    |          | 77.93                 | 0.10995             | YES | YES   |
| 19 | a    |          | 83.73                 | 0.90023             | YES | YES   |
| 20 | a    |          | 90.22                 | 0.23146             | YES | YES   |
| 21 | a    |          | 94.80                 | 0.17699             | YES | YES   |
| 22 | a    |          | 98.30                 | 0.47627             | YES | YES   |
| 23 | a    |          | 104.33                | 0.89218             | YES | YES   |
| 24 | a    |          | 109.49                | 0.93333             | YES | YES   |
| 25 | a    |          | 118.15                | 1.82754             | YES | YES   |
| 26 | a    |          | 146.42                | 1.64226             | YES | YES   |
| 27 | a    |          | 150.95                | 1.34614             | YES | YES   |
| 28 | a    |          | 158.67                | 0.88868             | YES | YES   |
| 29 | a    |          | 169.35                | 2.88200             | YES | YES   |
| 30 | a    |          | 181.04                | 2.40710             | YES | YES   |
| 31 | a    |          | 188.68                | 3.26368             | YES | YES   |
| 32 | a    |          | 191.67                | 1.53467             | YES | YES   |
| 33 | a    |          | 206.86                | 0.62635             | YES | YES   |
| 34 | a    |          | 230.76                | 3.27932             | YES | YES   |
| 35 | a    |          | 234.86                | 2.02230             | YES | YES   |
| 36 | a    |          | 248.55                | 0.36116             | YES | YES   |
| 37 | a    |          | 253.94                | 1.23472             | YES | YES   |
| 38 | a    |          | 267.87                | 0.75825             | YES | YES   |
| 39 | a    |          | 296.61                | 3.74998             | YES | YES   |
| 40 | a    |          | 320.41                | 2.34102             | YES | YES   |
| 41 | a    |          | 341.10                | 0.88454             | YES | YES   |
| 42 | a    |          | 360.93                | 5.44085             | YES | YES   |
| 43 | a    |          | 376.09                | 10.14822            | YES | YES   |
| 44 | a    |          | 382.42                | 32.74494            | YES | YES   |
| 45 | a    |          | 401.20                | 0.01273             | YES | YES   |
| 46 | a    |          | 402.61                | 0.11511             | YES | YES   |
| 47 | a    |          | 415.93                | 2.26611             | YES | YES   |
| 48 | a    |          | 421.73                | 1.09551             | YES | YES   |
|   |   |       |   |     |     |
|---|---|-------|---|-----|-----|
| 49| a | 440.76| 4.23288| YES | YES |
| 50| a | 453.33| 1.25458| YES | YES |
2fa'

SCF Energy (au) BP86/SV(P) -2391.959491985
SCF Energy (au) PBE0/def2-TZVPP -2391.516131723
SCF Energy (au) PBE0/def2-TZVPP -2391.5242788848 (Toluene Correction)
Zero Point Energy (au) 0.3212083
Chemical Potential (kJ mol⁻¹) 690.67
Dispersion Correction (au) PBE0/def2-TZVPP -0.06847143

xyz coordinates

| Element | x     | y     | z     |
|---------|-------|-------|-------|
| Mn      | 1.3963769 | 1.3583796 | 0.3444836 |
| C       | 1.4957594 | 1.7909642 | 2.0933701 |
| C       | 3.1423484 | 1.0164151 | 0.2487564 |
| C       | 1.6670801 | 3.0927734 | -0.1289336 |
| O       | 1.9417192 | 4.1914285 | -0.4091898 |
| O       | 4.2810258 | 0.7630211 | 0.1844692 |
| O       | 1.5645760 | 2.0826934 | 3.2182820 |
| C       | -1.3013999 | 0.2766545 | 1.0687616 |
| C       | -1.5652880 | 2.3506976 | -0.0038004 |
| C       | -2.9709816 | 2.2805102 | 0.0915204 |
| C       | -3.5348398 | 1.1533677 | 0.7050525 |
| C       | -2.7031045 | 0.1460634 | 1.1961401 |
| C       | -0.3361981 | -0.7167661 | 1.5532949 |
| C       | 1.0401974 | -0.4292863 | 1.3235092 |
| C       | 1.9895755 | -1.3493861 | 2.8491260 |
| O       | 1.5987860 | -2.5251865 | 2.4814980 |
| C       | 0.2347955 | -2.8085505 | 2.6814675 |
| C       | -0.7272833 | -1.9041925 | 2.2201260 |
| O       | -0.9183472 | 3.3876342 | -0.5742201 |
| H       | 3.6082712 | 3.0827651 | -0.3038207 |
| H       | -4.6300732 | 1.0672355 | 0.7956806 |
| H       | -3.1312896 | -0.7437030 | 1.6772621 |
| O       | 3.0679694 | -1.1558228 | 1.6898941 |
| H       | 2.3676865 | -3.2262140 | 2.8491260 |
| H       | -0.0759951 | -3.7294558 | 3.2012154 |
| H       | -1.7934148 | -2.1283994 | 2.3874980 |
| O       | -0.7487716 | 1.3797544 | 0.4702178 |
| H       | 1.2478329 | 2.1441806 | -2.5348533 |
| C       | 1.1781634 | 1.3641921 | -1.7754152 |
| C       | 1.0614090 | 0.1419872 | -1.4550057 |
| C       | 0.8178416 | -1.2600164 | -1.7094089 |
| C       | 0.3304515 | -3.9864540 | -2.2994260 |
| C       | 1.5879058 | -3.5794731 | -1.8181482 |
| C       | 1.8312532 | -2.2322700 | -1.5175448 |
| C       | -0.4470777 | -1.6804654 | -2.1938190 |
| C       | -0.6847403 | -3.0319935 | -2.4845658 |
| H       | 0.1423019 | -5.0482405 | -2.5298388 |
| H       | 2.3899640 | -4.3218948 | -1.6721158 |
| H       | 2.8161788 | -1.9143457 | -1.1427412 |
| H       | -1.2399391 | -0.9305886 | -2.3445678 |
| H       | -1.6733543 | -3.3420701 | -2.8625993 |
| C       | -1.6486398 | 4.5142629 | -1.0398888 |
| H       | -2.3272451 | 4.2424261 | -1.8811164 |
| H       | -0.8856423 | 5.2328984 | -1.3989641 |
| H       | -2.2390287 | 4.9844696 | -0.2201868 |

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|-----------------|
| 1 | 0.00 | 0.00000  | -           | -            |
| 2 | 0.00 | 0.00000  | -           | -            |
| 3 | 0.00 | 0.00000  | -           | -            |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7  | a | 17.56 | 0.32176 | YES | YES |
| 8  | a | 30.56 | 0.34957 | YES | YES |
| 9  | a | 35.61 | 0.34595 | YES | YES |
| 10 | a | 46.86 | 0.06387 | YES | YES |
| 11 | a | 53.70 | 0.06745 | YES | YES |
| 12 | a | 73.53 | 1.80693 | YES | YES |
| 13 | a | 80.07 | 0.76770 | YES | YES |
| 14 | a | 92.33 | 0.60385 | YES | YES |
| 15 | a | 96.13 | 0.24797 | YES | YES |
| 16 | a | 101.05 | 0.13766 | YES | YES |
| 17 | a | 109.72 | 0.88510 | YES | YES |
| 18 | a | 118.53 | 0.25899 | YES | YES |
| 19 | a | 120.29 | 0.21308 | YES | YES |
| 20 | a | 126.82 | 0.65942 | YES | YES |
| 21 | a | 156.16 | 0.25574 | YES | YES |
| 22 | a | 164.73 | 0.43699 | YES | YES |
| 23 | a | 176.58 | 2.86296 | YES | YES |
| 24 | a | 184.23 | 1.52408 | YES | YES |
| 25 | a | 219.10 | 0.21957 | YES | YES |
| 26 | a | 232.13 | 1.09117 | YES | YES |
| 27 | a | 233.24 | 1.55831 | YES | YES |
| 28 | a | 263.08 | 0.18058 | YES | YES |
| 29 | a | 289.97 | 0.69181 | YES | YES |
| 30 | a | 308.04 | 0.41727 | YES | YES |
| 31 | a | 325.07 | 11.81392 | YES | YES |
| 32 | a | 334.42 | 1.62532 | YES | YES |
| 33 | a | 400.32 | 0.77081 | YES | YES |
| 34 | a | 407.09 | 10.83810 | YES | YES |
| 35 | a | 409.88 | 5.26984 | YES | YES |
| 36 | a | 430.73 | 0.31742 | YES | YES |
| 37 | a | 458.21 | 1.77025 | YES | YES |
| 38 | a | 461.90 | 4.09505 | YES | YES |
| 39 | a | 472.38 | 4.53511 | YES | YES |
| 40 | a | 482.55 | 7.02191 | YES | YES |
| 41 | a | 493.96 | 3.82026 | YES | YES |
| 42 | a | 498.09 | 3.42824 | YES | YES |
| 43 | a | 506.42 | 21.10995 | YES | YES |
| 44 | a | 508.51 | 0.81419 | YES | YES |
| 45 | a | 529.26 | 8.32951 | YES | YES |
| 46 | a | 537.81 | 17.08554 | YES | YES |
| 47 | a | 541.32 | 2.62297 | YES | YES |
| 48 | a | 568.59 | 3.32784 | YES | YES |
| 49 | a | 581.32 | 2.91337 | YES | YES |
| 50 | a | 612.10 | 26.50879 | YES | YES |
2ga
SCF Energy (au) BP86/SV(P) -2508.397058357
SCF Energy (au) PBE0/def2-TZVPP -2507.918314687
SCF Energy (au) PBE0/def2-TZVPP -2507.9263616631 (Toluene Correction)
Zero Point Energy (au) 0.3679099
Chemical Potential (kJ mol\(-1\)) 804.72
Dispersion Correction (au) PBE0/def2-TZVPP -0.08238683

xyz coordinates

Mn 1.4627019 -0.6136569 0.6719518
C 1.9354949 0.0695481 2.2687287
C 3.0921388 -1.2780301 0.4018875
C 1.9643077 0.8904391 -0.2341898
O 2.4492548 1.7919919 -0.7928015
O 4.1559398 -1.7320077 0.2404221
O 2.2409436 0.4997903 3.3074133
C -1.2743036 -1.2048065 1.6578451
C -2.7339246 0.9150606 0.6335650
C -3.4234327 -0.1952212 1.1390735
C -2.6868249 -1.2467250 1.6858767
C -0.4209420 -2.2522340 2.2349893
O 0.9717282 -2.1633040 1.9506955
C 1.8238570 -3.1294950 2.5254005
C 1.3197737 -4.1548839 3.344704
C -0.0604725 -4.2411538 3.608029
C -0.9265764 -3.2923808 3.0539203
C -0.6419949 2.2018926 0.2795213
H -3.2694568 1.8023745 0.2637775
H -4.5254493 -0.2231023 1.1354352
H -3.1980078 -2.1159172 2.1239789
H 2.9098132 -3.0934209 2.3361770
H 2.0124835 -4.8924719 3.7849519
H -0.4575073 -5.0421799 4.2535378
H -2.0039605 -3.3563542 3.2794642
N -0.6094863 -0.1505738 1.0806026
C 0.3156615 -0.4401438 -2.5752413
C 1.2673483 0.2390870 -3.3774685
C 0.8691893 0.8875930 -4.5549764
C -0.4793001 0.8733101 -4.9545738
C -1.4323542 0.2068282 -4.1678224
C -1.0430860 -0.4459915 -2.9889960
H 2.3248815 0.2482745 -3.0744248
H 1.6234532 1.4069923 -5.1688521
H -0.7868842 1.3911799 -5.8809002
H -2.4908057 0.1869449 -4.4772127
H -1.7867481 -0.9773241 -2.3740579
C 0.6874200 -1.1659350 -1.3824163
C 0.7767075 -2.1594344 -0.6038190
C 0.7188242 -3.2323749 -0.4197090
C 0.4681783 4.7342046 -0.2978530
C 0.6605090 4.1523752 0.9671899
C 0.1111930 2.8946908 1.2554809
C -0.8466833 2.8017314 -0.9816079
C -0.2847516 4.0553750 -1.2705521
H 0.9067758 5.7197436 -0.5261296
H 1.2440403 4.6821833 1.7380140
H 0.2553213 2.4465547 2.2516542
H -1.4278246 2.2673028 -1.7507523
H -0.4336055 4.5026189 -2.2672091
| # | mode | symmetry | wave number (cm\(^{-1}\)) | IR intensity (km/mol) | selection rules |
|---|------|----------|-----------------|---------------------|-----------------|
| 1 | 1    |          | 0.00            | 0.00000             | -                |
| 2 | 2    |          | 0.00            | 0.00000             | -                |
| 3 | 3    |          | 0.00            | 0.00000             | -                |
| 4 | 4    |          | 0.00            | 0.00000             | -                |
| 5 | 5    |          | 0.00            | 0.00000             | -                |
| 6 | 6    |          | 0.00            | 0.00000             | -                |
| 7 | a    | a        | 10.36           | 0.19938             | YES              |
| 8 | a    | a        | 27.51           | 0.04880             | YES              |
| 9 | a    | a        | 38.08           | 0.05465             | YES              |
| 10| a    | a        | 42.39           | 0.27325             | YES              |
| 11| a    | a        | 57.15           | 0.17486             | YES              |
| 12| a    | a        | 68.93           | 0.12536             | YES              |
| 13| a    | a        | 74.12           | 0.12933             | YES              |
| 14| a    | a        | 75.27           | 0.85869             | YES              |
| 15| a    | a        | 81.84           | 0.06469             | YES              |
| 16| a    | a        | 89.05           | 0.58480             | YES              |
| 17| a    | a        | 93.51           | 0.42378             | YES              |
| 18| a    | a        | 111.22          | 0.16990             | YES              |
| 19| a    | a        | 113.13          | 0.03525             | YES              |
| 20| a    | a        | 117.12          | 0.61225             | YES              |
| 21| a    | a        | 121.99          | 0.37536             | YES              |
| 22| a    | a        | 139.20          | 0.58041             | YES              |
| 23| a    | a        | 155.50          | 4.72657             | YES              |
| 24| a    | a        | 160.00          | 0.76063             | YES              |
| 25| a    | a        | 175.36          | 1.07927             | YES              |
| 26| a    | a        | 210.04          | 0.69555             | YES              |
| 27| a    | a        | 220.26          | 0.16892             | YES              |
| 28| a    | a        | 237.95          | 1.93218             | YES              |
| 29| a    | a        | 242.94          | 2.19533             | YES              |
| 30| a    | a        | 294.11          | 2.09996             | YES              |
| 31| a    | a        | 314.01          | 0.68797             | YES              |
| 32| a    | a        | 321.10          | 19.21421            | YES              |
| 33| a    | a        | 337.85          | 1.48906             | YES              |
| 34| a    | a        | 372.54          | 1.02664             | YES              |
| 35| a    | a        | 400.01          | 0.24974             | YES              |
| 36| a    | a        | 401.56          | 0.02427             | YES              |
| 37| a    | a        | 410.61          | 5.14172             | YES              |
| 38| a    | a        | 431.09          | 4.52154             | YES              |
| 39| a    | a        | 450.68          | 15.38779            | YES              |
| 40| a    | a        | 459.24          | 1.28575             | YES              |
| 41| a    | a        | 465.75          | 4.47669             | YES              |
| 42| a    | a        | 476.92          | 5.61536             | YES              |
| 43| a    | a        | 477.59          | 5.69098             | YES              |
| 44| a    | a        | 489.88          | 4.79517             | YES              |
| 45| a    | a        | 498.86          | 8.36890             | YES              |
| 46| a    | a        | 505.49          | 15.89184            | YES              |
| 47| a    | a        | 512.07          | 0.41507             | YES              |
| 48| a    | a        | 525.04          | 22.93634            | YES              |
| 49| a    | a        | 539.12          | 9.81531             | YES              |
| 50| a    | a        | 545.76          | 4.36875             | YES              |
\(2ga'\)

SCF Energy (au) BP86/SV(P) -2508.396040454
SCF Energy (au) PBE0/def2-TZVPP -2507.916677625
SCF Energy (au) PBE0/def2-TZVPP -2507.9248487015 (Toluene Correction)
Zero Point Energy (au) 0.3677349
Chemical Potential (kJ mol\(^{-1}\)) 803.07
Dispersion Correction (au) PBE0/def2-TZVPP -0.08281505

xyz coordinates
51

Mn 1.4391057 0.6238850 0.2962395
C 1.6057090 1.2800530 1.9682203
C 3.1384581 0.0991255 0.2177723
C 1.9242572 2.2136855 -0.4425164
O 2.3853360 3.1769319 -0.9117753
O 4.2454900 -0.2706716 0.1786023
O 1.7088666 1.7165425 3.0427783
C -1.3073847 -0.3107272 0.9690128
C -1.5041005 1.7935720 2.1640286
C -2.8934610 -1.8698532 -0.2371849
C -3.4956725 0.4332819 3.0476429
C -0.8663112 -2.3526857 2.3985808
C -0.9366685 3.1277568 -0.4318752
H -3.4886153 2.4275855 0.8463202
H -4.5799235 0.2729178 0.0967109
H -3.144796 -1.4512244 1.2310743
H 2.9721522 -1.7048341 2.1004869
H 2.1417944 -3.6047800 3.4502864
H -0.3304881 -4.0452930 3.6506908
H -1.9468188 -2.5412764 2.5099494
N -0.7183081 0.8205497 0.4609888
H 1.1918898 1.0978682 -2.6496469
C 1.1094174 0.4155304 -1.8019133
C 0.9619543 -0.7563221 -1.339748
C 0.6429493 -2.1626103 -1.4536003
C 0.0072647 -4.9014407 -1.7918630
C 1.2330252 -4.5245521 -1.2139585
C 1.5483836 -3.1703207 -1.0374688
C -0.5901544 -2.5528379 -2.0368187
C -0.9018073 -3.9104278 -2.2019866
H -0.2391899 -5.9682252 -1.9226733
H 1.9521015 -5.2959201 -0.8921393
H 2.5079090 -2.8774387 -0.5853995
H -1.2990600 -1.7747098 -2.3615368
H -1.8639889 -4.1971431 -2.6585568
C -0.0654151 5.7462825 -1.0362026
C 0.0314850 5.2560744 0.2776686
C -0.3981314 3.9555611 0.5794579
C -1.0496052 3.6351764 -1.7444527
C -0.6052271 4.9326472 -2.0465734
H 0.2807037 6.7657957 -1.2734075
H 0.4487774 5.8915806 1.0758772
H -0.3250503 3.5756515 1.611820
H -1.4787104 2.9993103 -2.5369369
H -0.6819526 5.3106181 -3.0795345
| # | mode | symmetry | wave number (cm**(-1)) | IR intensity (km/mol) | IR intensity (km/mol) | IR intensity (km/mol) | selection rules |
|---|------|----------|------------------------|----------------------|----------------------|----------------------|-----------------|
| 1 |      |          |                        |                      |                      |                      |                 |
| 2 |      |          |                        |                      |                      |                      |                 |
| 3 |      |          |                        |                      |                      |                      |                 |
| 4 |      |          |                        |                      |                      |                      |                 |
| 5 |      |          |                        |                      |                      |                      |                 |
| 6 |      |          |                        |                      |                      |                      |                 |
| 7 | a    |          | 14.68                  | 0.02458              | YES                  | YES                  |                 |
| 8 | a    |          | 20.00                  | 0.02170              | YES                  | YES                  |                 |
| 9 | a    |          | 26.94                  | 0.27393              | YES                  | YES                  |                 |
| 10| a    |          | 44.89                  | 0.09041              | YES                  | YES                  |                 |
| 11| a    |          | 52.65                  | 0.10546              | YES                  | YES                  |                 |
| 12| a    |          | 55.18                  | 0.14935              | YES                  | YES                  |                 |
| 13| a    |          | 68.98                  | 0.10168              | YES                  | YES                  |                 |
| 14| a    |          | 75.19                  | 0.90378              | YES                  | YES                  |                 |
| 15| a    |          | 80.23                  | 0.43735              | YES                  | YES                  |                 |
| 16| a    |          | 95.98                  | 0.04786              | YES                  | YES                  |                 |
| 17| a    |          | 96.61                  | 0.15507              | YES                  | YES                  |                 |
| 18| a    |          | 105.08                 | 0.15543              | YES                  | YES                  |                 |
| 19| a    |          | 111.34                 | 0.29671              | YES                  | YES                  |                 |
| 20| a    |          | 118.14                 | 0.38801              | YES                  | YES                  |                 |
| 21| a    |          | 124.61                 | 0.95451              | YES                  | YES                  |                 |
| 22| a    |          | 137.24                 | 0.09103              | YES                  | YES                  |                 |
| 23| a    |          | 158.46                 | 0.86799              | YES                  | YES                  |                 |
| 24| a    |          | 174.47                 | 1.38164              | YES                  | YES                  |                 |
| 25| a    |          | 183.09                 | 1.57158              | YES                  | YES                  |                 |
| 26| a    |          | 200.25                 | 0.43881              | YES                  | YES                  |                 |
| 27| a    |          | 216.64                 | 0.84383              | YES                  | YES                  |                 |
| 28| a    |          | 229.46                 | 1.29740              | YES                  | YES                  |                 |
| 29| a    |          | 240.10                 | 0.08552              | YES                  | YES                  |                 |
| 30| a    |          | 297.63                 | 0.15925              | YES                  | YES                  |                 |
| 31| a    |          | 311.68                 | 0.62241              | YES                  | YES                  |                 |
| 32| a    |          | 330.86                 | 11.24064             | YES                  | YES                  |                 |
| 33| a    |          | 337.66                 | 1.74335              | YES                  | YES                  |                 |
| 34| a    |          | 370.52                 | 1.39688              | YES                  | YES                  |                 |
| 35| a    |          | 399.39                 | 0.24768              | YES                  | YES                  |                 |
| 36| a    |          | 399.93                 | 0.79518              | YES                  | YES                  |                 |
| 37| a    |          | 407.82                 | 14.42548             | YES                  | YES                  |                 |
| 38| a    |          | 426.95                 | 0.94010              | YES                  | YES                  |                 |
| 39| a    |          | 453.00                 | 0.03982              | YES                  | YES                  |                 |
| 40| a    |          | 459.14                 | 3.39036              | YES                  | YES                  |                 |
| 41| a    |          | 462.50                 | 8.72856              | YES                  | YES                  |                 |
| 42| a    |          | 476.80                 | 6.22106              | YES                  | YES                  |                 |
| 43| a    |          | 481.75                 | 0.17525              | YES                  | YES                  |                 |
| 44| a    |          | 490.98                 | 5.09356              | YES                  | YES                  |                 |
| 45| a    |          | 499.22                 | 0.51778              | YES                  | YES                  |                 |
| 46| a    |          | 505.01                 | 18.43589             | YES                  | YES                  |                 |
| 47| a    |          | 512.38                 | 4.66827              | YES                  | YES                  |                 |
| 48| a    |          | 531.55                 | 4.58873              | YES                  | YES                  |                 |
| 49| a    |          | 541.02                 | 12.91639             | YES                  | YES                  |                 |
| 50| a    |          | 549.53                 | 3.33764              | YES                  | YES                  |                 |
SCF Energy (au) BP86/SV(P) -2354.867702753
SCF Energy (au) PBE0/def2-TZVPP -2354.415337120
SCF Energy (au) PBE0/def2-TZVPP -2354.423622997 (Toluene Correction)
Zero Point Energy (au) 0.3227920
Chemical Potential (kJ mol\(^{-1}\)) 692.09
Dispersion Correction (au) PBE0/def2-TZVPP 0.06448300

xyz coordinates

| atom | x         | y         | z         |
|------|-----------|-----------|-----------|
| Mn   | 1.9844632 | 0.3615964 | 0.2805713 |
| C    | 2.4729053 | 0.7706078 | 1.9633091 |
| C    | 3.6802028 | -0.0913158| -0.1161913|
| C    | 2.1691997 | 2.0841028 | -0.2778616|
| O    | 2.2954408 | 3.2028442 | -0.5801308|
| O    | 4.7776609 | -0.3989431| -0.3667064|
| O    | 2.7934382 | 1.0254737 | 3.0533302 |
| C    | -0.6474250| -0.2993731| 1.3472536 |
| C    | -0.0987172| -0.1416954| 1.6399885 |
| C    | 0.1625301 | -1.4533976| 1.7369729 |
| C    | 1.5284218 | -1.3774515| 1.314167  |
| C    | 2.3774492 | -2.4442437| 1.6743531 |
| C    | 1.8981386 | -3.5411240| 2.4143880 |
| C    | 0.5545604 | -3.5942075| 2.8362105 |
| C    | -0.3123366| -2.5468645| 2.5030714 |
| H    | 2.5876445 | -4.3616677| 2.6781061 |
| H    | 0.1908380 | -4.4464731| 3.4329670 |
| H    | -1.3580410| -2.5659727| 2.8511029 |
| N    | 0.0191421 | 0.6347120 | 0.7090967 |
| C    | 0.9878452 | 1.0097481 | -2.9360200|
| C    | 1.9878171 | 1.7884232 | -3.5718213|
| C    | 1.6561809 | 2.6351458 | -4.6380820|
| C    | 0.3254007 | 2.7326849 | -5.0831244|
| C    | -0.6758427| 1.9707337 | -4.4556397|
| C    | -0.3522845| 1.1163009 | -3.3916256|
| H    | 3.0304467 | 1.7157479 | -3.2248581|
| H    | 2.4468762 | 3.2286812 | -5.1259904|
| H    | 0.0691267 | 3.4043029 | -5.9190083|
| H    | -1.7212712| 2.0399266 | -4.7997030|
| H    | -1.1341259| 0.5134927 | -2.9024547|
| C    | 1.3062087 | 0.0918749 | -1.8676401|
| C    | 1.4093925 | -1.0031709| -1.2426333|
| H    | 1.3803549 | -2.0928587| -1.2210400|
| C    | -4.8598289| 0.2380123 | 2.1238249 |
| C    | -4.4023850| -0.9573970| 1.5420035 |
| C    | -3.0322054| -1.1508820| 1.3058817 |
| C    | -2.5709113| 1.0600181 | 2.2188912 |
| C    | -3.9402320| 1.2457316 | 2.4628171 |
| H    | -5.9358974| 0.3841697 | 2.3141531 |
| H    | -5.1204428| -1.7467476| 1.2648043 |
| H    | -2.6820451| -2.0814766| 0.8311990 |
| H    | -1.8499617| 1.8443132 | 2.5038226 |
| H    | -4.2907055| 2.1823146 | 2.9268384 |
| H    | -0.5475650| 1.4430989 | 0.4124348 |

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|----------------|
| 1 |      |          | 0.00        | 0.00000      | -              |
| 2 |      |          | 0.00        | 0.00000      | -              |
| 3 |      |          | 0.00        | 0.00000      | -              |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 4 | a | 0.00 | 0.00000 | - | - |
| 5 | a | 0.00 | 0.00000 | - | - |
| 6 | a | 0.00 | 0.00000 | - | - |
| 7 | a | 13.29 | 0.15192 | YES | YES |
| 8 | a | 23.03 | 0.07633 | YES | YES |
| 9 | a | 33.10 | 0.10247 | YES | YES |
|10 | a | 43.98 | 0.05862 | YES | YES |
|11 | a | 51.74 | 0.15394 | YES | YES |
|12 | a | 61.36 | 0.17907 | YES | YES |
|13 | a | 71.43 | 0.28741 | YES | YES |
|14 | a | 78.72 | 0.06019 | YES | YES |
|15 | a | 85.78 | 0.82130 | YES | YES |
|16 | a | 91.19 | 0.05240 | YES | YES |
|17 | a | 99.69 | 0.24511 | YES | YES |
|18 | a | 109.24 | 0.33295 | YES | YES |
|19 | a | 115.10 | 0.66219 | YES | YES |
|20 | a | 126.70 | 0.21360 | YES | YES |
|21 | a | 150.72 | 0.94188 | YES | YES |
|22 | a | 160.87 | 5.74710 | YES | YES |
|23 | a | 185.99 | 0.60228 | YES | YES |
|24 | a | 204.17 | 1.78023 | YES | YES |
|25 | a | 214.52 | 2.04916 | YES | YES |
|26 | a | 236.75 | 1.95956 | YES | YES |
|27 | a | 274.26 | 2.42220 | YES | YES |
|28 | a | 308.38 | 1.57647 | YES | YES |
|29 | a | 317.62 | 23.99863 | YES | YES |
|30 | a | 353.85 | 0.52186 | YES | YES |
|31 | a | 399.49 | 0.02689 | YES | YES |
|32 | a | 403.76 | 0.21821 | YES | YES |
|33 | a | 410.32 | 4.31237 | YES | YES |
|34 | a | 421.74 | 6.72909 | YES | YES |
|35 | a | 446.90 | 9.46617 | YES | YES |
|36 | a | 451.86 | 1.39235 | YES | YES |
|37 | a | 464.55 | 11.74879 | YES | YES |
|38 | a | 477.59 | 6.21398 | YES | YES |
|39 | a | 488.60 | 4.57895 | YES | YES |
|40 | a | 490.74 | 0.53493 | YES | YES |
|41 | a | 495.96 | 12.78844 | YES | YES |
|42 | a | 501.78 | 3.93526 | YES | YES |
|43 | a | 503.02 | 13.71281 | YES | YES |
|44 | a | 524.14 | 33.20199 | YES | YES |
|45 | a | 536.84 | 10.50917 | YES | YES |
|46 | a | 546.50 | 11.89717 | YES | YES |
|47 | a | 584.32 | 10.55322 | YES | YES |
|48 | a | 609.23 | 6.23246 | YES | YES |
|49 | a | 611.60 | 6.04316 | YES | YES |
|50 | a | 618.08 | 26.29849 | YES | YES |
2ha'

SCF Energy (au) BP86/SV(P) -2354.864921936
SCF Energy (au) PBE0/def2-TZVPP -2354.412686755
SCF Energy (au) PBE0/def2-TZVPP -2354.420595661 (Toluene Correction)
Zero Point Energy (au) 0.3226891
Chemical Potential (kJ mol⁻¹) 689.13
Dispersion Correction (au) PBE0/def2-TZVPP -0.06741741

xyz coordinates
45

Mn  1.7370355  1.9156621  -0.0185669
C  1.9577555  2.3012045  1.7280394
C  3.5025465  1.6204490 -0.1985573
C  1.8152550  3.6694973 -0.4796261
O  1.8576291  4.8024604 -0.7541614
O  4.6427294  1.396452  -0.3138999
O  2.1139695  2.5589014  2.8526198
C  -0.9128298  0.9532138  0.7371207
C  -0.0320248 -0.1264507  1.1817887
C  1.3579263  0.1145890  0.9381381
C  2.2687341 -0.8681919  1.3733419
C  1.8252121 -2.0586472  1.9791169
C  0.4511831 -2.3013110  2.1698957
C  -0.4790054 -1.3349730  2.6299379
H  3.3531148 -0.7201772  1.2347946
H  2.5643202 -2.8133496  2.2986332
H  0.1092259 -3.2436898  2.6277984
H  -1.5577047 -1.5208744  1.8999189
N  -0.2877921  1.9497253  0.1541413
H  1.4157086  2.6834474 -2.9025956
C  1.4505005  1.8998432 -2.1490172
C  1.4570271  0.6712439 -1.8394499
C  1.3933284 -0.7536490 -2.0724049
C  1.2754370 -3.5277641 -2.6245405
C  2.5071684 -2.9174475 -2.3265894
C  2.5693084 -1.545561 -2.0451657
C  0.1564402 -1.3787876 -2.3703728
C  0.1022075 -2.7536656 -2.6432421
H  1.2301733 -4.6077036 -2.8416829
H  3.4320346 -3.5175530 -2.3114330
H  3.5339045 -1.0675370 -1.8131480
H  -0.7618670 -0.7708876 -2.3936988
H  -0.8675413 -3.2241721 -2.8760245
C  -2.3914229  0.9752072  0.9151925
C  -5.1970723  1.1358492  1.2411788
C  -4.3794026  0.8234653  2.3378931
C  -2.9827916  0.7378493  2.1781861
C  -3.2278479  1.2961468 -0.1798602
C  -4.6198514  1.3707898 -0.0187747
H  -6.2904248  1.1971927  1.3691612
H  -4.8210463  0.6497995  3.3310303
H  -2.3425002  0.5151240  3.0466631
H  -2.7787729  1.4666498 -1.1727490
H  -5.2587493  1.6098494 -0.8848484
H  -0.8957280  2.7306852 -0.1336224

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number (cm⁻¹) | IR intensity (km/mol) | selection rules |
|---|------|---------|-------------------|----------------------|-----------------|
| 1 |      |         | 0.00              | 0.00000              | -               |
| 2 |      |         | 0.00              | 0.00000              | -               |
| 3 |      |         | 0.00              | 0.00000              | -               |
|   | 0.00 | 0.00000 | - | - |
|---|------|---------|---|---|
| 10 | 0.00 | 0.00000 | - | - |
| 7  | a    | 5.23    | 0.02192 | YES | YES |
| 8  | a    | 16.44   | 0.10699 | YES | YES |
| 9  | a    | 38.20   | 0.10104 | YES | YES |
| 10 | a    | 42.72   | 0.17829 | YES | YES |
| 11 | a    | 54.28   | 0.13952 | YES | YES |
| 12 | a    | 54.98   | 0.02477 | YES | YES |
| 13 | a    | 69.67   | 0.51001 | YES | YES |
| 14 | a    | 79.26   | 0.02376 | YES | YES |
| 15 | a    | 85.42   | 0.70115 | YES | YES |
| 16 | a    | 94.94   | 0.21828 | YES | YES |
| 17 | a    | 99.78   | 0.07365 | YES | YES |
| 18 | a    | 104.02  | 0.58385 | YES | YES |
| 19 | a    | 112.90  | 0.20273 | YES | YES |
| 20 | a    | 127.26  | 0.35518 | YES | YES |
| 21 | a    | 157.98  | 1.20516 | YES | YES |
| 22 | a    | 169.08  | 0.84161 | YES | YES |
| 23 | a    | 175.46  | 2.55549 | YES | YES |
| 24 | a    | 203.10  | 0.94757 | YES | YES |
| 25 | a    | 216.55  | 1.45099 | YES | YES |
| 26 | a    | 229.83  | 0.29463 | YES | YES |
| 27 | a    | 272.63  | 3.00912 | YES | YES |
| 28 | a    | 305.65  | 0.53639 | YES | YES |
| 29 | a    | 312.82  | 13.43462 | YES | YES |
| 30 | a    | 353.75  | 0.62675 | YES | YES |
| 31 | a    | 397.88  | 2.80142 | YES | YES |
| 32 | a    | 400.74  | 9.57004 | YES | YES |
| 33 | a    | 404.39  | 1.69232 | YES | YES |
| 34 | a    | 419.99  | 0.68333 | YES | YES |
| 35 | a    | 447.42  | 0.40847 | YES | YES |
| 36 | a    | 455.05  | 2.94910 | YES | YES |
| 37 | a    | 471.57  | 3.81417 | YES | YES |
| 38 | a    | 482.56  | 9.46046 | YES | YES |
| 39 | a    | 483.31  | 3.76855 | YES | YES |
| 40 | a    | 490.41  | 6.60203 | YES | YES |
| 41 | a    | 496.41  | 2.36391 | YES | YES |
| 42 | a    | 499.52  | 17.06561 | YES | YES |
| 43 | a    | 504.97  | 7.12513 | YES | YES |
| 44 | a    | 520.67  | 15.02069 | YES | YES |
| 45 | a    | 535.37  | 8.58747 | YES | YES |
| 46 | a    | 560.04  | 8.32210 | YES | YES |
| 47 | a    | 586.03  | 3.19765 | YES | YES |
| 48 | a    | 610.13  | 0.63566 | YES | YES |
| 49 | a    | 612.40  | 6.56616 | YES | YES |
| 50 | a    | 619.97  | 64.61582 | YES | YES |
SCF Energy (au) BP86/SV(P) -2183.122606432
SCF Energy (au) PBE0/def2-TZVPP -2182.706625903
SCF Energy (au) PBE0/def2-TZVPP -2182.7132650811 (Toluene Correction)
Zero Point Energy (au) 0.2582288
Chemical Potential (kJ mol\(^{-1}\)) 536.57
Dispersion Correction (au) PBE0/def2-TZVPP -0.05063461

xyz coordinates
37

Mn  1.0276323  0.3512433  0.9392188
C   1.1370934  0.6341023  2.717790
C   2.7601907 -0.0495923  0.8708951
C   1.3101813  2.1264881  0.5941055
O   1.5153634  3.2602778  0.436312
O   3.8873994 -0.3513020  0.8262138
O   1.2212734  0.7993244  3.8667371
C  -1.7321304 -0.3567563  1.336582
C  -3.2367423  2.7601907  0.8708951
C  -1.0221630 -1.5557674  1.7671824
C   0.4036238 -1.4598931  1.6766759
C   1.1509095 -2.5788773  2.1038483
C   0.5148944 -3.7386671  2.5790587
C  -0.8932832 -3.8219904  2.6497290
C  -1.6626598 -2.7286071  2.244057
H   2.2532812 -2.5552058  2.0663755
H   1.1268527 -4.5975959  2.9050630
H  -1.3780831 -4.7378682  3.0247820
H  -2.7632359 -2.7795799  2.2979940
O  -0.1463227  0.6258788  0.9473827
C   0.5587890  1.3296505 -2.2859772
C   1.3550578  1.2794408 -3.4595080
C   1.1786239  2.2285641 -4.4762772
C   0.2087685  3.2381839 -4.3436773
C  -0.5854823  3.2952924 -3.1842105
C  -0.4119255  2.3550292 -2.1598384
H   2.1150387  0.4882493 -3.5600353
H   1.8061901  2.1801339 -5.3817235
H   0.0737329  3.9844462 -5.1440526
H  -1.3470002  4.0851299 -3.0747019
H  -1.0301008  2.3943804 -1.2493785
C   0.7254424  0.3200752 -1.2659808
C   0.8311265 -0.8453558 -0.7786278
H   0.8181768 -1.9306874 -0.8852514
H  -3.5372666  0.7642561  0.9869631
H  -3.6380547 -0.3971449  2.3717041
H  -3.6951916 -1.0151920  0.6922219

#  mode  symmetry  wave number  IR intensity  selection rules
#      cm**(-1)  km/mol  IR   RAMAN
1     0.00  0.00000  -  -
2     0.00  0.00000  -  -
3     0.00  0.00000  -  -
4     0.00  0.00000  -  -
5     0.00  0.00000  -  -
6     0.00  0.00000  -  -
7     a  22.87  0.42459  YES  YES
8     a  33.85  0.18411  YES  YES
9     a  46.95  0.12673  YES  YES
10    a  57.10  0.04978  YES  YES
11    a  67.42  0.90009  YES  YES
|   | a | 77.84 | 0.13583 | YES | YES |
|---|---|-------|--------|-----|-----|
| 13 | a | 88.20 | 0.66367 | YES | YES |
| 14 | a | 95.47 | 0.27775 | YES | YES |
| 15 | a | 106.01 | 0.31080 | YES | YES |
| 16 | a | 109.13 | 0.52012 | YES | YES |
| 17 | a | 117.66 | 0.08236 | YES | YES |
| 18 | a | 119.11 | 0.12682 | YES | YES |
| 19 | a | 132.46 | 0.08321 | YES | YES |
| 20 | a | 169.13 | 3.07848 | YES | YES |
| 21 | a | 170.62 | 1.97929 | YES | YES |
| 22 | a | 210.75 | 1.15734 | YES | YES |
| 23 | a | 222.46 | 1.43356 | YES | YES |
| 24 | a | 242.47 | 1.64021 | YES | YES |
| 25 | a | 254.89 | 0.37087 | YES | YES |
| 26 | a | 288.22 | 0.78470 | YES | YES |
| 27 | a | 325.61 | 19.55637 | YES | YES |
| 28 | a | 402.00 | 0.15435 | YES | YES |
| 29 | a | 405.50 | 0.34124 | YES | YES |
| 30 | a | 411.25 | 1.72472 | YES | YES |
| 31 | a | 418.63 | 4.36502 | YES | YES |
| 32 | a | 440.28 | 9.11232 | YES | YES |
| 33 | a | 459.61 | 9.70023 | YES | YES |
| 34 | a | 470.59 | 1.75045 | YES | YES |
| 35 | a | 477.20 | 2.96730 | YES | YES |
| 36 | a | 488.01 | 10.85217 | YES | YES |
| 37 | a | 495.04 | 2.33308 | YES | YES |
| 38 | a | 505.71 | 2.73942 | YES | YES |
| 39 | a | 519.54 | 19.67222 | YES | YES |
| 40 | a | 524.75 | 36.41111 | YES | YES |
| 41 | a | 536.80 | 13.03176 | YES | YES |
| 42 | a | 548.38 | 3.82310 | YES | YES |
| 43 | a | 600.77 | 14.13686 | YES | YES |
| 44 | a | 608.60 | 4.43846 | YES | YES |
| 45 | a | 610.84 | 39.97431 | YES | YES |
| 46 | a | 613.49 | 3.98419 | YES | YES |
| 47 | a | 633.19 | 2.48601 | YES | YES |
| 48 | a | 649.36 | 55.39115 | YES | YES |
| 49 | a | 661.00 | 16.37113 | YES | YES |
| 50 | a | 677.34 | 63.83913 | YES | YES |
2ia’

SCF Energy (au) BP86/SV(P) -2183.119255411
SCF Energy (au) PBE0/def2-TZVPP -2182.703507634
SCF Energy (au) PBE0/def2-TZVPP -2182.710242209 (Toluene Correction)
Zero Point Energy (au) 0.2582085
Chemical Potential (kJ mol\textsuperscript{-1}) 535.77
Dispersion Correction (au) PBE0/def2-TZVPP -0.05302657

xyz coordinates
37

Mn 0.8983506 2.1448421 0.2688325
C 0.9141654 2.6039852 2.0158285
C 2.6524396 1.8402962 0.2910139
C 1.0410226 3.8978391 -0.2149611
O 3.7932662 1.5904865 0.3081505
O 0.9364859 2.9056166 3.1391041
C -1.8075626 1.2690843 0.7174211
C -3.3169564 1.2705979 0.7003573
C -1.0157638 0.1978747 1.3120318
C 0.3991048 0.3910100 1.2188449
C 1.2199172 -0.5869534 1.8179770
C 0.6658534 -1.7165200 2.4456782
C -0.7312506 -1.9033912 2.5086360
C -1.5737069 -0.9425776 1.9432115
H 2.3172948 -0.4767215 1.8032392
H 1.3356915 -2.4674974 2.8992107
H -1.1522350 -2.7932599 3.0039253
H -2.6680678 -1.0712190 1.9941553
O -1.1936215 2.2423079 0.2064007
H 0.8117751 2.896123 -2.6174311
C 0.7709592 2.1278030 -1.8471192
C 0.7261974 0.9043305 -1.5060129
C 0.5963222 -0.5095824 -1.7921790
H -3.6832412 2.1744501 0.1742166
H -3.7192499 1.2647297 1.7380287
H -3.708763 0.3619751 0.1922516
C 0.3439853 -3.2490311 -2.4608312
C -0.6892896 -2.3484622 -2.7736553
C -0.5671662 -0.9900332 -2.4453026
C 1.6281109 -1.4273549 -1.4744203
C 1.5025775 -2.7816281 -1.8145887
H 0.2475396 -4.3157889 -2.7222773
H -1.5990167 -2.7059184 -3.2843124
H -1.3704902 -0.2800854 -2.6988473
H 2.5380412 -1.0612958 -0.9746253
H 2.3193148 -3.4812396 -1.5712059

# mode symmetry wave number IR intensity selection rules
# cm**(-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 a 16.26 0.07232 YES YES
8 a 27.27 0.39170 YES YES
9 a 49.44 0.19270 YES YES
10 a 59.02 0.06082 YES YES
11 a 63.52 0.04027 YES YES
|   |   |   |   |   |
|---|---|---|---|---|
|12 | a | 73.78 | 1.26466 | YES | YES |
|13 | a | 88.99 | 0.65309 | YES | YES |
|14 | a | 97.88 | 0.16892 | YES | YES |
|15 | a | 104.69 | 0.28633 | YES | YES |
|16 | a | 115.69 | 0.22641 | YES | YES |
|17 | a | 117.80 | 0.85020 | YES | YES |
|18 | a | 127.99 | 0.10742 | YES | YES |
|19 | a | 131.86 | 0.42863 | YES | YES |
|20 | a | 165.40 | 1.61920 | YES | YES |
|21 | a | 182.02 | 1.60815 | YES | YES |
|22 | a | 201.91 | 0.59779 | YES | YES |
|23 | a | 222.49 | 1.74088 | YES | YES |
|24 | a | 231.59 | 1.17169 | YES | YES |
|25 | a | 254.48 | 0.63146 | YES | YES |
|26 | a | 291.18 | 0.61839 | YES | YES |
|27 | a | 328.62 | 12.16511 | YES | YES |
|28 | a | 400.08 | 0.31887 | YES | YES |
|29 | a | 406.66 | 6.49271 | YES | YES |
|30 | a | 409.60 | 3.66119 | YES | YES |
|31 | a | 416.98 | 3.55152 | YES | YES |
|32 | a | 450.74 | 2.33025 | YES | YES |
|33 | a | 460.02 | 1.33503 | YES | YES |
|34 | a | 470.60 | 3.95403 | YES | YES |
|35 | a | 478.52 | 6.71100 | YES | YES |
|36 | a | 492.43 | 11.27503 | YES | YES |
|37 | a | 497.15 | 3.54688 | YES | YES |
|38 | a | 502.61 | 9.37704 | YES | YES |
|39 | a | 511.36 | 10.56242 | YES | YES |
|40 | a | 526.42 | 16.87395 | YES | YES |
|41 | a | 535.87 | 6.33441 | YES | YES |
|42 | a | 566.15 | 5.67608 | YES | YES |
|43 | a | 601.71 | 15.77670 | YES | YES |
|44 | a | 608.29 | 5.91649 | YES | YES |
|45 | a | 612.50 | 14.51577 | YES | YES |
|46 | a | 616.09 | 56.93462 | YES | YES |
|47 | a | 633.33 | 2.95790 | YES | YES |
|48 | a | 647.28 | 41.26479 | YES | YES |
|49 | a | 652.92 | 19.21428 | YES | YES |
|50 | a | 679.40 | 77.09036 | YES | YES |
SCF Energy (au) BP86/SV(P) -2452.080768239
SCF Energy (au) PBE0/def2-TZVPP -2451.62092726
SCF Energy (au) PBE0/def2-TZVPP -2451.6286920118 (Toluene Correction)
Zero Point Energy (au) 0.3431713
Chemical Potential (kJ mol\(^{-1}\)) 738.84
Dispersion Correction (au) PBE0/def2-TZVPP -0.06762876

xyz coordinates

48

Mn 1.3428078 0.8045502 0.5807547
C 1.3783701 1.2227344 2.3336199
C 3.1025940 0.4977164 0.5670520
C 1.5688369 2.5632149 0.1210029
O 1.7224449 3.6913483 -0.1112692
O 4.2521930 0.2995053 0.5355771
O 1.4098099 1.4889051 3.4667047
O 1.3953526 0.0611476 0.8785204
C -2.8797304 0.1605952 0.8509716
C -0.6783374 -1.0867017 1.3610949
C 0.7053038 -0.9939985 1.3398313
C 1.5223928 -2.1348688 1.7934017
O -0.7101442 1.0584446 0.4739061
C 0.9310357 1.5353758 -2.7143732
C 1.7985379 1.5006747 -3.8368380
C 1.6046139 2.3843498 -4.9078489
C 0.5482648 3.3121502 -4.8796436
C -0.3155739 3.357136 3.7703583
C -0.1271098 2.4784202 -2.6927061
H 2.6264471 0.7741179 -3.8549566
H 2.2867829 2.3491936 -5.7734986
H 0.3997020 4.0069114 -5.7228199
H -1.1450905 4.0795798 -3.7432425
H -0.7977290 2.5028749 -1.8197662
C 1.1209643 0.5937250 -1.6368683
C 1.2891557 -0.5235868 -1.0649263
H 1.3650205 -1.6113508 -1.0932481
H -1.2044599 -1.9612831 1.7807001
C -5.6935604 0.4280399 0.7868146
C -4.8732260 1.5569739 0.6043783
C -3.4791073 1.4241220 0.6323170
C -3.7145290 -0.9672559 1.0353129
C -5.1103379 -0.8335910 0.9991676
H -6.7910934 0.5322035 0.7635136
H -5.3271954 2.5483246 0.4407592
H -2.8247368 2.2988518 0.4958738
H -3.3278656 -1.9635792 1.1913143
H -5.7485923 -1.7217179 1.1370152
C 3.0580313 -4.3695410 2.6573743
C 3.4298663 -3.0650970 3.0284627
C 2.6845134 -1.9624397 2.5882318
C 1.1570995 -3.4620276 1.4377184
C 1.9212272 -4.5624642 1.8534064
H 3.6573577 -5.2335446 2.9890534
H 4.3184064 -2.9022364 3.6605160
H 2.9930370 -0.9498948 2.8854907
H 0.2687670 -3.6236172 0.8047863
H 1.6251862 -5.5798783 1.5477199
| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|-----------------|
| 1 |      |          | 0.00        | 0.00000      | -               |
| 2 |      |          | 0.00        | 0.00000      | -               |
| 3 |      |          | 0.00        | 0.00000      | -               |
| 4 |      |          | 0.00        | 0.00000      | -               |
| 5 |      |          | 0.00        | 0.00000      | -               |
| 6 |      |          | 0.00        | 0.00000      | -               |
| 7 | a    |          | 19.34       | 0.18328      | YES             |
| 8 | a    |          | 29.78       | 0.20821      | YES             |
| 9 | a    |          | 32.91       | 0.04331      | YES             |
| 10| a    |          | 34.27       | 0.08747      | YES             |
| 11| a    |          | 41.54       | 0.19343      | YES             |
| 12| a    |          | 48.66       | 0.55510      | YES             |
| 13| a    |          | 57.82       | 0.19647      | YES             |
| 14| a    |          | 63.27       | 0.31881      | YES             |
| 15| a    |          | 74.34       | 0.11516      | YES             |
| 16| a    |          | 92.61       | 0.34213      | YES             |
| 17| a    |          | 95.48       | 0.14209      | YES             |
| 18| a    |          | 98.31       | 1.04767      | YES             |
| 19| a    |          | 104.50      | 0.24461      | YES             |
| 20| a    |          | 116.99      | 0.52529      | YES             |
| 21| a    |          | 124.52      | 0.20012      | YES             |
| 22| a    |          | 145.07      | 0.11716      | YES             |
| 23| a    |          | 154.08      | 0.65564      | YES             |
| 24| a    |          | 175.28      | 4.49094      | YES             |
| 25| a    |          | 193.75      | 0.92811      | YES             |
| 26| a    |          | 215.30      | 0.74143      | YES             |
| 27| a    |          | 221.97      | 0.42138      | YES             |
| 28| a    |          | 232.00      | 1.96209      | YES             |
| 29| a    |          | 259.41      | 0.65432      | YES             |
| 30| a    |          | 265.94      | 0.65064      | YES             |
| 31| a    |          | 318.81      | 19.77363     | YES             |
| 32| a    |          | 364.90      | 3.81450      | YES             |
| 33| a    |          | 396.90      | 1.90010      | YES             |
| 34| a    |          | 399.97      | 0.14845      | YES             |
| 35| a    |          | 401.99      | 0.35826      | YES             |
| 36| a    |          | 405.08      | 2.76880      | YES             |
| 37| a    |          | 417.70      | 8.06474      | YES             |
| 38| a    |          | 441.71      | 6.07106      | YES             |
| 39| a    |          | 453.03      | 1.48347      | YES             |
| 40| a    |          | 468.08      | 5.77371      | YES             |
| 41| a    |          | 476.58      | 1.52319      | YES             |
| 42| a    |          | 485.08      | 6.65317      | YES             |
| 43| a    |          | 488.75      | 9.69227      | YES             |
| 44| a    |          | 503.43      | 1.20446      | YES             |
| 45| a    |          | 509.22      | 27.45127     | YES             |
| 46| a    |          | 521.79      | 15.92382     | YES             |
| 47| a    |          | 534.58      | 10.70216     | YES             |
| 48| a    |          | 539.24      | 4.13881      | YES             |
| 49| a    |          | 563.79      | 5.43094      | YES             |
| 50| a    |          | 575.98      | 25.67458     | YES             |
3aa

SCF Energy (au) BP86/SV(P) -2427.897218753
SCF Energy (au) PBE0/def2-TZVPP -2427.461062227
SCF Energy (au) PBE0/def2-TZVPP -2427.472378136 (Toluene Correction)
Zero Point Energy (au) 0.2981519
Chemical Potential (kJ mol\(^{-1}\)) 630.17
Dispersion Correction (au) PBE0/def2-TZVPP 0.06351537

xyz coordinates
43

Mn 1.1810811 0.7159650 0.5661474
C 1.6598767 0.9219215 2.3218986
C 2.8124931 0.1034934 0.0877373
C 1.6285850 2.3714621 0.1740137
O 1.8910188 3.4873282 -0.0653848
O 3.8648482 -0.2685205 -0.2369390
O 1.9970452 1.0639864 3.4301209
C -1.3639759 0.0004371 1.3595888
C -1.5344690 2.2323180 0.6746315
C -2.8999818 2.2629891 0.9887676
C -3.5043130 1.1126164 1.5220845
C -2.7223835 -0.0387250 1.7130407
C -0.4323711 -1.1556316 1.4903727
C 0.2282191 -1.6852839 2.9014701
C -0.3120505 -1.8039179 2.7701581
H -1.0105112 3.1111142 0.2663304
H -3.4764221 3.1855249 0.8182644
H -4.5749929 1.1091453 1.7824192
H -3.1549511 -0.9672730 2.1167805
O 1.4408513 -3.6214689 -0.3846887
O 0.7252502 -3.6793587 4.1700191
H -0.7993238 -1.3709488 3.6556688
N -0.7869478 1.1259126 0.8682712
C 0.4306811 0.7439951 -2.5882684
C 1.4333479 1.6346543 -3.0505655
C 1.3607196 2.2088200 -4.3280906
C 0.2732415 1.9259245 -5.1739001
C -0.7390712 1.0556150 -4.7303850
C -0.6602454 0.4704662 -3.4584866
H 2.2928458 1.8603887 -2.4004361
H 2.161960 2.8881582 -4.6656384
H 0.2122367 2.3866509 -6.1738962
H -1.6002679 0.8323011 -5.3826107
H -1.4631317 -0.2007728 -3.1113904
C 0.5017330 0.1159829 -1.2647706
C 0.1302878 -1.1756697 -1.0245816
H -0.0776536 -1.9218985 -1.8186780
H 0.1921505 -3.2179402 5.0253523
H 1.8172426 -3.6823528 4.3875594
H 0.4118588 -4.7430222 4.0740278

$\text{vibrational spectrum}$

| #  | mode | symmetry | wave number (cm$^{-1}$) | IR intensity (km/mol) | IR | RAMAN |
|----|------|----------|-------------------------|-----------------------|----|--------|
| 1  | 0.00 | 0.00000  | -                       | -                     | -  | -      |
| 2  | 0.00 | 0.00000  | -                       | -                     | -  | -      |
| 3  | 0.00 | 0.00000  | -                       | -                     | -  | -      |
| 4  | 0.00 | 0.00000  | -                       | -                     | -  | -      |
| 5  | 0.00 | 0.00000  | -                       | -                     | -  | -      |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 6 | 0.00 | 0.00000 | - | - |
| 7 | a | 27.13 | 0.22894 | YES | YES |
| 8 | a | 31.31 | 1.15888 | YES | YES |
| 9 | a | 38.64 | 0.09170 | YES | YES |
| 10 | a | 47.06 | 3.23123 | YES | YES |
| 11 | a | 51.03 | 0.03444 | YES | YES |
| 12 | a | 65.80 | 0.31219 | YES | YES |
| 13 | a | 70.64 | 0.62300 | YES | YES |
| 14 | a | 83.70 | 0.71523 | YES | YES |
| 15 | a | 85.74 | 0.30667 | YES | YES |
| 16 | a | 98.66 | 0.91459 | YES | YES |
| 17 | a | 100.41 | 0.85868 | YES | YES |
| 18 | a | 105.58 | 0.32114 | YES | YES |
| 19 | a | 122.03 | 0.32392 | YES | YES |
| 20 | a | 142.13 | 0.21008 | YES | YES |
| 21 | a | 147.67 | 1.31379 | YES | YES |
| 22 | a | 154.77 | 0.60684 | YES | YES |
| 23 | a | 164.90 | 0.61796 | YES | YES |
| 24 | a | 168.59 | 1.02392 | YES | YES |
| 25 | a | 204.03 | 1.34226 | YES | YES |
| 26 | a | 234.09 | 0.82969 | YES | YES |
| 27 | a | 264.90 | 0.57805 | YES | YES |
| 28 | a | 271.62 | 0.42055 | YES | YES |
| 29 | a | 287.09 | 2.49634 | YES | YES |
| 30 | a | 306.14 | 0.94595 | YES | YES |
| 31 | a | 337.11 | 1.05520 | YES | YES |
| 32 | a | 370.70 | 2.97965 | YES | YES |
| 33 | a | 395.16 | 8.92298 | YES | YES |
| 34 | a | 408.27 | 0.68182 | YES | YES |
| 35 | a | 432.09 | 0.64404 | YES | YES |
| 36 | a | 450.92 | 2.19969 | YES | YES |
| 37 | a | 458.61 | 0.68661 | YES | YES |
| 38 | a | 471.99 | 2.82716 | YES | YES |
| 39 | a | 480.60 | 1.00547 | YES | YES |
| 40 | a | 486.92 | 0.72672 | YES | YES |
| 41 | a | 495.74 | 7.17728 | YES | YES |
| 42 | a | 498.30 | 3.06704 | YES | YES |
| 43 | a | 520.60 | 3.47485 | YES | YES |
| 44 | a | 534.57 | 2.34487 | YES | YES |
| 45 | a | 543.14 | 2.48022 | YES | YES |
| 46 | a | 552.57 | 3.12640 | YES | YES |
| 47 | a | 564.04 | 1.11003 | YES | YES |
| 48 | a | 599.29 | 2.19529 | YES | YES |
| 49 | a | 613.24 | 1.04141 | YES | YES |
| 50 | a | 616.73 | 25.69378 | YES | YES |
### 3aa'

**SCF Energy (au) BP86/SV(P)**  
-2427.892694005

**SCF Energy (au) PBE0/def2-TZVPP**  
-2427.457091685

**SCF Energy (au) PBE0/def2-TZVPP**  
-2427.4689841208 (Toluene Correction)

**Zero Point Energy (au)**  
0.2981446

**Chemical Potential (kJ mol\(^{-1}\))**  
631.41

**Dispersion Correction (au) PBE0/def2-TZVPP**  
0.06308410

**xyz coordinates**

|   |   |   |   |
|---|---|---|---|
| Mn | 1.3171493 | 1.8585225 | 0.5296280 |
| C  | 1.6298756 | 2.1496790 | 2.3126624 |
| C  | 3.0307253 | 1.3974938 | 0.2029409 |
| C  | 1.6464497 | 3.5272692 | 0.0470398 |
| O  | 1.8291102 | 4.6279022 | -0.3021686 |
| O  | 4.1385152 | 1.1270452 | -0.0289385 |
| O  | 1.8701931 | 2.3678615 | 3.4338012 |
| C  | 1.1847137 | 0.8917145 | 1.0692971 |
| C  | 1.5637281 | 3.1280814 | 0.5011556 |
| C  | 2.9455932 | 2.9756846 | 0.6882717 |
| C  | 3.4474210 | 1.7276430 | 1.0919780 |
| C  | 2.5502800 | 0.6634518 | 1.2902467 |
| O  | 0.0090156 | -0.1110759 | 1.2427467 |
| O  | 0.7083217 | -0.4934816 | 0.1437899 |
| O  | 1.7304981 | -1.5486002 | 0.3443189 |
| C  | 4.1898373 | -2.0854507 | 1.6614893 |
| C  | 1.0341846 | -1.7118421 | 2.6908435 |
| C  | 0.0741113 | -0.7478401 | 2.5256006 |
| H  | -1.168883 | 4.0879769 | 0.1958499 |
| H  | -3.6155793 | 3.8331442 | 0.5201520 |
| H  | -4.5236314 | 1.4817486 | 1.2486277 |
| H  | -2.8986445 | -0.3361000 | 1.6009322 |
| O  | 2.4712274 | -2.0071104 | -0.4899417 |
| C  | 1.3433680 | -2.4441814 | 3.9587961 |
| H  | -0.5466861 | -0.4406024 | 3.3791964 |
| N  | -0.7096453 | 2.1048080 | 0.6960981 |
| C  | 0.8184261 | 1.8829236 | -2.3052401 |
| C  | 0.8588662 | 1.3098571 | -1.3604264 |
| C  | 0.5171987 | -0.0004278 | -1.2695444 |
| C  | -0.0323389 | -0.9242508 | -2.3214178 |
| H  | 0.6553275 | -2.1414774 | 4.7733723 |
| H  | 2.3902219 | -2.2377382 | 4.2764703 |
| H  | 1.2642493 | -3.5430963 | 3.8012614 |
| C  | -0.9610834 | -2.6689967 | -4.3362568 |
| C  | -0.2837614 | -1.4860245 | -4.6880366 |
| C  | 0.2098940 | -0.6288371 | -3.6958179 |
| C  | -0.6469555 | -2.1199279 | -1.9851720 |
| C  | -1.1373039 | -2.9824307 | -2.9782057 |
| H  | -1.3423396 | -3.3459983 | -5.1185200 |
| H  | -0.1273649 | -1.2356769 | -5.7508757 |
| H  | 0.7615512 | 0.2801757 | -3.9854026 |
| H  | -0.8033312 | -2.3761770 | -0.9232676 |
| H  | -1.6618697 | -3.9081283 | -2.6873795 |

### Vibrational Spectrum

| #  | Mode | Symmetry | Wave Number (cm\(^{-1}\)) | IR Intensity (km/mol) | Selection Rules |
|----|------|----------|-----------------------------|-----------------------|-----------------|
| 1  |     |          | 0.00                        | 0.00000               |                 |
| 2  |     |          | 0.00                        | 0.00000               |                 |
| 3  |     |          | 0.00                        | 0.00000               |                 |
| 4  |     |          | 0.00                        | 0.00000               |                 |
| 5  |     |          | 0.00                        | 0.00000               |                 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
|   |   |   |   |   |   |   |
| 6 | a | 0.00 | 0.00000 | - | - |   |
| 7 | a | 29.19 | 0.39689 | YES | YES |   |
| 8 | a | 37.85 | 0.18530 | YES | YES |   |
| 9 | a | 42.04 | 0.53987 | YES | YES |   |
| 10 | a | 45.28 | 2.33284 | YES | YES |   |
| 11 | a | 55.60 | 0.07883 | YES | YES |   |
| 12 | a | 71.08 | 1.12178 | YES | YES |   |
| 13 | a | 72.97 | 0.64680 | YES | YES |   |
| 14 | a | 81.99 | 0.64645 | YES | YES |   |
| 15 | a | 89.08 | 0.10909 | YES | YES |   |
| 16 | a | 92.22 | 0.21892 | YES | YES |   |
| 17 | a | 97.74 | 1.15302 | YES | YES |   |
| 18 | a | 104.90 | 0.38369 | YES | YES |   |
| 19 | a | 125.99 | 0.51286 | YES | YES |   |
| 20 | a | 140.22 | 2.69414 | YES | YES |   |
| 21 | a | 149.69 | 0.95855 | YES | YES |   |
| 22 | a | 161.56 | 1.03869 | YES | YES |   |
| 23 | a | 166.50 | 1.04911 | YES | YES |   |
| 24 | a | 189.68 | 0.39795 | YES | YES |   |
| 25 | a | 206.72 | 0.93187 | YES | YES |   |
| 26 | a | 226.68 | 0.48747 | YES | YES |   |
| 27 | a | 253.12 | 0.35894 | YES | YES |   |
| 28 | a | 281.86 | 1.61657 | YES | YES |   |
| 29 | a | 285.37 | 0.53583 | YES | YES |   |
| 30 | a | 303.63 | 3.70548 | YES | YES |   |
| 31 | a | 340.15 | 0.60494 | YES | YES |   |
| 32 | a | 346.30 | 1.04459 | YES | YES |   |
| 33 | a | 403.46 | 0.16006 | YES | YES |   |
| 34 | a | 423.67 | 1.61991 | YES | YES |   |
| 35 | a | 429.09 | 3.27110 | YES | YES |   |
| 36 | a | 452.70 | 3.31077 | YES | YES |   |
| 37 | a | 466.50 | 1.35906 | YES | YES |   |
| 38 | a | 473.72 | 1.84264 | YES | YES |   |
| 39 | a | 484.93 | 2.26677 | YES | YES |   |
| 40 | a | 487.33 | 1.39886 | YES | YES |   |
| 41 | a | 502.24 | 2.90579 | YES | YES |   |
| 42 | a | 519.55 | 11.89092 | YES | YES |   |
| 43 | a | 524.12 | 11.54128 | YES | YES |   |
| 44 | a | 535.06 | 2.93645 | YES | YES |   |
| 45 | a | 543.20 | 2.59277 | YES | YES |   |
| 46 | a | 556.86 | 3.38187 | YES | YES |   |
| 47 | a | 573.17 | 2.88697 | YES | YES |   |
| 48 | a | 600.66 | 33.06235 | YES | YES |   |
| 49 | a | 612.22 | 2.75040 | YES | YES |   |
| 50 | a | 619.54 | 32.55359 | YES | YES |   |
3ba

SCF Energy (au) BP86/SV(P)  -2277.545461326
SCF Energy (au) PBE0/def2-TZVPP -2277.10429156
SCF Energy (au) PBE0/def2-TZVPP -2277.1124730146 (Toluene Correction)
Zero Point Energy (au) 0.2916084
Chemical Potential (kJ mol⁻¹) 622.44
Dispersion Correction (au) PBE0/def2-TZVPP 0.06485876

xyz coordinates

Mn  1.2035844  0.6105743  0.8523064
C   1.6744913  0.8965522  2.5994236
C   2.8473894  0.0456107  0.3779394
C   1.5909450  2.2597372  0.4049332
O   1.8148923  3.3744824  0.1207876
O   3.9082864 -0.3109878  0.0515739
O   2.0053768  1.0941946  3.7003449
C   1.3227434 -0.2381294  1.6401022
C   1.5436521  2.0144170  1.0274230
C   2.9081022  2.0114590  1.3451955
C   3.4882403  0.8327062  1.8409466
O   2.6826732 -0.3079262  1.9888013
O   3.2684065 -1.9506208  0.6110439
C   1.0047266 -3.1538226  0.7947706
C   1.268247  -3.7633542  2.0457343
C   0.5024462 -3.1928078  3.1746501
H   1.0387463  2.9154439  0.6443993
H   3.5013098  2.9283945  1.2048881
H   4.5582313  0.7983263  2.1223647
H   3.0974068 -1.2591955  2.3566214
H   1.4894977 -3.6036451 -0.0875664
H   1.7150206 -4.6901783  2.1490020
H   0.6024968 -3.6636841  4.1659042
H  -0.7641460 -1.5865805  3.8980022
N  -0.7722237  0.9178227  1.1841217
C   0.4618578  0.5683655 -2.2841753
C   1.4959925  1.4046476 -2.7766900
C   1.4177823  1.9803452 -4.0533923
C   0.2933206  1.7557737 -4.8679978
C  -0.7509429  0.9425426 -4.3928556
C  -0.6676157  0.3551167 -3.1214676
H   2.3837147  1.5872005 -2.1510279
H   2.2430676  2.6168488 -4.4154145
H   0.2281842  2.2194463 -5.8664202
H  -1.6426649  0.7667664 -5.0182869
H  -1.4952286 -0.2693487 -2.7481429
C   0.5384954  0.0687245  0.9062239
C   0.1581614 -1.3606470  0.7491599
H  -0.1018175 -2.0549193  1.5772156

$vibrational spectrum

# mode    symmetry wave number  IR intensity  selection rules
  #    cm⁻¹ (kJ mol⁻¹)       IR     RAMAN
1         0.00    0.000000  - -
2         0.00    0.000000  - -
3         0.00    0.000000  - -
4         0.00    0.000000  - -
5         0.00    0.000000  - -
6         0.00    0.000000  - -
7         30.29   0.176730  YES YES
| n  | a              | Value 1  | Value 2  | Value 3  | Value 4  | Value 5  | Value 6  |
|----|----------------|----------|----------|----------|----------|----------|----------|
| 8  | a              | 36.56    | 0.28054  | YES      | YES      |
| 9  | a              | 45.25    | 0.15305  | YES      | YES      |
| 10 | a              | 53.89    | 0.01637  | YES      | YES      |
| 11 | a              | 59.66    | 0.18616  | YES      | YES      |
| 12 | a              | 71.73    | 0.36929  | YES      | YES      |
| 13 | a              | 75.91    | 0.28811  | YES      | YES      |
| 14 | a              | 85.61    | 0.08148  | YES      | YES      |
| 15 | a              | 95.08    | 1.34750  | YES      | YES      |
| 16 | a              | 100.20   | 0.89084  | YES      | YES      |
| 17 | a              | 106.07   | 0.11045  | YES      | YES      |
| 18 | a              | 109.81   | 0.57321  | YES      | YES      |
| 19 | a              | 145.93   | 0.39554  | YES      | YES      |
| 20 | a              | 164.63   | 1.78407  | YES      | YES      |
| 21 | a              | 176.37   | 0.65124  | YES      | YES      |
| 22 | a              | 201.46   | 0.39912  | YES      | YES      |
| 23 | a              | 225.54   | 0.91587  | YES      | YES      |
| 24 | a              | 241.40   | 1.04718  | YES      | YES      |
| 25 | a              | 290.50   | 0.84951  | YES      | YES      |
| 26 | a              | 305.46   | 0.62450  | YES      | YES      |
| 27 | a              | 340.85   | 1.99622  | YES      | YES      |
| 28 | a              | 359.19   | 1.66423  | YES      | YES      |
| 29 | a              | 407.29   | 0.27628  | YES      | YES      |
| 30 | a              | 411.67   | 2.09351  | YES      | YES      |
| 31 | a              | 430.32   | 2.45243  | YES      | YES      |
| 32 | a              | 448.20   | 0.79627  | YES      | YES      |
| 33 | a              | 458.90   | 0.39531  | YES      | YES      |
| 34 | a              | 476.54   | 0.32414  | YES      | YES      |
| 35 | a              | 479.07   | 5.08508  | YES      | YES      |
| 36 | a              | 491.65   | 1.11876  | YES      | YES      |
| 37 | a              | 505.52   | 7.79304  | YES      | YES      |
| 38 | a              | 505.80   | 6.78980  | YES      | YES      |
| 39 | a              | 534.99   | 0.55830  | YES      | YES      |
| 40 | a              | 540.90   | 5.74478  | YES      | YES      |
| 41 | a              | 548.34   | 4.66755  | YES      | YES      |
| 42 | a              | 555.32   | 0.92651  | YES      | YES      |
| 43 | a              | 564.16   | 0.93785  | YES      | YES      |
| 44 | a              | 613.20   | 0.87636  | YES      | YES      |
| 45 | a              | 621.73   | 35.32377 | YES      | YES      |
| 46 | a              | 622.92   | 1.41328  | YES      | YES      |
| 47 | a              | 630.49   | 26.57959 | YES      | YES      |
| 48 | a              | 633.57   | 21.9976  | YES      | YES      |
| 49 | a              | 644.97   | 6.16252  | YES      | YES      |
| 50 | a              | 696.03   | 24.05804 | YES      | YES      |
3ba'

SCF Energy (au) BP86/SV(P)  -2277.542842618
SCF Energy (au) PBE0/def2-TZVPP  -2277.102650356
SCF Energy (au) PBE0/def2-TZVPP  -2277.1108568307 (Toluene Correction)
Zero Point Energy (au)  0.2916320
Chemical Potential (kJ mol\(^{-1}\))  621.89
Dispersion Correction (au) PBE0/def2-TZVPP  0.06426298

xyz coordinates

41

Mn  1.4885199  1.7045119  0.8181604
C   1.8265077  2.1026966  2.5777115
C   3.1454414  1.0652797  0.5205397
C   1.9444044  3.2939881  0.2327303
O   2.2063876  4.3558369  0.1870421
O   4.2131739  0.6509773  0.3046883
O   2.0888999  0.8846646  1.3480670
O   1.0888999  3.1519178  0.7822458
C   2.6578844  3.1277864  1.3523987
C   3.2731840  1.9291202  1.3523987
C   2.4749497  0.7896866  1.5512143
C   0.1314261  0.2465627  1.5563800
C   0.5976287  0.8229594  0.4644390
C   1.4042200  1.9613386  0.7375116
C   1.5023706  2.0212514  3.0902786
C   0.0299553  0.8176980  2.8543520
H   0.7337819  4.0677567  0.4807180
H   3.2445334  4.0438220  0.7866494
H   4.3641253  1.8787612  1.4995791
H   2.9143293  0.1741581  1.8509878
H   1.9574847  2.4179608  0.0991123
H   2.1457900  3.3806853  2.1980356
H   0.8584594  2.3507146  4.1052713
H   0.6028304  0.3658125  3.6809242
N   0.5072126  2.0562722  0.9820539
H   1.0338613  1.5503658  1.9838215
C   0.9936968  1.0196038  1.0131345
C   0.5364100  0.2610022  0.9328100
C   0.0626639  1.1237395  2.0460919
C   0.8974941  2.7471965  4.1820293
C   1.2411541  3.0468770  2.8531537
C   0.7671295  2.2467719  1.8009977
C   0.4052510  0.8428378  3.3933402
C   0.0706512  1.6385431  4.4441504
H   1.2564379  3.3762956  5.0093935
H   1.8885083  3.9120274  2.6308809
H   1.0556802  2.4909255  0.7649647
H   1.0720201  0.0063175  3.6141987
H   0.2169276  1.3980867  5.4816012

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number (cm\(^{-1}\)) | IR intensity (km/mol) | selection rules |
|---|------|----------|--------------------------|----------------------|-----------------|
| 1 |      |          | 0.00                     | 0.00000              |                 |
| 2 |      |          | 0.00                     | 0.00000              |                 |
| 3 |      |          | 0.00                     | 0.00000              |                 |
| 4 |      |          | 0.00                     | 0.00000              |                 |
| 5 |      |          | 0.00                     | 0.00000              |                 |
| 6 |      |          | 0.00                     | 0.00000              |                 |
| 7 | a    |          | 27.98                    | 0.21000              | YES             | YES             |

581
|   |   |   |   |
|---|---|---|---|
| 8 | a | 35.88 | 0.03719 | YES | YES |
| 9 | a | 42.40 | 0.53053 | YES | YES |
| 10 | a | 53.71 | 0.17874 | YES | YES |
| 11 | a | 55.09 | 0.13841 | YES | YES |
| 12 | a | 75.80 | 0.23442 | YES | YES |
| 13 | a | 77.98 | 0.89256 | YES | YES |
| 14 | a | 86.90 | 0.33696 | YES | YES |
| 15 | a | 91.37 | 0.61055 | YES | YES |
| 16 | a | 95.14 | 0.10495 | YES | YES |
| 17 | a | 100.47 | 0.86115 | YES | YES |
| 18 | a | 108.09 | 0.34828 | YES | YES |
| 19 | a | 143.97 | 1.32281 | YES | YES |
| 20 | a | 172.24 | 0.81078 | YES | YES |
| 21 | a | 181.93 | 0.53638 | YES | YES |
| 22 | a | 212.56 | 0.77347 | YES | YES |
| 23 | a | 220.47 | 0.60037 | YES | YES |
| 24 | a | 260.51 | 0.31917 | YES | YES |
| 25 | a | 268.38 | 0.73732 | YES | YES |
| 26 | a | 316.09 | 0.36434 | YES | YES |
| 27 | a | 330.62 | 2.16754 | YES | YES |
| 28 | a | 355.25 | 0.15889 | YES | YES |
| 29 | a | 404.05 | 0.10322 | YES | YES |
| 30 | a | 415.22 | 2.55529 | YES | YES |
| 31 | a | 433.11 | 3.82045 | YES | YES |
| 32 | a | 454.83 | 1.38103 | YES | YES |
| 33 | a | 460.18 | 0.75567 | YES | YES |
| 34 | a | 471.42 | 3.55094 | YES | YES |
| 35 | a | 475.30 | 0.66048 | YES | YES |
| 36 | a | 491.02 | 1.76918 | YES | YES |
| 37 | a | 518.76 | 7.99125 | YES | YES |
| 38 | a | 517.19 | 10.00528 | YES | YES |
| 39 | a | 530.15 | 2.93397 | YES | YES |
| 40 | a | 543.68 | 6.69378 | YES | YES |
| 41 | a | 551.17 | 0.59449 | YES | YES |
| 42 | a | 572.72 | 7.04324 | YES | YES |
| 43 | a | 608.23 | 17.58280 | YES | YES |
| 44 | a | 612.63 | 17.55498 | YES | YES |
| 45 | a | 618.95 | 10.36268 | YES | YES |
| 46 | a | 624.31 | 3.62383 | YES | YES |
| 47 | a | 627.60 | 41.99112 | YES | YES |
| 48 | a | 636.32 | 10.37859 | YES | YES |
| 49 | a | 654.78 | 7.29210 | YES | YES |
| 50 | a | 693.78 | 26.60027 | YES | YES |
3bb
SCF Energy (au) BP86/SV(P) -2505.270959872
SCF Energy (au) PBE0/def2-TZVPP -2504.828741005
SCF Energy (au) PBE0/def2-TZVPP -2504.8384434576 (Toluene Correction)
Zero Point Energy (au) 0.000000
Chemical Potential (kJ mol⁻¹) 711.91
Dispersion Correction (au) PBE0/def2-TZVPP 0.000000

xyz coordinates
47
Mn 1.6477972 1.0275833 2.0605900
C 1.8976650 1.2694763 3.8608441
C 3.3020158 0.3626725 1.8050471
C 2.1780726 2.6512926 1.6683046
O 2.4926516 3.7462634 1.3914971
O 4.3695223 -0.0656815 1.6159589
O 2.0955334 1.4417486 4.9969535
C -0.9715380 2.473441 2.4287731
C -1.0499351 2.5466755 1.9737597
C -2.4450362 2.567129 2.1013274
C -3.1157768 1.3761657 2.4180761
C -2.3670369 0.1994742 2.5838918
C -0.0896805 -0.9507204 2.589833
C 0.6497980 -1.495271 1.4829103
C 1.2885120 -2.748776 1.6746996
C 1.2464445 -3.420783 2.8987807
C 0.5497269 -2.861959 3.9908379
C -0.1201860 -1.647293 3.8279927
H -0.4745746 3.4555027 1.7362322
H -2.9910714 3.5119022 1.9514598
H -4.2122738 1.356749 2.5266123
H -2.8516628 -0.761371 2.8163959
H 1.8354101 -3.186493 0.8232017
H 1.7644995 -4.386886 3.0112949
H 0.5233452 -3.822485 4.9618903
H -0.6904628 -1.215145 4.6692787
N -0.3372492 1.4146770 2.1450505
C 1.4343270 1.2627304 -1.0908466
C 1.2152329 0.4607538 0.1506046
C 0.7394831 -0.8075673 0.1684062
H 0.5149719 -1.394225 0.7454952
H 2.5194542 1.4570064 -1.2394867
O 1.0014743 0.5985720 -2.3075364
H 0.9106454 2.2410176 -1.0240664
H -0.2351374 0.9166963 -2.7772483
O -0.9697675 1.7454896 -2.2628037
C -0.5837036 0.1342317 -4.0072151
C -1.3420827 -1.2767439 -6.3224652
C -2.2226665 -0.332637 -5.7518477
C -1.8439204 0.364561 -4.5991023
C 0.2965975 -0.8071567 -4.5836955
C -0.0844649 -1.5091943 -5.7374509
H -1.6386221 -1.8296577 -7.2298127
H -3.2068873 -0.1543811 -6.2108652
H -2.5123797 1.1056769 -4.1330868
H 1.2790184 -0.9804965 -4.1195620
H 0.6052185 -2.2437876 -6.1854283

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number cm⁻¹ | IR intensity km/mol | selection rules |
|---|------|----------|------------------|---------------------|-----------------|
| 1 |      |          | 0.00             | 0.000000            | -                |
| 2 |      |          | 0.00             | 0.000000            | -                |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
|3  |0.00|0.00000|  - |  - |
|4  |0.00|0.00000|  - |  - |
|5  |0.00|0.00000|  - |  - |
|6  |0.00|0.00000|  - |  - |
|7  |a  |10.78|1.10029| YES| YES|
|8  |a  |21.30|0.05131| YES| YES|
|9  |a  |25.19|0.81352| YES| YES|
|10 |a  |39.40|0.01817| YES| YES|
|11 |a  |42.14|0.18979| YES| YES|
|12 |a  |55.45|0.68925| YES| YES|
|13 |a  |57.90|0.38211| YES| YES|
|14 |a  |64.94|0.45207| YES| YES|
|15 |a  |74.83|0.18833| YES| YES|
|16 |a  |83.62|0.12810| YES| YES|
|17 |a  |86.40|0.08338| YES| YES|
|18 |a  |93.65|1.00408| YES| YES|
|19 |a  |95.93|0.76442| YES| YES|
|20 |a  |107.74|0.05519| YES| YES|
|21 |a  |117.15|0.46782| YES| YES|
|22 |a  |146.24|0.38746| YES| YES|
|23 |a  |155.71|0.99850| YES| YES|
|24 |a  |175.99|1.34711| YES| YES|
|25 |a  |190.00|1.81081| YES| YES|
|26 |a  |214.51|0.56787| YES| YES|
|27 |a  |237.60|1.83998| YES| YES|
|28 |a  |276.57|2.56669| YES| YES|
|29 |a  |290.70|0.88472| YES| YES|
|30 |a  |311.95|3.93747| YES| YES|
|31 |a  |331.38|17.34403| YES| YES|
|32 |a  |354.47|0.52693| YES| YES|
|33 |a  |365.80|4.48850| YES| YES|
|34 |a  |374.44|1.17807| YES| YES|
|35 |a  |404.85|0.01467| YES| YES|
|36 |a  |434.65|1.57511| YES| YES|
|37 |a  |441.25|0.43459| YES| YES|
|38 |a  |446.29|0.05822| YES| YES|
|39 |a  |455.43|0.59858| YES| YES|
|40 |a  |466.19|2.35891| YES| YES|
|41 |a  |475.71|2.30286| YES| YES|
|42 |a  |477.44|2.93109| YES| YES|
|43 |a  |489.91|1.94362| YES| YES|
|44 |a  |495.82|6.22667| YES| YES|
|45 |a  |511.62|5.83307| YES| YES|
|46 |a  |522.82|10.20532| YES| YES|
|47 |a  |538.10|1.68865| YES| YES|
|48 |a  |549.48|1.99689| YES| YES|
|49 |a  |576.38|3.85253| YES| YES|
|50 |a  |610.28|0.55554| YES| YES|
3bb'

| SCF Energy (au) BP86/SV(P)          | -2505.262474030 |
|------------------------------------|-----------------|
| SCF Energy (au) PBE0/def2-TZVPP   | -2504.821881763 |
| SCF Energy (au) PBE0/def2-TZVPP   | -2504.8324982709 (Toluene Correction) |
| Zero Point Energy (au)             | 0.332973        |
| Chemical Potential (kJ mol⁻¹)      | 707.95          |
| Dispersion Correction (au) PBE0/def2-TZVPP | -0.06822560 |

xyz coordinates

|   |   |   |
|---|---|---|
| Mn | 1.4239376 | 1.6744286 | 1.8220771 |
| C  | 1.8865455 | 2.2627008 | 3.4965058 |
| C  | 3.1056942 | 1.2035792 | 1.3873430 |
| C  | 1.6306999 | 3.2445483 | 1.0746210 |
| O  | 1.7262686 | 4.2893934 | 0.5526978 |
| O  | 4.1875927 | 0.8961212 | 1.0815572 |
| O  | 2.2210702 | 2.6565818 | 4.5424955 |
| O  | -0.9950372 | 0.6248463 | 2.6735470 |
| C  | -1.4576079 | 2.8078057 | 1.9592185 |
| C  | -2.8176036 | 2.6651682 | 2.2663124 |
| C  | -3.2690759 | 1.4505949 | 2.8065614 |
| C  | -2.3417691 | 0.4156411 | 3.0134971 |
| C  | 0.0764247 | -0.3995511 | 2.8792772 |
| C  | 0.7681943 | -0.9957410 | 1.7734712 |
| C  | 1.6808274 | -2.0469290 | 2.0566569 |
| C  | 1.9203980 | -2.4827095 | 3.3635035 |
| C  | 1.2444866 | -1.8825392 | 4.449250 |
| C  | 0.3280167 | -0.8567160 | 4.1995850 |
| H  | -1.0510607 | 3.7420424 | 1.5401705 |
| H  | -3.5079445 | 3.5031200 | 2.0827257 |
| H  | -4.3320018 | 1.3072214 | 3.0598091 |
| H  | -2.6511245 | -0.5576994 | 3.4248795 |
| H  | 2.2192233 | -2.5183200 | 1.2184258 |
| H  | 2.6466862 | -3.2935919 | 3.5462002 |
| H  | 1.4342444 | -2.2179514 | 5.4773143 |
| H  | -0.2138813 | -0.3881755 | 5.0377423 |
| N  | -0.5713820 | 1.8119713 | 2.1663599 |
| H  | 0.7444662 | 1.1648687 | -0.9101610 |
| C  | 0.8359730 | 0.7575780 | 0.1133129 |
| C  | 0.5410352 | -0.5397815 | 0.3604814 |
| C  | 0.0598516 | -1.5885711 | -0.6198576 |
| H  | 0.7383530 | -2.4370668 | -0.6561824 |
| O  | -0.0366306 | -1.0211831 | -1.9346468 |
| H  | -0.9394416 | -1.9890683 | -0.3240467 |
| C  | -0.3792417 | -1.8897228 | -2.9238423 |
| C  | -0.4612079 | -1.2276167 | -4.2638339 |
| O  | -0.5948285 | -3.0752282 | -2.7243464 |
| C  | -0.6481598 | -0.0957918 | -6.8346892 |
| C  | -0.2881988 | 0.7066557 | -5.7371038 |
| C  | -0.1944030 | 0.1455912 | -4.4542450 |
| C  | -0.8217122 | -2.0287012 | -5.3688646 |
| C  | -0.9151381 | -1.4646325 | -6.6486519 |
| H  | -0.7204377 | 0.3484577 | -7.8416054 |
| H  | -0.0772928 | 1.7790471 | -5.8830349 |
| H  | 0.0882734 | 0.7675542 | -3.5916822 |
| H  | -1.0240530 | -3.0975207 | -5.1960703 |
| H  | -1.1970123 | -2.0947084 | -7.5084098 |

$vibrational spectrum$

| # | mode | symmetry | wave number cm⁻¹ | IR intensity km/mol | selection rules |
|---|------|----------|------------------|---------------------|-----------------|
| 1 | 0.00 | 0.00000   | -                 | -                   | -               |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 2 | 0.00 | 0.00000 | - | - |
| 3 | 0.00 | 0.00000 | - | - |
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | a | 4.99 | 0.87779 | YES | YES |
| 8 | a | 14.98 | 0.49000 | YES | YES |
| 9 | a | 27.14 | 0.57272 | YES | YES |
| 10 | a | 41.47 | 0.03971 | YES | YES |
| 11 | a | 43.34 | 0.10929 | YES | YES |
| 12 | a | 50.05 | 0.78132 | YES | YES |
| 13 | a | 62.65 | 1.08905 | YES | YES |
| 14 | a | 73.73 | 0.24892 | YES | YES |
| 15 | a | 76.33 | 0.74414 | YES | YES |
| 16 | a | 80.36 | 0.19552 | YES | YES |
| 17 | a | 93.09 | 0.68049 | YES | YES |
| 18 | a | 93.15 | 0.12074 | YES | YES |
| 19 | a | 97.84 | 0.99353 | YES | YES |
| 20 | a | 107.09 | 0.42463 | YES | YES |
| 21 | a | 113.49 | 0.31746 | YES | YES |
| 22 | a | 138.60 | 0.77426 | YES | YES |
| 23 | a | 163.63 | 2.56034 | YES | YES |
| 24 | a | 165.67 | 1.61550 | YES | YES |
| 25 | a | 186.51 | 1.09764 | YES | YES |
| 26 | a | 199.15 | 1.39561 | YES | YES |
| 27 | a | 209.75 | 1.17396 | YES | YES |
| 28 | a | 255.17 | 3.35363 | YES | YES |
| 29 | a | 265.72 | 1.06408 | YES | YES |
| 30 | a | 299.42 | 3.21550 | YES | YES |
| 31 | a | 320.48 | 2.42530 | YES | YES |
| 32 | a | 331.95 | 3.75774 | YES | YES |
| 33 | a | 364.98 | 1.97094 | YES | YES |
| 34 | a | 379.24 | 1.10255 | YES | YES |
| 35 | a | 403.35 | 0.00028 | YES | YES |
| 36 | a | 434.60 | 4.97223 | YES | YES |
| 37 | a | 445.03 | 0.12190 | YES | YES |
| 38 | a | 451.78 | 0.68727 | YES | YES |
| 39 | a | 458.23 | 2.59165 | YES | YES |
| 40 | a | 474.34 | 0.99981 | YES | YES |
| 41 | a | 479.67 | 3.72907 | YES | YES |
| 42 | a | 482.22 | 7.97386 | YES | YES |
| 43 | a | 491.27 | 4.35792 | YES | YES |
| 44 | a | 515.35 | 9.18263 | YES | YES |
| 45 | a | 525.91 | 1.57433 | YES | YES |
| 46 | a | 529.50 | 3.93818 | YES | YES |
| 47 | a | 538.23 | 2.59232 | YES | YES |
| 48 | a | 562.36 | 3.58769 | YES | YES |
| 49 | a | 564.16 | 4.23410 | YES | YES |
| 50 | a | 610.15 | 0.24927 | YES | YES |
3bc

SCF Energy (au) BP86/SV(P) -2281.135995277
SCF Energy (au) PBE0/def2-TZVPP -2280.709892308
SCF Energy (au) PBE0/def2-TZVPP -2280.7163380043 (Toluene Correction)
Zero Point Energy (au) 0.3591834
Chemical Potential (kJ mol\(^{-1}\)) 796.63
Dispersion Correction (au) PBE0/def2-TZVPP -0.07061984

xyz coordinates
47

Mn  
C  
C  
O  
O  
O  
C  
-1.4787280 -0.6152415 2.0577329
C  
-1.8374708 1.6433332 1.5472334
C  
-3.1878842 1.5579354 1.9092559
C  
-3.6919294 0.3292394 2.3653486
C  
-2.8228319 -0.7705066 2.4414410
C  
-0.4767104 -1.7177011 2.1490224
C  
0.2007391 0.9609250 4.0552737
C  
1.1880167 -3.9861117 2.3980705
C  
0.5382259 -3.4679615 3.5375738
C  
-0.2931455 -2.3530503 3.4052073
H  
H  
H  
H  
H  
H  
N  
-1.0056886 0.5825233 1.6225377
C  
C  
C  
C  
C  
C  
H  
H  
H  
H  
H  
H  
C  
2.4660993 -0.0490734 2.2881233
C  
-0.3841621 2.3961246 -3.2829140
H  
H  
H  
H  
H  
C  
0.4245959 2.3216262 -5.3197810
H  
-0.3844579 0.8306588 -4.7848120
$vibrational spectrum$

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|----------------|
| 1 |      |          | 0.00        | 0.00000      | -              |
| 2 |      |          | 0.00        | 0.00000      | -              |
| 3 |      |          | 0.00        | 0.00000      | -              |
| 4 |      |          | 0.00        | 0.00000      | -              |
| 5 |      |          | 0.00        | 0.00000      | -              |
| 6 |      |          | 0.00        | 0.00000      | -              |
| 7 | a    |          | 35.36       | 0.26877      | YES            |
| 8 | a    |          | 37.03       | 0.11738      | YES            |
| 9 | a    |          | 48.25       | 0.04837      | YES            |
| 10| a    |          | 51.60       | 0.02182      | YES            |
| 11| a    |          | 60.04       | 0.43157      | YES            |
| 12| a    |          | 65.10       | 0.52792      | YES            |
| 13| a    |          | 76.48       | 0.13860      | YES            |
| 14| a    |          | 88.60       | 0.05733      | YES            |
| 15| a    |          | 96.20       | 0.79255      | YES            |
| 16| a    |          | 100.71      | 0.79076      | YES            |
| 17| a    |          | 107.42      | 0.45034      | YES            |
| 18| a    |          | 108.57      | 0.28856      | YES            |
| 19| a    |          | 123.15      | 0.04763      | YES            |
| 20| a    |          | 142.86      | 0.45196      | YES            |
| 21| a    |          | 161.33      | 1.25089      | YES            |
| 22| a    |          | 171.62      | 0.05950      | YES            |
| 23| a    |          | 187.52      | 0.39619      | YES            |
| 24| a    |          | 212.63      | 1.39349      | YES            |
| 25| a    |          | 223.89      | 0.51838      | YES            |
| 26| a    |          | 259.86      | 0.08106      | YES            |
| 27| a    |          | 290.14      | 1.01879      | YES            |
| 28| a    |          | 295.14      | 1.52142      | YES            |
| 29| a    |          | 333.21      | 1.70194      | YES            |
| 30| a    |          | 355.39      | 1.34461      | YES            |
| 31| a    |          | 403.43      | 0.50782      | YES            |
| 32| a    |          | 419.53      | 7.20342      | YES            |
| 33| a    |          | 443.13      | 1.20729      | YES            |
| 34| a    |          | 451.04      | 0.97650      | YES            |
| 35| a    |          | 462.27      | 1.80215      | YES            |
| 36| a    |          | 464.56      | 0.30656      | YES            |
| 37| a    |          | 473.55      | 0.91469      | YES            |
| 38| a    |          | 481.66      | 5.21201      | YES            |
| 39| a    |          | 493.70      | 2.55763      | YES            |
| 40| a    |          | 503.71      | 8.88712      | YES            |
| 41| a    |          | 510.53      | 8.46111      | YES            |
| 42| a    |          | 528.20      | 0.73778      | YES            |
| 43| a    |          | 537.71      | 0.57584      | YES            |
| 44| a    |          | 548.05      | 1.17087      | YES            |
| 45| a    |          | 550.95      | 2.53395      | YES            |
| 46| a    |          | 567.38      | 2.39919      | YES            |
| 47| a    |          | 621.92      | 28.4105        | YES            |
| 48| a    |          | 622.65      | 2.27148      | YES            |
| 49| a    |          | 629.06      | 34.3454      | YES            |
| 50| a    |          | 634.10      | 7.22001      | YES            |
3bc'

SCF Energy (au) BP86/SV(P) -2281.140662981
SCF Energy (au) PBE0/def2-TZVPP -2280.715719323
SCF Energy (au) PBE0/def2-TZVPP -2280.7223820342 (Toluene Correction)
Zero Point Energy (au) 0.3590261
Chemical Potential (kJ mol$^{-1}$) 795.17
Dispersion Correction (au) PBE0/def2-TZVPP -0.06962776

xyz coordinates

Mn  1.7008294  1.9178340  1.2440537
C  1.9464929  2.2382414  3.0331653
C  3.3315730  1.1960531  1.0180863
C  2.2868389  3.4888898  0.7343215
O  2.6405981  4.5418127  0.3602348
O  4.3846566  0.7258024  0.8452115
O  2.1525111  2.4639907  4.1595807

H  -0.9782636  1.2554733  1.5666412
C  -0.9342414  3.5476428  1.0845970
C  -2.3307824  3.6335022  1.1661203
C  -3.0673510  2.4772899  1.4704893
O  -0.1295595  0.0478783  1.8081275
C  -0.6845288  -0.5178141  0.7703939
C  -1.4519761 -1.6688415  1.1034235
C  -1.3975069 -2.2547954  2.3717161
C   0.5680687  -1.7075987  3.3710144
C  -0.1827243  -0.5644054  3.0883288
H  -0.3100682  4.4267213  0.8574934
H  -2.8276646  4.6011997  0.9947426
H  -4.1662721  2.5132506  1.5450442
H  -2.9131136  -0.3353467  1.9044298
H   2.1172542  -2.0946194  0.3373892
H   2.0127821  -3.1433835  2.5897974
H   0.5222532  -2.1657562  4.3723103
H  -0.8209259  -0.1154719  3.8673750
N  -0.2777518  2.3872866  1.2903563
H   1.3996283  1.8612120  -1.6028164
C   1.2783893  1.3182463  -0.6440395
C   0.7292965  0.0806393  -0.6157631
C   0.1674180  -0.6703298  -1.8229329
C   0.9487741  -1.9443464  -2.2328460
H   0.2553998  0.0463469  -2.6744401
C  -1.3354527  -1.0109098  -1.6610256
H   2.0263430  -1.6978684  -2.3658397
C   0.3755887  -2.5712595  -3.5174003
H   0.8866761  -2.6995264  -1.4128483
C  -1.9210119  -1.6584808  -2.9299712
H   -1.9023449  -0.0867089  -1.4056220
H  -1.4595226  -1.7099529  -0.7988130
C  -1.1197359  -2.8983627  -3.3627757
H  -1.9112953  -0.9089820  -3.7575255
H  -2.9896957  -1.9259817  -2.7643687
H   0.9474940  -3.4898021  -3.7824158
H   0.5125164  -1.8597757  -4.3661075
H  -1.5283127  -3.3092554  -4.3136337
H  -1.2408158  -3.7001716  -2.5951562
| #  | mode | symmetry | wave number | IR intensity | selection rules |
|----|------|----------|-------------|--------------|-----------------|
| 1  |      |          | 0.00        | 0.00000      | -               |
| 2  |      |          | 0.00        | 0.00000      | -               |
| 3  |      |          | 0.00        | 0.00000      | -               |
| 4  |      |          | 0.00        | 0.00000      | -               |
| 5  |      |          | 0.00        | 0.00000      | -               |
| 6  |      |          | 0.00        | 0.00000      | -               |
| 7  | a    |          | 23.50       | 0.32533      | YES YES        |
| 8  | a    |          | 31.99       | 0.01860      | YES YES        |
| 9  | a    |          | 44.13       | 0.24008      | YES YES        |
| 10 | a    |          | 51.06       | 0.22408      | YES YES        |
| 11 | a    |          | 51.84       | 0.35126      | YES YES        |
| 12 | a    |          | 69.06       | 0.38263      | YES YES        |
| 13 | a    |          | 77.41       | 0.09042      | YES YES        |
| 14 | a    |          | 87.88       | 0.23113      | YES YES        |
| 15 | a    |          | 93.53       | 0.67250      | YES YES        |
| 16 | a    |          | 96.45       | 0.52594      | YES YES        |
| 17 | a    |          | 100.05      | 0.08474      | YES YES        |
| 18 | a    |          | 106.99      | 0.49804      | YES YES        |
| 19 | a    |          | 131.13      | 0.27875      | YES YES        |
| 20 | a    |          | 157.94      | 0.90602      | YES YES        |
| 21 | a    |          | 169.99      | 1.48451      | YES YES        |
| 22 | a    |          | 203.07      | 0.56503      | YES YES        |
| 23 | a    |          | 210.99      | 0.25113      | YES YES        |
| 24 | a    |          | 220.28      | 0.40385      | YES YES        |
| 25 | a    |          | 238.63      | 0.03352      | YES YES        |
| 26 | a    |          | 268.33      | 0.02872      | YES YES        |
| 27 | a    |          | 306.85      | 0.86862      | YES YES        |
| 28 | a    |          | 314.02      | 0.39462      | YES YES        |
| 29 | a    |          | 337.59      | 1.09218      | YES YES        |
| 30 | a    |          | 353.62      | 1.49040      | YES YES        |
| 31 | a    |          | 389.14      | 0.87982      | YES YES        |
| 32 | a    |          | 428.20      | 1.24568      | YES YES        |
| 33 | a    |          | 436.17      | 3.80539      | YES YES        |
| 34 | a    |          | 439.55      | 1.18578      | YES YES        |
| 35 | a    |          | 458.00      | 1.66801      | YES YES        |
| 36 | a    |          | 463.29      | 0.79979      | YES YES        |
| 37 | a    |          | 471.05      | 1.32839      | YES YES        |
| 38 | a    |          | 476.24      | 1.22475      | YES YES        |
| 39 | a    |          | 491.21      | 2.23124      | YES YES        |
| 40 | a    |          | 515.51      | 7.94809      | YES YES        |
| 41 | a    |          | 518.27      | 3.62172      | YES YES        |
| 42 | a    |          | 522.65      | 6.67053      | YES YES        |
| 43 | a    |          | 537.87      | 3.65551      | YES YES        |
| 44 | a    |          | 546.13      | 2.31482      | YES YES        |
| 45 | a    |          | 582.34      | 2.57348      | YES YES        |
| 46 | a    |          | 604.22      | 21.23873     | YES YES        |
| 47 | a    |          | 620.00      | 8.90392      | YES YES        |
| 48 | a    |          | 627.22      | 38.83376     | YES YES        |
| 49 | a    |          | 629.79      | 7.92577      | YES YES        |
| 50 | a    |          | 637.71      | 8.14397      | YES YES        |
SCF Energy (au) BP86/SV(P) \(-2411.413617596\)
SCF Energy (au) PBE0/def2-TZVPP \(-2410.960779076\)
SCF Energy (au) PBE0/def2-TZVPP \(-2410.9697888395\) (Toluene Correction)
Zero Point Energy (au) \(0.3619092\)
Chemical Potential (kJ mol\(^{-1}\)) \(789.69\)
Dispersion Correction (au) PBE0/def2-TZVPP \(0.07292669\)

xyz coordinates
49

Mn  1.1580946   0.2533469   2.0022092
C   1.6348367   0.5380953   3.7484200
C   2.7925991  -0.3277689   1.5176508
C   1.5653154   1.8951322   1.5564534
O   1.8040972   3.0097385   1.2778736
O   3.8473452  -0.6948563   1.1821893
O   1.9709921   0.7309954   4.8490138
C  -1.4026967  -0.5179689   2.8343411
C  -1.5531558   1.7099038   2.1187935
C  -2.9141328   1.7686986   2.4427297
C  -3.5306391   0.6351080   2.9973705
C  -2.7627536  -0.5232472   3.1929938
C  -0.5156184  -1.7030816   2.9964020
C   0.1482835  -2.2987802   3.5441020
C   0.2704004  -3.5109000   4.4591501
C  -0.4399921  -2.3227292   4.2706203
H   1.0218140   2.5749738   1.6915378
H   3.4766530   2.6978981   2.2619131
H   4.5994638   0.6490149   3.2655475
H  -3.2072983  -1.4427180   3.6042513
H   1.3250606  -4.0080314   1.2309236
H   1.4531173  -5.0665573   3.4859650
H   0.3288523  -3.9680690   5.4600933
H  -0.9536017  -1.8474087   5.1229669
N  -0.8152995   0.5974297   2.3241413
C   0.4378693   0.0956152  -1.1362323
C   1.4061952   1.0155642  -1.6139407
C   1.3827041   1.5187134  -2.9174912
C   0.3575769   1.1454161  -3.8349631
C  -0.6344641   0.2388594  -3.3573499
C  -0.5845963  -0.2648783  -2.0551730
H   2.2229875   1.3305442  -0.9460467
H   2.1765766   2.2157761  -3.2215062
N   0.3208918   1.6473731  -5.1284990
H  -1.4644746  -0.0724593  -4.0085269
H  -1.3814464  -0.9508668  -1.7224392
C   0.4823353  -0.4694157   0.2148392
C   0.0874268  -1.7501554   0.4903919
H  -0.1313716  -2.4849103  -0.3141261
C  -0.7211384   1.2196232  -6.0429968
C   1.3460939   2.5724649  -5.5760493
H   1.3697334   3.5021422  -4.9580529
H   1.1409724   2.8697347  -6.6241407
H   2.3674314   2.1205057  -5.5435120
H  -0.5728768   1.7113929  -7.0250688
H  -1.7409551   1.4924086  -5.6775268
H  -0.7084804   0.1148478  -6.2100478
| # | mode | symmetry | wave number (cm\(^{-1}\)) | IR intensity (km/mol) | IR intensity (IR) | Raman intensity (Raman) |
|---|---|---|---|---|---|---|
| 1 | 0.00 | 0.00000 | - | - |
| 2 | 0.00 | 0.00000 | - | - |
| 3 | 0.00 | 0.00000 | - | - |
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | a | 21.08 | 0.31267 | YES | YES |
| 8 | a | 25.20 | 1.16210 | YES | YES |
| 9 | a | 39.43 | 0.37353 | YES | YES |
| 10 | a | 43.29 | 0.93927 | YES | YES |
| 11 | a | 49.24 | 0.06683 | YES | YES |
| 12 | a | 55.98 | 0.63821 | YES | YES |
| 13 | a | 65.09 | 0.47275 | YES | YES |
| 14 | a | 74.16 | 0.64624 | YES | YES |
| 15 | a | 75.81 | 0.02333 | YES | YES |
| 16 | a | 85.58 | 0.10151 | YES | YES |
| 17 | a | 93.05 | 2.03898 | YES | YES |
| 18 | a | 98.03 | 0.55357 | YES | YES |
| 19 | a | 100.07 | 1.20359 | YES | YES |
| 20 | a | 107.45 | 0.07850 | YES | YES |
| 21 | a | 121.05 | 0.15239 | YES | YES |
| 22 | a | 134.11 | 0.51650 | YES | YES |
| 23 | a | 153.22 | 1.04832 | YES | YES |
| 24 | a | 174.25 | 0.48049 | YES | YES |
| 25 | a | 197.72 | 1.30506 | YES | YES |
| 26 | a | 213.05 | 0.33096 | YES | YES |
| 27 | a | 214.24 | 1.50010 | YES | YES |
| 28 | a | 222.78 | 0.43599 | YES | YES |
| 29 | a | 261.15 | 3.97850 | YES | YES |
| 30 | a | 287.96 | 1.54180 | YES | YES |
| 31 | a | 300.00 | 6.92838 | YES | YES |
| 32 | a | 309.55 | 1.05348 | YES | YES |
| 33 | a | 351.99 | 0.36710 | YES | YES |
| 34 | a | 365.35 | 3.37415 | YES | YES |
| 35 | a | 411.90 | 2.31770 | YES | YES |
| 36 | a | 419.13 | 3.32007 | YES | YES |
| 37 | a | 423.46 | 0.65970 | YES | YES |
| 38 | a | 443.47 | 1.55412 | YES | YES |
| 39 | a | 455.43 | 1.10299 | YES | YES |
| 40 | a | 462.10 | 0.58427 | YES | YES |
| 41 | a | 469.99 | 3.00002 | YES | YES |
| 42 | a | 477.73 | 5.04355 | YES | YES |
| 43 | a | 483.03 | 11.93955 | YES | YES |
| 44 | a | 492.17 | 1.18165 | YES | YES |
| 45 | a | 505.41 | 6.49846 | YES | YES |
| 46 | a | 511.22 | 3.50146 | YES | YES |
| 47 | a | 532.30 | 1.08792 | YES | YES |
| 48 | a | 539.35 | 4.13962 | YES | YES |
| 49 | a | 541.66 | 10.15662 | YES | YES |
| 50 | a | 553.79 | 0.72502 | YES | YES |
3bd'

SCF Energy (au) BP86/SV(P) -2411.410447430
SCF Energy (au) PBE0/def2-TZVPP -2410.9683234203
SCF Energy (au) PBE0/def2-TZVPP -2410.958998524 (Toluene Correction)
Zero Point Energy (au) 0.3619800
Chemical Potential (kJ mol\(^{-1}\)) 789.09
Dispersion Correction (au) PBE0/def2-TZVPP -0.07249849

xyz coordinates
49

Mn  1.7594811  2.3780870  1.7905522
C   2.1164445  2.7676239  3.5463937
C   3.4076023  1.7338603  1.4632533
C   2.2143365  3.9673582  1.2063758
O   2.4755736  5.0305307  0.7878539
O   4.4702473  1.3172361  1.2254476
O   2.3853366  3.0343150  4.6505127
C   0.8169518  1.5653483  2.3349170
C   0.9917541  3.8351141  1.7792212
C   2.3812763  3.8152428  1.9639769
C   2.9979374  2.6172537  2.3586792
C   2.2019531  1.4746599  2.5473014
C   0.1367893  0.4292305  2.5314332
O   0.8530995 -0.1481106  1.4311450
O   1.6521145 -1.2944059  1.6949435
O   1.7573642 -1.8404689  2.9760550
C   0.2446318 -0.1468652  3.8269131
H  -0.4570121  4.7502102  1.4776112
H  -2.9658978  4.7302021  1.8005746
H  -4.0880015  2.5700200  2.5135215
H  -2.6421761  0.5107777  2.8463223
H   2.1936939 -1.7523519  0.8514653
H   2.3962216 -2.7231491  3.1449226
H   1.1324764 -1.6894560  5.0665279
H  -0.3183687  0.3068091  4.6593589
N  -0.2338650  2.7364166  1.9696384
H   1.2873711  2.2305719 -1.0112830
C   1.2436783  1.6982825 -0.0416089
C   0.7855325  0.4171385  0.0359651
C   0.3205685 -0.4499935 -1.0740953
C  -0.6403717 -2.1028271 -3.2470443
C  -0.9730280 -2.3859338 -1.8917463
C  -0.5033633 -1.5792577 -0.8481322
C   0.6575204 -0.1811621 -2.4238388
C   0.1967957 -0.9714930 -3.4795579
N  -1.1012140 -2.8933772 -4.2925653
H  -1.6118688 -3.2452270 -1.6415554
H  -0.8003567 -1.8353762  0.1830288
H   1.3209240  0.6686278 -2.6539594
H   0.5086177 -0.7108120 -4.5012067
C  -0.7156781 -2.5868255 -5.6574505
C  -1.9011040 -4.0696289 -4.0099143
H  -1.3570415 -4.8108492 -3.3737167
H  -2.1675748 -4.5714991 -4.9617157
H  -2.8533116 -3.8128451 -3.4853204
H  -1.0397056 -1.5628749 -5.9622423
H  -1.1969285 -3.3097895 -6.3461398
H   0.3896025 -2.6504176 -5.8141060
| #  | mode | symmetry | wave number | IR intensity | selection rules |
|----|------|----------|-------------|--------------|----------------|
| 1  |      |          | 0.00        | 0.00000      | -              |
| 2  |      |          | 0.00        | 0.00000      | -              |
| 3  |      |          | 0.00        | 0.00000      | -              |
| 4  |      |          | 0.00        | 0.00000      | -              |
| 5  |      |          | 0.00        | 0.00000      | -              |
| 6  |      |          | 0.00        | 0.00000      | -              |
| 7  | a    |          | 18.99       | 0.66596      | YES            |
| 8  | a    |          | 27.88       | 0.03399      | YES            |
| 9  | a    |          | 33.40       | 0.36254      | YES            |
| 10 | a    |          | 42.85       | 0.76193      | YES            |
| 11 | a    |          | 51.37       | 0.25743      | YES            |
| 12 | a    |          | 53.18       | 0.34361      | YES            |
| 13 | a    |          | 67.75       | 1.47722      | YES            |
| 14 | a    |          | 73.69       | 0.26541      | YES            |
| 15 | a    |          | 78.21       | 0.05442      | YES            |
| 16 | a    |          | 79.66       | 0.15106      | YES            |
| 17 | a    |          | 85.98       | 0.22070      | YES            |
| 18 | a    |          | 91.80       | 0.36237      | YES            |
| 19 | a    |          | 96.10       | 1.06830      | YES            |
| 20 | a    |          | 100.26      | 0.00276      | YES            |
| 21 | a    |          | 125.52      | 1.17836      | YES            |
| 22 | a    |          | 136.18      | 0.61147      | YES            |
| 23 | a    |          | 165.06      | 0.63800      | YES            |
| 24 | a    |          | 188.52      | 0.75308      | YES            |
| 25 | a    |          | 194.01      | 1.12099      | YES            |
| 26 | a    |          | 200.97      | 0.76149      | YES            |
| 27 | a    |          | 215.44      | 0.05230      | YES            |
| 28 | a    |          | 225.48      | 0.35162      | YES            |
| 29 | a    |          | 262.85      | 0.32014      | YES            |
| 30 | a    |          | 285.40      | 0.22519      | YES            |
| 31 | a    |          | 304.78      | 1.10759      | YES            |
| 32 | a    |          | 318.87      | 3.40583      | YES            |
| 33 | a    |          | 351.60      | 0.75539      | YES            |
| 34 | a    |          | 359.42      | 1.44456      | YES            |
| 35 | a    |          | 386.42      | 0.45695      | YES            |
| 36 | a    |          | 419.25      | 0.06425      | YES            |
| 37 | a    |          | 430.54      | 2.55204      | YES            |
| 38 | a    |          | 435.88      | 3.72607      | YES            |
| 39 | a    |          | 457.39      | 1.39231      | YES            |
| 40 | a    |          | 465.04      | 0.70328      | YES            |
| 41 | a    |          | 474.90      | 1.30233      | YES            |
| 42 | a    |          | 477.20      | 5.66843      | YES            |
| 43 | a    |          | 489.75      | 4.52679      | YES            |
| 44 | a    |          | 507.07      | 4.70699      | YES            |
| 45 | a    |          | 515.39      | 6.35917      | YES            |
| 46 | a    |          | 519.83      | 12.09470     | YES            |
| 47 | a    |          | 528.54      | 3.87924      | YES            |
| 48 | a    |          | 540.13      | 3.23204      | YES            |
| 49 | a    |          | 545.49      | 2.69293      | YES            |
| 50 | a    |          | 565.39      | 3.44381      | YES            |
SCF Energy (au) BP86/SV(P) -2391.988619360
SCF Energy (au) PBE0/def2-TZVPP -2391.5574436897
SCF Energy (au) PBE0/def2-TZVPP -2391.548466315 (Toluene Correction)
Zero Point Energy (au) 0.3230463
Chemical Potential (kJ mol\(^{-1}\)) 696.07
Dispersion Correction (au) PBE0/def2-TZVPP -0.06844294

xyz coordinates

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number (cm\(^{-1}\)) | IR intensity (km/mol) | selection rules |
|---|------|----------|---------------------------|-----------------------|------------------|
| 1 | 0.00 | 0.00000  | -                         | -                     | -                |
| 2 | 0.00 | 0.00000  | -                         | -                     | -                |
| 3 | 0.00 | 0.00000  | -                         | -                     | -                |
|    |    |    |    |    |    |
|---|---|---|---|---|---|
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | a | 24.73 | 0.42575 | YES | YES |
| 8 | a | 32.77 | 0.77416 | YES | YES |
| 9 | a | 42.59 | 0.15089 | YES | YES |
|10 | a | 46.02 | 0.87848 | YES | YES |
|11 | a | 52.13 | 0.24975 | YES | YES |
|12 | a | 63.43 | 0.74685 | YES | YES |
|13 | a | 74.81 | 0.35220 | YES | YES |
|14 | a | 85.09 | 0.23384 | YES | YES |
|15 | a | 92.76 | 2.26815 | YES | YES |
|16 | a | 96.37 | 0.91130 | YES | YES |
|17 | a | 99.38 | 0.70388 | YES | YES |
|18 | a | 107.24 | 0.04566 | YES | YES |
|19 | a | 110.33 | 0.13395 | YES | YES |
|20 | a | 134.31 | 0.77873 | YES | YES |
|21 | a | 149.52 | 0.77319 | YES | YES |
|22 | a | 156.88 | 0.95919 | YES | YES |
|23 | a | 184.06 | 2.13859 | YES | YES |
|24 | a | 207.19 | 1.35787 | YES | YES |
|25 | a | 225.26 | 0.81501 | YES | YES |
|26 | a | 245.18 | 1.33807 | YES | YES |
|27 | a | 261.34 | 0.08205 | YES | YES |
|28 | a | 288.42 | 1.41136 | YES | YES |
|29 | a | 299.88 | 4.71848 | YES | YES |
|30 | a | 309.29 | 1.51426 | YES | YES |
|31 | a | 355.99 | 0.36497 | YES | YES |
|32 | a | 374.05 | 3.39132 | YES | YES |
|33 | a | 416.93 | 2.14670 | YES | YES |
|34 | a | 420.58 | 1.90198 | YES | YES |
|35 | a | 442.85 | 1.75952 | YES | YES |
|36 | a | 449.83 | 0.82556 | YES | YES |
|37 | a | 458.49 | 1.00003 | YES | YES |
|38 | a | 460.39 | 0.68765 | YES | YES |
|39 | a | 477.03 | 2.82516 | YES | YES |
|40 | a | 481.12 | 4.21536 | YES | YES |
|41 | a | 491.75 | 0.15798 | YES | YES |
|42 | a | 505.02 | 7.51385 | YES | YES |
|43 | a | 510.10 | 5.19666 | YES | YES |
|44 | a | 531.44 | 9.00323 | YES | YES |
|45 | a | 539.68 | 6.37763 | YES | YES |
|46 | a | 543.52 | 12.21052 | YES | YES |
|47 | a | 553.19 | 0.47352 | YES | YES |
|48 | a | 562.70 | 0.53993 | YES | YES |
|49 | a | 606.89 | 11.00156 | YES | YES |
|50 | a | 622.36 | 39.86735 | YES | YES |
3be'

SCF Energy (au) BP86/SV(P) -2391.985428432
SCF Energy (au) PBE0/def2-TZVPP -2391.546398574
SCF Energy (au) PBE0/def2-TZVPP -2391.5556957408 (Toluene Correction)
Zero Point Energy (au) 0.3230217
Chemical Potential (kJ mol⁻¹) 695.14
Dispersion Correction (au) PBE0/def2-TZVPP 0.06784260

xyz coordinates
45

Mn  1.8122988  1.9480148  1.4147212
C   2.1633410  2.2412118  3.1914086
C   3.4260367  1.2198082  1.0881766
C   2.3708124  3.5311227  0.9087900
O   2.7033871  4.5923569  0.5400796
O   4.4661979  0.7486149  0.8543723
O   2.4275983  2.4515952  4.3083436
C   0.8078624  1.2543860  1.8906140
C   0.8508899  3.5589190  1.4669078
C   2.9257347  2.4251631  1.6471064
C   2.1967927  1.2302014  2.0941101
C   0.0787136  0.0554271  2.0244011
C   0.7642242  0.5020519  0.8946779
C   1.4890464  1.7088776  1.0928999
C   1.5535021  2.3326115  2.3409788
C   0.8802061  1.7743965  3.4486059
C   0.1461699  0.9818966  3.2855988
H   -0.2635877  4.4578431  1.2194019
H   -2.7712795  4.5652525  1.5367376
H   -4.0175570  2.4309466  2.1193480
H   -2.6923763  0.2773633  2.3364265
H   -2.0070467 -2.1502731  0.2261206
H   -2.1351046 -3.2617665  2.4597967
H   -0.9310593 -2.2610244  4.4360588
H   -0.3910429 -0.1582303  3.4486059
N   -0.1578763  2.4098254  1.5956229
C   -1.3642422  1.9902530 -1.3918890
C   -1.2834493  1.4028131 -0.4572734
C   -0.7459051  0.1595959 -0.4625141
C   -0.2320746 -0.6096878 -1.6295954
C   -0.8102307 -2.0339223 -3.8802903
C   -1.1850094 -2.3990410 -2.5709966
C   -0.6648818 -1.6912546 -1.4726317
C   -0.5997018 -0.2684207 -2.9589371
C   -0.0913856 -0.9579672 -4.0959224
O   -1.2465295 -2.6482198 -5.0190950
H   -1.8836455 -3.2294423 -2.3891168
H   -0.9813916 -1.9900963 -0.4593405
H   -1.3172506  0.5508679 -3.1272071
H   -0.3890617 -0.6920816 -5.0863897
C   -2.1423304 -3.7371722 -4.8997078
H   -3.0985747 -3.4365554 -4.4077426
H   -1.6928093 -4.5843190 -4.3276767
H   -2.3592397 -4.0745133 -5.9335893

$vibrational spectrum

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|-----------------|
| 1 | 0.00 | 0.000000 | - | - | - |
| 2 | 0.00 | 0.000000 | - | - | - |
| 3 | 0.00 | 0.000000 | - | - | - |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | a  | 23.52 | 0.30109 | YES | YES |
| 8 | a  | 30.01 | 0.16593 | YES | YES |
| 9 | a  | 36.90 | 0.27643 | YES | YES |
| 10| a   | 50.51 | 0.00623 | YES | YES |
| 11| a   | 52.27 | 0.21524 | YES | YES |
| 12| a   | 67.09 | 1.22178 | YES | YES |
| 13| a   | 74.68 | 0.28231 | YES | YES |
| 14| a   | 78.64 | 0.28640 | YES | YES |
| 15| a   | 86.87 | 0.22244 | YES | YES |
| 16| a   | 92.50 | 0.63221 | YES | YES |
| 17| a   | 95.52 | 1.22483 | YES | YES |
| 18| a   | 100.13| 0.02259 | YES | YES |
| 19| a   | 110.64| 1.46995 | YES | YES |
| 20| a   | 134.65| 0.58483 | YES | YES |
| 21| a   | 154.92| 1.77198 | YES | YES |
| 22| a   | 168.01| 0.43068 | YES | YES |
| 23| a   | 191.21| 2.88992 | YES | YES |
| 24| a   | 204.06| 0.04844 | YES | YES |
| 25| a   | 218.20| 1.83517 | YES | YES |
| 26| a   | 245.89| 0.16399 | YES | YES |
| 27| a   | 264.59| 0.28702 | YES | YES |
| 28| a   | 281.62| 1.29168 | YES | YES |
| 29| a   | 306.04| 1.87473 | YES | YES |
| 30| a   | 320.05| 2.46467 | YES | YES |
| 31| a   | 349.10| 0.07857 | YES | YES |
| 32| a   | 357.62| 0.91673 | YES | YES |
| 33| a   | 411.52| 3.23641 | YES | YES |
| 34| a   | 413.58| 0.11381 | YES | YES |
| 35| a   | 433.61| 2.99339 | YES | YES |
| 36| a   | 453.82| 0.36253 | YES | YES |
| 37| a   | 458.11| 0.55712 | YES | YES |
| 38| a   | 465.67| 0.55181 | YES | YES |
| 39| a   | 475.22| 1.37219 | YES | YES |
| 40| a   | 489.37| 4.35182 | YES | YES |
| 41| a   | 505.21| 4.77785 | YES | YES |
| 42| a   | 515.59| 11.10122| YES | YES |
| 43| a   | 519.17| 12.44789| YES | YES |
| 44| a   | 530.62| 5.92420 | YES | YES |
| 45| a   | 540.35| 11.68463| YES | YES |
| 46| a   | 545.26| 3.48926 | YES | YES |
| 47| a   | 563.04| 5.39888 | YES | YES |
| 48| a   | 606.72| 24.11151| YES | YES |
| 49| a   | 615.07| 18.59324| YES | YES |
| 50| a   | 622.05| 7.04463 | YES | YES |
### 3bf

**SCF Energy (au) BP86/SV(P)**
-2376.715791997

**SCF Energy (au) PBE0/def2-TZVPP**
-2376.297634233

**SCF Energy (au) PBE0/def2-TZVPP**
-2376.3055857295 (Toluene Correction)

**Zero Point Energy (au)**
0.2836993

**Chemical Potential (kJ mol^{-1})**
598.37

**Dispersion Correction (au) PBE0/def2-TZVPP**
0.06503775

**xyz coordinates**

| Atoms | x               | y               | z               |
|-------|-----------------|-----------------|-----------------|
| Mn    | 1.2193489       | 0.6020264       | 0.8606017       |
| C     | 1.6842037       | 0.8796677       | 2.6111754       |
| C     | 2.8635536       | 0.0347297       | 0.3892382       |
| C     | 1.6136558       | 2.2512375       | 0.4220448       |
| O     | 1.8430488       | 3.3662344       | 0.1421678       |
| O     | 3.9243350       | -0.3226417      | 0.0636773       |
| O     | 2.0099078       | 1.0716719       | 3.7144017       |
| C     | -1.3157925      | -0.2381116      | 1.6367694       |
| C     | -1.5220768      | 2.0153745       | 1.0217826       |
| C     | -2.8892199      | 2.0182225       | 1.3273910       |
| C     | -3.4786214      | 0.8418555       | 1.8179138       |
| C     | -2.6790387      | -0.3019325      | 1.9735991       |
| C     | -0.3847977      | -1.3973172      | 1.7667139       |
| O     | 0.2790332       | -1.9556667      | 0.6205201       |
| O     | 1.0105745       | -3.1603577      | 0.8100076       |
| C     | 1.1196397       | -3.7711764      | 2.0612806       |
| C     | 0.4856663       | -3.2003028      | 3.1849117       |
| C     | -0.2675173      | -2.0340653      | 3.029354        |
| H     | -1.0102054      | 2.9143696       | 0.6432601       |
| H     | -3.4772754      | 2.9376370       | 1.1816374       |
| H     | -4.5511404      | 0.8118623       | 2.0692392       |
| H     | -3.101102       | -1.2513266      | 2.3378737       |
| H     | 1.5021338       | -3.6107959      | -0.0682391      |
| H     | 1.7046006       | -4.6994786      | 2.1693927       |
| H     | 0.5748327       | -3.6726192      | 4.1765020       |
| H     | -0.7836713      | -1.5916614      | 3.8981051       |
| N     | -0.7566698      | 0.9154196       | 1.1849338       |
| C     | 0.4638524       | 0.5641322       | -2.2739335      |
| C     | 1.4741388       | 1.4300413       | -2.7659224      |
| C     | 1.3859130       | 2.0136955       | -4.0373997      |
| C     | 0.2610546       | 1.7505013       | -4.8313512      |
| C     | -0.7671117      | 0.9135563       | -4.3806572      |
| C     | -0.6592671      | 0.3264455       | -3.1124551      |
| H     | 2.3588837       | 1.6352477       | -2.1437123      |
| H     | 2.1767868       | 2.6771795       | -4.4209382      |
| F     | 0.1600023       | 2.3228520       | -6.0494858      |
| H     | -1.6444173      | 0.7381501       | -5.0252582      |
| H     | -1.4724362      | -0.3201573      | -2.7445602      |
| C     | 0.5549493       | -0.0746596      | -0.9524162      |
| C     | 0.1756649       | -1.3671346      | -0.7406668      |
| H     | -0.0825691      | -2.0627050      | -1.5680801      |

$\text{vibrational spectrum}$

| #  | mode | symmetry | wave number (cm\(^{-1}\)) | IR intensity (km/mol) | selection rules |
|----|------|----------|---------------------------|----------------------|-----------------|
| 1  |      |          | 0.00                      | 0.00000              | -               |
| 2  |      |          | 0.00                      | 0.00000              | -               |
| 3  |      |          | 0.00                      | 0.00000              | -               |
| 4  |      |          | 0.00                      | 0.00000              | -               |
| 5  |      |          | 0.00                      | 0.00000              | -               |
| 6  |      |          | 0.00                      | 0.00000              | -               |
| 7  | a    |          | 26.77                     | 0.20929              | YES             |

**vibrational spectrum**

| #  | mode | symmetry | wave number (cm\(^{-1}\)) | IR intensity (km/mol) | selection rules |
|----|------|----------|---------------------------|----------------------|-----------------|
| 1  |      |          | 0.00                      | 0.00000              | -               |
| 2  |      |          | 0.00                      | 0.00000              | -               |
| 3  |      |          | 0.00                      | 0.00000              | -               |
| 4  |      |          | 0.00                      | 0.00000              | -               |
| 5  |      |          | 0.00                      | 0.00000              | -               |
| 6  |      |          | 0.00                      | 0.00000              | -               |
| 7  | a    |          | 26.77                     | 0.20929              | YES             |
|   |   |         |         |        |     |     |
|---|---|---------|---------|--------|-----|-----|
|   | a | 35.17   | 0.34218 | YES    | YES |
| 9 | a | 43.76   | 0.07449 | YES    | YES |
| 10| a | 51.77   | 0.04781 | YES    | YES |
| 11| a | 56.52   | 0.02224 | YES    | YES |
| 12| a | 65.03   | 0.45307 | YES    | YES |
| 13| a | 75.62   | 0.26948 | YES    | YES |
| 14| a | 85.39   | 0.07668 | YES    | YES |
| 15| a | 94.89   | 1.43426 | YES    | YES |
| 16| a | 99.61   | 0.91990 | YES    | YES |
| 17| a | 104.50  | 0.18700 | YES    | YES |
| 18| a | 107.39  | 0.10932 | YES    | YES |
| 19| a | 139.09  | 0.09849 | YES    | YES |
| 20| a | 144.26  | 0.18890 | YES    | YES |
| 21| a | 160.21  | 1.62454 | YES    | YES |
| 22| a | 191.69  | 1.00490 | YES    | YES |
| 23| a | 214.21  | 1.03482 | YES    | YES |
| 24| a | 232.05  | 0.45241 | YES    | YES |
| 25| a | 285.99  | 2.11397 | YES    | YES |
| 26| a | 294.17  | 1.63832 | YES    | YES |
| 27| a | 303.39  | 2.14950 | YES    | YES |
| 28| a | 353.23  | 0.16027 | YES    | YES |
| 29| a | 365.44  | 1.32245 | YES    | YES |
| 30| a | 401.71  | 4.96093 | YES    | YES |
| 31| a | 416.92  | 0.44825 | YES    | YES |
| 32| a | 425.01  | 1.63155 | YES    | YES |
| 33| a | 443.83  | 0.90585 | YES    | YES |
| 34| a | 457.88  | 0.43720 | YES    | YES |
| 35| a | 459.00  | 0.25517 | YES    | YES |
| 36| a | 476.86  | 0.88823 | YES    | YES |
| 37| a | 479.54  | 4.53331 | YES    | YES |
| 38| a | 488.56  | 0.74087 | YES    | YES |
| 39| a | 503.99  | 5.66997 | YES    | YES |
| 40| a | 505.86  | 8.85895 | YES    | YES |
| 41| a | 520.33  | 11.79803| YES    | YES |
| 42| a | 537.67  | 2.67685 | YES    | YES |
| 43| a | 541.17  | 10.51813| YES    | YES |
| 44| a | 552.49  | 0.41224 | YES    | YES |
| 45| a | 558.84  | 0.56721 | YES    | YES |
| 46| a | 604.48  | 10.51765| YES    | YES |
| 47| a | 622.15  | 39.45123| YES    | YES |
| 48| a | 622.69  | 5.24592 | YES    | YES |
| 49| a | 628.44  | 20.32636| YES    | YES |
| 50| a | 633.02  | 19.60220| YES    | YES |
### SCF Energy (au) BP86/SV(P)
-2376.712862759

### SCF Energy (au) PBE0/def2-TZVPP
-2376.295538110

### SCF Energy (au) PBE0/def2-TZVPP (Toluene Correction)
-2376.3037174351

### Zero Point Energy (au)
0.2837056

### Chemical Potential (kJ mol⁻¹)
597.71

### Dispersion Correction (au)
PBE0/def2-TZVPP
-0.06440518

### xyz coordinates

| 41 | Mn  | 1.4841279 | 1.7117603 | 0.8161645 |
|----|-----|-----------|-----------|-----------|
|    | C   | 1.8347473 | 2.1095485 | 2.5732290 |
|    | C   | 3.1379523 | 1.0696799 | 0.5072899 |
|    | C   | 1.9390421 | 3.3004134 | 0.2278432 |
|    | O   | 2.2002880 | 4.3615391 | -0.1939786 |
|    | O   | 4.2031005 | 0.6530320 | 0.2834789 |
|    | O   | 2.0980604 | 2.3800517 | 3.6768443 |
|    | C   | -1.0912426 | 0.8955884 | 1.3618890 |
|    | C   | -1.2679949 | 3.1650984 | 0.8042767 |
|    | C   | -2.6571279 | 3.1446433 | 0.9918775 |
|    | C   | -3.2723958 | 1.9467289 | 1.3888197 |
|    | C   | -2.4757778 | 0.8045197 | 1.5771501 |
|    | C   | -0.1360325 | -0.2393286 | 1.5618573 |
|    | C   | 0.5855734 | -0.8182385 | 0.4695734 |
|    | C   | 1.3878778 | -1.9607722 | 0.7345586 |
|    | C   | 1.4896605 | -2.5042610 | 2.0172579 |
|    | C   | 0.7777799 | -1.9268438 | 3.0901668 |
|    | C   | -0.0303131 | -0.8122031 | 2.8587612 |
|    | H   | -0.7343996 | 4.0804218 | 0.5014531 |
|    | H   | -3.2424425 | 4.0630071 | 0.8290436 |
|    | H   | -4.3620244 | 1.8993039 | 1.5462304 |
|    | H   | -2.9154253 | -0.1586595 | 1.8792875 |
|    | H   | 1.9362159 | -2.4188131 | -0.1045801 |
|    | H   | 2.1299847 | -3.3849637 | 2.1900484 |
|    | H   | 0.8566168 | -2.3503587 | 4.1044705 |
|    | H   | -0.5971524 | -0.3585124 | 3.6884911 |
|    | N   | -0.5095354 | 2.0663137 | 0.9942040 |
|    | H   | 1.0145027 | 1.5569886 | -1.9830248 |
|    | C   | 0.9763957 | 1.0270270 | -1.0116645 |
|    | C   | 0.5225045 | -0.2547710 | -0.9302930 |
|    | C   | 0.0619967 | -1.1225549 | -2.049167 |
|    | C   | -0.8527700 | -2.7478115 | -4.1697179 |
|    | C   | -1.2287016 | -3.0580846 | -2.8570813 |
|    | C   | -0.7701515 | -2.2457407 | -1.8084125 |
|    | C   | 0.4233886 | -0.8492925 | -3.3891059 |
|    | C   | -0.0298422 | -1.6463722 | -4.4476822 |
|    | F   | -1.2820083 | -3.5260240 | -5.1857821 |
|    | H   | -1.8773332 | -3.9283335 | -2.6700729 |
|    | H   | -1.0765659 | -2.4870338 | -0.7772746 |
|    | H   | 1.0912536 | -0.0008119 | -3.6073525 |
|    | H   | 0.2581675 | -1.4362164 | -5.4897271 |

### Vibrational spectrum

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|-----------------|
| 1 |      |          | 0.00        | 0.00000      | -               |
| 2 |      |          | 0.00        | 0.00000      | -               |
| 3 |      |          | 0.00        | 0.00000      | -               |
| 4 |      |          | 0.00        | 0.00000      | -               |
| 5 |      |          | 0.00        | 0.00000      | -               |
| 6 |      |          | 0.00        | 0.00000      | -               |
| 7 | a    |          | 24.62       | 0.36777      | YES YES         |

$\text{vibrational spectrum}$
| 8 | a | 34.24 | 0.13052 | YES | YES |
| 9 | a | 40.74 | 0.50128 | YES | YES |
|10 | a | 52.69 | 0.03101 | YES | YES |
|11 | a | 53.24 | 0.17478 | YES | YES |
|12 | a | 71.92 | 1.11648 | YES | YES |
|13 | a | 76.77 | 0.25782 | YES | YES |
|14 | a | 83.21 | 0.23343 | YES | YES |
|15 | a | 89.53 | 0.46304 | YES | YES |
|16 | a | 93.28 | 0.18580 | YES | YES |
|17 | a | 97.80 | 0.77714 | YES | YES |
|18 | a | 103.60 | 0.00812 | YES | YES |
|19 | a | 137.41 | 1.20567 | YES | YES |
|20 | a | 153.58 | 0.57525 | YES | YES |
|21 | a | 171.04 | 1.05843 | YES | YES |
|22 | a | 203.77 | 0.97908 | YES | YES |
|23 | a | 207.67 | 0.08842 | YES | YES |
|24 | a | 243.63 | 0.46889 | YES | YES |
|25 | a | 260.86 | 0.45042 | YES | YES |
|26 | a | 303.88 | 1.62775 | YES | YES |
|27 | a | 320.42 | 1.57653 | YES | YES |
|28 | a | 340.64 | 0.35798 | YES | YES |
|29 | a | 357.53 | 0.88841 | YES | YES |
|30 | a | 395.13 | 2.68512 | YES | YES |
|31 | a | 412.39 | 0.02398 | YES | YES |
|32 | a | 424.94 | 0.63912 | YES | YES |
|33 | a | 435.67 | 3.16904 | YES | YES |
|34 | a | 457.09 | 0.86556 | YES | YES |
|35 | a | 462.47 | 0.17062 | YES | YES |
|36 | a | 475.11 | 1.19513 | YES | YES |
|37 | a | 487.90 | 3.87155 | YES | YES |
|38 | a | 496.79 | 17.14149 | YES | YES |
|39 | a | 503.35 | 5.61634 | YES | YES |
|40 | a | 517.87 | 11.40446 | YES | YES |
|41 | a | 525.85 | 8.38907 | YES | YES |
|42 | a | 536.67 | 2.63981 | YES | YES |
|43 | a | 544.98 | 3.90885 | YES | YES |
|44 | a | 563.85 | 6.90296 | YES | YES |
|45 | a | 605.97 | 20.59872 | YES | YES |
|46 | a | 615.23 | 21.57449 | YES | YES |
|47 | a | 622.45 | 6.64940 | YES | YES |
|48 | a | 624.34 | 31.15951 | YES | YES |
|49 | a | 631.27 | 3.33761 | YES | YES |
|50 | a | 635.77 | 17.39122 | YES | YES |
3bg

SCF Energy (au) BP86/SV(P)  -2614.359816251
SCF Energy (au) PBE0/def2-TZVPP  -2613.984795259
SCF Energy (au) PBE0/def2-TZVPP  -2613.992371345 (Toluene Correction)
Zero Point Energy (au)  0.2962443
Chemical Potential (kJ mol\(^{-1}\))  619.21
Dispersion Correction (au) PBE0/def2-TZVPP  -0.06852295

xyz coordinates
44

Mn  1.1861921  0.4233087  1.3165635
C   1.6496781  0.7318831  3.0615198
C   2.8324442 -0.1503251  0.8592402
C   1.5764145  2.0672875  0.8494133
O   1.8015756  3.1767450  0.5480063
O   3.8942168 -0.5116914  0.5419882
O   1.5764145  2.0672875  0.8494133
C   0.2601682 -2.1423136  1.0719082
C   1.0035837 -3.3393906  1.2618963
C   1.1376889 -3.9351896  2.5189698
C   0.5185693 -3.527583  3.6456958
C  -0.2463025 -2.1942099  3.4885463
H  -1.0640941  2.7313999  1.1019798
H  -3.5317034  2.7268438  1.6427157
H  -4.5812509  0.5846999  2.5276280
H  -3.1091275 -1.4598707  2.7922637
H   1.4842035 -3.7967404  0.3812146
H   1.709746 -4.8562239  2.6289410
H   0.6280887 -3.8119977  4.6413336
H  -0.7523739 -1.7459878  4.3605277
N  -0.7901591  0.7339893  1.6397458
C   0.4502444  0.3771908 -1.8134071
C   1.5031279  1.1820141 -2.3181999
C   1.4211083  1.7775904 -3.5819796
C   0.2699348  1.6042905 -4.3750452
C   -0.7943677  0.8213249 -3.8886097
C  -0.7019962  0.2157855 -2.6292994
H   2.4086376  1.3296299 -1.7098435
H   2.2543302  2.391246 -3.9533462
C   0.1970226  2.2168518 -5.7520544
H  -1.7037872  0.6935105 -4.4967259
H  -1.5460078 -0.3813972 -2.2477264
C   0.5271147 -0.2669150 -0.4950082
C   0.1438119 -1.5578492 -0.2905013
H  -0.1236005 -2.2496742 -1.1179296
F   0.9269758  3.3565088 -5.8407486
F  -1.0778491  2.5221585 -6.1055511
F   0.6739844  1.3706320 -6.7049893

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number cm\(^{-1}\) | IR intensity km/mol | selection rules |
|---|------|----------|---------------------------|---------------------|-----------------|
| 1 |      |          | 0.00                      | 0.00000             | -               |
| 2 |      |          | 0.00                      | 0.00000             | -               |
| 3 |      |          | 0.00                      | 0.00000             | -               |
| 4 |      |          | 0.00                      | 0.00000             | -               |
|   |   |   |   |
|---|---|---|---|
| 5 | 0.00 | 0.00000 | - |
| 6 | 0.00 | 0.00000 | - |
| 7 | a  | 21.16 | 0.19647 | YES | YES |
| 8 | a  | 30.62 | 0.37460 | YES | YES |
| 9 | a  | 34.38 | 0.08761 | YES | YES |
| 10| a   | 43.31 | 0.02830 | YES | YES |
| 11| a   | 45.44 | 0.00144 | YES | YES |
| 12| a   | 52.76 | 0.09202 | YES | YES |
| 13| a   | 61.15 | 0.48361 | YES | YES |
| 14| a   | 76.48 | 0.23164 | YES | YES |
| 15| a   | 85.17 | 0.06903 | YES | YES |
| 16| a   | 89.14 | 0.08270 | YES | YES |
| 17| a   | 94.28 | 1.18713 | YES | YES |
| 18| a   | 97.77 | 0.86356 | YES | YES |
| 19| a   | 105.08| 0.11509 | YES | YES |
| 20| a   | 115.00| 0.60942 | YES | YES |
| 21| a   | 124.46| 0.08990 | YES | YES |
| 22| a   | 142.91| 1.09096 | YES | YES |
| 23| a   | 165.52| 0.91736 | YES | YES |
| 24| a   | 193.41| 1.03521 | YES | YES |
| 25| a   | 206.99| 1.04327 | YES | YES |
| 26| a   | 209.37| 0.23505 | YES | YES |
| 27| a   | 246.59| 0.58105 | YES | YES |
| 28| a   | 289.94| 0.90528 | YES | YES |
| 29| a   | 302.57| 1.09223 | YES | YES |
| 30| a   | 311.33| 4.35150 | YES | YES |
| 31| a   | 353.49| 1.33456 | YES | YES |
| 32| a   | 365.35| 0.63782 | YES | YES |
| 33| a   | 388.01| 1.67649 | YES | YES |
| 34| a   | 403.34| 2.38918 | YES | YES |
| 35| a   | 406.95| 2.43588 | YES | YES |
| 36| a   | 423.41| 3.80656 | YES | YES |
| 37| a   | 443.59| 2.53152 | YES | YES |
| 38| a   | 455.39| 0.11763 | YES | YES |
| 39| a   | 459.59| 0.25725 | YES | YES |
| 40| a   | 476.40| 0.49494 | YES | YES |
| 41| a   | 480.99| 4.10822 | YES | YES |
| 42| a   | 492.52| 2.78660 | YES | YES |
| 43| a   | 505.99| 5.85205 | YES | YES |
| 44| a   | 506.58| 9.33807 | YES | YES |
| 45| a   | 528.92| 2.64916 | YES | YES |
| 46| a   | 535.96| 1.06907 | YES | YES |
| 47| a   | 549.17| 2.80493 | YES | YES |
| 48| a   | 552.38| 1.11732 | YES | YES |
| 49| a   | 568.97| 0.13806 | YES | YES |
| 50| a   | 576.26| 6.76105 | YES | YES |
SCF Energy (au) BP86/SV(P) -2614.357206437
SCF Energy (au) PBE0/def2-TZVPP -2613.982644347
SCF Energy (au) PBE0/def2-TZVPP -2613.990778406 (Toluene Correction)
Zero Point Energy (au) 0.2962383
Chemical Potential (kJ mol⁻¹) 618.34
Dispersion Correction (au) PBE0/def2-TZVPP 0.06781524

xyz coordinates

Mn 1.6001682 1.9660958 1.2084954
C 1.9402133 2.3601237 2.9702089
C 3.2552590 1.3172544 0.9168275
C 2.0678143 3.5539099 0.6260754
O 2.3383040 4.6136584 0.2077755
O 4.3208450 0.8957304 0.7063910
O 2.1966241 2.6283642 4.0754364
C -0.9835461 1.1633802 1.7461958
C -1.1452378 3.4336904 1.1871035
C -2.5350874 3.4209000 1.3699211
C -3.1584688 2.2264742 1.7648633
C -2.3692137 1.0798174 1.9566628
C -0.0337177 0.0245597 1.9488109
O 0.6938366 -0.5506656 0.8554969
C 1.5003815 -1.6897805 1.1248842
C 1.5970839 -2.2362874 2.4068790
C 0.8769778 -1.6642491 3.4769506
C 0.0669285 -0.5510369 3.2447207
H -0.6057135 4.3459505 0.8855869
H -3.1147598 4.3424036 1.2049079
H -4.2489407 2.1851419 1.9179131
H -8.2155056 0.1192388 2.2572971
H 2.0553274 -2.1439724 0.2879564
H 2.2393663 -3.1152472 2.5808171
H 0.9515830 -2.0904040 4.4904534
H -0.5043819 -0.1005059 4.0730469
N -0.3937996 2.3309129 1.3799587
H 1.1424550 1.8252016 -1.5900900
C 1.1010036 1.2923378 -0.6205604
C 0.6327642 0.0146024 -0.5412096
C 0.1520765 -0.8394015 -1.6544086
C -0.8006482 -2.4659841 -3.7918210
C -1.1247657 -2.7817152 -2.4594137
C -0.6540416 -1.9806723 -1.4108200
C 0.4642913 -0.5384421 -3.0052720
C -0.0045216 -1.3329374 -4.0560291
C -1.2384704 -3.3710109 -4.9169275
H -1.7555102 -3.6578757 -2.2413575
H -0.9280730 -2.2405682 -0.3753446
H 1.1037146 0.3290837 -3.2325959
H 0.2560351 -1.0779295 -5.0951339
F -0.3354706 -4.3639575 -5.1412764
F -1.3787107 -2.6995453 -6.0876251
F -2.4244684 -3.9766473 -4.6518171

$\textbf{vibrational spectrum}$

| # | mode | symmetry | wave number (cm⁻¹) | IR intensity (km/mol) | selection rules |
|---|------|---------|-------------------|----------------------|-----------------|
| 1 | 0.00 | 0.00000 | - | - |
| 2 | 0.00 | 0.00000 | - | - |
| 3 | 0.00 | 0.00000 | - | - |
| 4 | 0.00 | 0.00000 | - | - |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | a | 19.68 | 0.52294 | YES | YES |
| 8 | a | 26.46 | 0.13913 | YES | YES |
| 9 | a | 32.03 | 0.26819 | YES | YES |
| 10 | a | 41.65 | 0.40771 | YES | YES |
| 11 | a | 48.83 | 0.05953 | YES | YES |
| 12 | a | 53.68 | 0.29348 | YES | YES |
| 13 | a | 63.35 | 1.14071 | YES | YES |
| 14 | a | 73.77 | 0.06558 | YES | YES |
| 15 | a | 77.85 | 0.22656 | YES | YES |
| 16 | a | 84.33 | 0.31054 | YES | YES |
| 17 | a | 91.53 | 0.39077 | YES | YES |
| 18 | a | 95.57 | 0.57094 | YES | YES |
| 19 | a | 99.41 | 0.23112 | YES | YES |
| 20 | a | 120.35 | 1.01401 | YES | YES |
| 21 | a | 132.15 | 0.20509 | YES | YES |
| 22 | a | 159.95 | 0.84835 | YES | YES |
| 23 | a | 171.94 | 1.33900 | YES | YES |
| 24 | a | 186.84 | 0.47245 | YES | YES |
| 25 | a | 195.29 | 0.80549 | YES | YES |
| 26 | a | 221.48 | 0.38611 | YES | YES |
| 27 | a | 263.02 | 1.98195 | YES | YES |
| 28 | a | 267.54 | 0.28038 | YES | YES |
| 29 | a | 301.13 | 0.31184 | YES | YES |
| 30 | a | 323.00 | 3.63535 | YES | YES |
| 31 | a | 348.55 | 0.80659 | YES | YES |
| 32 | a | 361.83 | 2.92247 | YES | YES |
| 33 | a | 382.91 | 0.74989 | YES | YES |
| 34 | a | 397.60 | 2.23162 | YES | YES |
| 35 | a | 404.48 | 1.12542 | YES | YES |
| 36 | a | 432.96 | 8.21703 | YES | YES |
| 37 | a | 436.02 | 5.05123 | YES | YES |
| 38 | a | 458.17 | 3.76486 | YES | YES |
| 39 | a | 461.98 | 3.13311 | YES | YES |
| 40 | a | 474.49 | 1.24921 | YES | YES |
| 41 | a | 482.14 | 4.98839 | YES | YES |
| 42 | a | 491.52 | 1.26753 | YES | YES |
| 43 | a | 515.90 | 6.81848 | YES | YES |
| 44 | a | 521.01 | 9.17935 | YES | YES |
| 45 | a | 531.91 | 0.61700 | YES | YES |
| 46 | a | 543.89 | 4.41968 | YES | YES |
| 47 | a | 555.20 | 2.97278 | YES | YES |
| 48 | a | 565.14 | 1.58730 | YES | YES |
| 49 | a | 577.77 | 1.37054 | YES | YES |
| 50 | a | 593.16 | 2.46991 | YES | YES |
SCF Energy (au) BP86/SV(P) -2505.273702407
SCF Energy (au) PBE0/def2-TZVPP -2504.831435415
SCF Energy (au) PBE0/def2-TZVPP -2504.8417586438 (Toluene Correction)
Zero Point Energy (au) 0.3330534
Chemical Potential (kJ mol\(^{-1}\)) 713.51
Dispersion Correction (au) PBE0/def2-TZVPP -0.07112017

xyz coordinates

47

Mn  1.1127105  0.1658704  1.8333390
C   1.5835667  0.4652460  3.5777114
C   2.7580751 -0.4013803  1.3658922
C   1.4987726  1.8125468  1.3726203
O   1.7223402  2.9241475  1.0778646
O   3.8197636 -0.7593539  1.0442834
O   1.9126438  0.6717683  4.6772089
C  -1.4083933 -0.6864908  2.6225665
C  -1.6393087  1.5654795  2.0113434
C  -3.0045365  1.5549963  2.3260552
C  -3.5795623  0.3725487  2.8187640
C  -2.7685323 -0.7641869  2.9680342
C  -0.4628153 -1.8353476  2.7491352
C   0.1903774  1.3658922  1.3726203
C   1.4987726  1.8125468  1.3726203
C   1.4987726  1.8125468  1.3726203
C  -0.4628153 -1.8353476  2.7491352
C   0.1903774  1.3658922  1.3726203
C   1.4987726  1.8125468  1.3726203
C  -0.4628153 -1.8353476  2.7491352
C  -1.4083933 -0.6864908  2.6225665
H  -1.1382390  2.4694458  1.6301879
H  -3.6023673  2.4687759  2.1851321
H  -4.6500949  0.3322759  3.0769977
H  -3.1792429 -1.7176700  3.346265
H   1.4210940 -4.0452573  0.9058355
H   1.6643287 -5.1139616  3.149300
H   0.5510143 -4.0825979  5.1629201
H  -0.8324425 -2.0179584  4.8870611
N  -0.8633106  0.4723700  2.1681784
C   0.3546108  0.1156761 -1.2967836
C   1.3937879  0.9355107 -1.8095598
C   1.3014148  1.5103666 -3.0781817
C   0.1508371  1.3199446 -3.8747206
C  -0.8979050  0.5181877 -3.3735738
C  -0.7967238 -0.0741491 -2.1133860
H   2.2977957  1.0998998 -1.2026855
H   2.1238572  2.1399783 -3.4621786
C  -0.0148038  1.9274728 -5.2272940
H  -1.7927646  0.3752723 -3.9999790
H  -1.6273941 -0.6863229 -1.7237034
C   0.4438958 -0.5211862  0.0233078
C   0.0692481 -1.8140045  0.2365671
H  -0.1943918 -2.5108049 -0.5878937
O   1.0685248  2.6674624 -5.5973594
O  -0.9976746  1.7912167 -5.9403573
C   0.9803481  3.2813351 -6.8872879
H   1.9278126  3.8392272 -7.0223537
H   0.1117819  3.9733183 -6.938616
H   0.8645159  2.5147030 -7.6840296
| #  | mode | symmetry | wave number | IR intensity | selection rules |
|----|------|----------|-------------|--------------|-----------------|
|    |      | cm**(-1) | km/mol      |              |                 |
| 1  |      | 0.00     | 0.00000     | -            | -               |
| 2  |      | 0.00     | 0.00000     | -            | -               |
| 3  |      | 0.00     | 0.00000     | -            | -               |
| 4  |      | 0.00     | 0.00000     | -            | -               |
| 5  |      | 0.00     | 0.00000     | -            | -               |
| 6  |      | 0.00     | 0.00000     | -            | -               |
| 7  | a    | 21.47    | 0.25461     | YES          | YES             |
| 8  | a    | 29.01    | 0.98577     | YES          | YES             |
| 9  | a    | 36.31    | 1.24804     | YES          | YES             |
| 10 | a    | 43.19    | 0.04438     | YES          | YES             |
| 11 | a    | 49.37    | 0.17824     | YES          | YES             |
| 12 | a    | 60.58    | 0.47438     | YES          | YES             |
| 13 | a    | 72.51    | 0.60654     | YES          | YES             |
| 14 | a    | 76.70    | 0.17487     | YES          | YES             |
| 15 | a    | 83.77    | 0.35492     | YES          | YES             |
| 16 | a    | 85.91    | 0.04484     | YES          | YES             |
| 17 | a    | 94.45    | 1.25210     | YES          | YES             |
| 18 | a    | 96.61    | 0.86233     | YES          | YES             |
| 19 | a    | 104.33   | 0.04465     | YES          | YES             |
| 20 | a    | 110.46   | 0.11004     | YES          | YES             |
| 21 | a    | 116.69   | 0.76729     | YES          | YES             |
| 22 | a    | 122.66   | 0.49100     | YES          | YES             |
| 23 | a    | 145.17   | 0.74573     | YES          | YES             |
| 24 | a    | 155.67   | 0.42430     | YES          | YES             |
| 25 | a    | 165.40   | 1.94312     | YES          | YES             |
| 26 | a    | 196.82   | 0.30048     | YES          | YES             |
| 27 | a    | 202.74   | 2.62503     | YES          | YES             |
| 28 | a    | 231.80   | 0.93245     | YES          | YES             |
| 29 | a    | 265.95   | 4.40239     | YES          | YES             |
| 30 | a    | 291.06   | 0.35258     | YES          | YES             |
| 31 | a    | 300.26   | 8.23611     | YES          | YES             |
| 32 | a    | 319.46   | 10.79951    | YES          | YES             |
| 33 | a    | 335.23   | 2.25638     | YES          | YES             |
| 34 | a    | 360.78   | 1.49515     | YES          | YES             |
| 35 | a    | 397.04   | 0.64580     | YES          | YES             |
| 36 | a    | 410.01   | 0.38725     | YES          | YES             |
| 37 | a    | 415.09   | 1.68924     | YES          | YES             |
| 38 | a    | 434.16   | 1.71597     | YES          | YES             |
| 39 | a    | 448.98   | 0.27168     | YES          | YES             |
| 40 | a    | 458.05   | 0.85427     | YES          | YES             |
| 41 | a    | 471.42   | 3.20674     | YES          | YES             |
| 42 | a    | 476.46   | 0.29819     | YES          | YES             |
| 43 | a    | 483.71   | 5.55441     | YES          | YES             |
| 44 | a    | 493.53   | 4.04021     | YES          | YES             |
| 45 | a    | 507.03   | 9.25964     | YES          | YES             |
| 46 | a    | 509.77   | 7.06654     | YES          | YES             |
| 47 | a    | 536.07   | 0.97439     | YES          | YES             |
| 48 | a    | 541.46   | 5.73429     | YES          | YES             |
| 49 | a    | 550.95   | 1.47145     | YES          | YES             |
| 50 | a    | 560.15   | 1.29427     | YES          | YES             |
| 51 | a    | 581.11   | 3.81664     | YES          | YES             |
3bh'

SCF Energy (au) BP86/SV(P) -2505.271309102
SCF Energy (au) PBE0/def2-TZVPP -2504.82959821
SCF Energy (au) PBE0/def2-TZVPP -2504.84071336 (Toluene Correction)
Zero Point Energy (au) 0.3330903
Chemical Potential (kJ mol$^{-1}$) 712.91
Dispersion Correction (au) PBE0/def2-TZVPP -0.0705338

xyz coordinates
47
Mn 1.6951515 2.2430586 1.7176277
C 2.0101655 2.6557657 3.4800857
C 3.3595998 1.6083577 1.4508410
C 2.1535237 3.8297089 1.1245673
O 2.4173128 4.8883301 0.6988351
O 4.4319548 1.1965283 1.2556827
O 2.2528970 2.9349053 4.5857533
C -0.8911553 1.4255255 2.2317931
C -1.0636848 3.6857983 1.6372204
C -2.4562428 3.6626635 1.7969004
C -3.0754853 2.4682106 2.1983456
C -2.2793436 1.3318583 2.4201525
C 0.0665331 0.2994706 2.4640724
C 0.8181627 -0.2785311 1.3889900
C 1.6377436 -1.4017069 1.6847080
C 1.7222910 -1.9311725 2.9746488
C 0.9762750 -1.357444 4.0261294
C 0.1542544 -0.2591693 3.7681922
H -0.5275454 4.5985734 1.3312333
H -3.0414274 4.5761381 1.6082466
H -4.1680748 2.4187907 2.3328839
H -2.7219556 0.3712217 2.7259262
H 2.2111109 -1.8581712 0.8615820
H 2.3743136 -2.7985375 3.1693147
H 1.0405027 -1.7712958 5.0455614
H -0.4361572 0.1931152 4.5820178
N -0.3055626 2.5929144 1.8583711
H 1.2733847 2.0659007 -1.0847791
C 1.2260194 1.5444683 -0.1094272
C 0.7639596 0.2647934 -0.0173071
C 0.2863037 -0.6035700 -1.1187124
C -0.6827035 -2.2508569 -3.2398217
C -0.9766216 -2.5633958 -1.8956706
C -0.5001765 -1.7566044 -0.8571930
C 0.5785651 -0.3053822 -2.4761989
C 0.1032394 -1.1077699 -3.5164954
C -1.2145995 -3.1489235 -4.3044051
H -1.5907120 -3.4538243 -1.6870042
H -0.7510834 -2.0168623 0.1842040
H 1.2080316 0.5669184 -2.7138496
H 0.3471571 -0.8613470 -4.5608105
O -0.8560241 -2.7367563 -5.540155
O -1.8957086 -4.1438773 -4.1059219
C -1.3314246 -3.5532820 -6.6293140
H -2.4423585 -3.5923027 -6.6363219
H -0.9454243 -4.5917947 -6.5390658
H -0.9549812 -3.0801377 -7.5575728
| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|---|---|---|---|---|
| 1 | 0.00 | 0.00000 | - | - |
| 2 | 0.00 | 0.00000 | - | - |
| 3 | 0.00 | 0.00000 | - | - |
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | 17.32 | 0.40677 | YES | YES |
| 8 | 30.33 | 0.77351 | YES | YES |
| 9 | 33.68 | 1.59592 | YES | YES |
| 10 | 45.15 | 0.07589 | YES | YES |
| 11 | 52.02 | 0.21572 | YES | YES |
| 12 | 61.41 | 0.36558 | YES | YES |
| 13 | 69.80 | 2.06162 | YES | YES |
| 14 | 73.43 | 0.09241 | YES | YES |
| 15 | 79.52 | 0.14497 | YES | YES |
| 16 | 84.06 | 0.11968 | YES | YES |
| 17 | 91.95 | 0.36492 | YES | YES |
| 18 | 95.46 | 0.71358 | YES | YES |
| 19 | 98.89 | 0.16745 | YES | YES |
| 20 | 112.27 | 0.74477 | YES | YES |
| 21 | 119.97 | 0.79742 | YES | YES |
| 22 | 124.94 | 0.35669 | YES | YES |
| 23 | 152.47 | 0.60793 | YES | YES |
| 24 | 161.11 | 2.48913 | YES | YES |
| 25 | 169.65 | 0.53274 | YES | YES |
| 26 | 192.71 | 1.55445 | YES | YES |
| 27 | 205.35 | 0.68783 | YES | YES |
| 28 | 252.07 | 1.34069 | YES | YES |
| 29 | 257.35 | 1.83314 | YES | YES |
| 30 | 282.23 | 2.78482 | YES | YES |
| 31 | 304.70 | 1.73210 | YES | YES |
| 32 | 315.40 | 14.71030 | YES | YES |
| 33 | 335.86 | 5.17570 | YES | YES |
| 34 | 354.76 | 1.22162 | YES | YES |
| 35 | 369.92 | 0.72028 | YES | YES |
| 36 | 408.22 | 0.34369 | YES | YES |
| 37 | 431.27 | 5.32783 | YES | YES |
| 38 | 438.07 | 5.17158 | YES | YES |
| 39 | 456.80 | 1.67779 | YES | YES |
| 40 | 461.73 | 5.07869 | YES | YES |
| 41 | 474.36 | 1.72360 | YES | YES |
| 42 | 478.04 | 4.53376 | YES | YES |
| 43 | 478.84 | 3.91006 | YES | YES |
| 44 | 492.21 | 2.50350 | YES | YES |
| 45 | 516.49 | 8.45721 | YES | YES |
| 46 | 521.47 | 8.82860 | YES | YES |
| 47 | 532.75 | 0.54265 | YES | YES |
| 48 | 544.48 | 4.99197 | YES | YES |
| 49 | 561.64 | 3.10440 | YES | YES |
| 50 | 598.51 | 1.83620 | YES | YES |
**3bi**

SCF Energy (au) BP86/SV(P)  \(-2508.437513184\)

SCF Energy (au) PBE0/def2-TZVPP  \(-2507.961431247\)

SCF Energy (au) PBE0/def2-TZVPP  \(-2507.9706202452\) (Toluene Correction)

Zero Point Energy (au)  \(0.3703473\)

Chemical Potential (kJ mol\(^{-1}\))  \(811.94\)

Dispersion Correction (au) PBE0/def2-TZVPP  \(-0.08161133\)

**xyz coordinates**

|    |    |    |
|----|----|----|
|Mn  | 1.3161635 | 1.1650105 | 1.4833797 |
|C   | 1.6593210 | 1.4842760 | 3.2533358 |
|C   | 2.9754658 | 0.5498513 | 1.1511691 |
|C   | 1.7828870 | 2.7957704 | 1.0178426 |
|O   | 2.0615356 | 3.8928395 | 0.7197043 |
|O   | 4.0508324 | 0.1662239 | 0.9123884 |
|O   | 1.9147016 | 1.7039945 | 4.3703257 |
|C   | -1.2654764 | 0.4009478 | 2.0629745 |
|C   | -1.4245780 | 2.6380882 | 1.3808562 |
|C   | -2.8135249 | 2.6368021 | 1.5736835 |
|C   | -3.4361283 | 1.4687205 | 2.0420246 |
|C   | -2.6486650 | 0.3311229 | 2.290335 |
|C   | -0.3040279 | -0.7176535 | 2.8149407 |
|C   | 0.4669182 | -1.2705477 | 1.2171751 |
|C   | 1.3111559 | -2.3784035 | 1.5152922 |
|C   | 1.4018540 | -2.9126801 | 2.8009692 |
|C   | 0.6286248 | -2.3680511 | 3.8499410 |
|C   | -0.2175971 | -1.2889934 | 3.5942423 |
|H   | -0.8858776 | 3.5305258 | 1.0244945 |
|H   | -3.3930862 | 3.5481466 | 1.3592108 |
|H   | -4.5253477 | 1.4398180 | 2.2066012 |
|H   | -3.0952519 | -0.6107349 | 2.6451183 |
|H   | 1.8933520 | -2.8203291 | 0.6906032 |
|H   | 2.0741194 | -3.7644823 | 2.9952703 |
|H   | 0.6930241 | -2.7894471 | 4.8662471 |
|H   | -0.8236213 | -0.8558833 | 4.4069113 |
|N   | -0.6742083 | 1.5465764 | 1.6342579 |
|C   | 0.7019729 | 1.2990344 | -1.6199975 |
|C   | 1.8435003 | 1.9545775 | -2.1486610 |
|C   | 1.7585213 | 2.7274754 | -3.3162998 |
|C   | 0.5255875 | 2.8925712 | -3.9729487 |
|C   | -0.6211451 | 2.2676907 | -3.4516204 |
|C   | -0.5348133 | 1.4762490 | -2.2960780 |
|H   | 2.8126037 | 1.8416152 | -1.6360318 |
|H   | 2.6650371 | 3.2152519 | -3.7125717 |
|H   | 0.4580007 | 3.5111171 | -4.8832601 |
|H   | -1.5954982 | 2.3933875 | -3.9537007 |
|H   | -1.4352166 | 0.9794639 | -1.8993542 |
|C   | 0.7706214 | 0.5081032 | -0.3822832 |
|C   | 0.3582104 | -0.7845400 | -0.2063863 |
|C   | -0.0842868 | -1.7713981 | -1.2312206 |
|C   | -0.9525822 | -3.6806862 | -3.1567423 |
|C   | -1.4574443 | -3.7174792 | -1.8456476 |
|C   | -1.0252052 | -2.7783581 | -0.8960580 |
|C   | 0.4245111 | -1.7590372 | -2.5546917 |
|C   | -0.0064244 | -2.6984375 | -3.5026079 |
|H   | -1.2879851 | -4.1868489 | -3.9042361 |
|H   | -2.1964495 | -4.4845197 | -1.5584149 |
|H   | -1.4334390 | -2.8176048 | 0.1279640 |
|H   | 1.1795737 | -1.0088331 | -2.8347555 |
|H   | 0.4097852 | -2.6684663 | -4.5236090 |
| # | mode | symmetry | wave number (cm\(^{-1}\)) | IR intensity (km/mol) | IR intensity (km/mol) | selection rules |
|---|------|----------|-----------------------------|----------------------|----------------------|-----------------|
| 1 |      |          | 0.00                         | 0.00000              | -                    | -               |
| 2 |      |          | 0.00                         | 0.00000              | -                    | -               |
| 3 |      |          | 0.00                         | 0.00000              | -                    | -               |
| 4 |      |          | 0.00                         | 0.00000              | -                    | -               |
| 5 |      |          | 0.00                         | 0.00000              | -                    | -               |
| 6 |      |          | 0.00                         | 0.00000              | -                    | -               |
| 7 | a    |          | 25.86                        | 0.09436              | YES                  | YES             |
| 8 | a    |          | 29.50                        | 0.18490              | YES                  | YES             |
| 9 | a    |          | 40.32                        | 0.30306              | YES                  | YES             |
| 10| a    |          | 41.33                        | 0.44143              | YES                  | YES             |
| 11| a    |          | 52.94                        | 0.08549              | YES                  | YES             |
| 12| a    |          | 54.89                        | 0.03200              | YES                  | YES             |
| 13| a    |          | 59.74                        | 0.25229              | YES                  | YES             |
| 14| a    |          | 68.71                        | 0.07958              | YES                  | YES             |
| 15| a    |          | 77.02                        | 1.14270              | YES                  | YES             |
| 16| a    |          | 82.37                        | 0.69631              | YES                  | YES             |
| 17| a    |          | 86.47                        | 0.49161              | YES                  | YES             |
| 18| a    |          | 95.32                        | 0.27536              | YES                  | YES             |
| 19| a    |          | 97.69                        | 0.57342              | YES                  | YES             |
| 20| a    |          | 104.79                       | 0.29736              | YES                  | YES             |
| 21| a    |          | 108.64                       | 0.81777              | YES                  | YES             |
| 22| a    |          | 145.85                       | 0.50143              | YES                  | YES             |
| 23| a    |          | 161.14                       | 0.79578              | YES                  | YES             |
| 24| a    |          | 176.47                       | 0.59376              | YES                  | YES             |
| 25| a    |          | 190.30                       | 0.24471              | YES                  | YES             |
| 26| a    |          | 213.84                       | 0.19749              | YES                  | YES             |
| 27| a    |          | 222.98                       | 0.33355              | YES                  | YES             |
| 28| a    |          | 229.16                       | 0.75418              | YES                  | YES             |
| 29| a    |          | 250.61                       | 0.27012              | YES                  | YES             |
| 30| a    |          | 262.46                       | 0.46384              | YES                  | YES             |
| 31| a    |          | 322.56                       | 0.72430              | YES                  | YES             |
| 32| a    |          | 331.75                       | 1.46288              | YES                  | YES             |
| 33| a    |          | 362.43                       | 0.29753              | YES                  | YES             |
| 34| a    |          | 402.26                       | 0.16382              | YES                  | YES             |
| 35| a    |          | 405.84                       | 0.12806              | YES                  | YES             |
| 36| a    |          | 423.68                       | 4.33802              | YES                  | YES             |
| 37| a    |          | 440.44                       | 1.56353              | YES                  | YES             |
| 38| a    |          | 446.26                       | 0.33748              | YES                  | YES             |
| 39| a    |          | 456.75                       | 2.33162              | YES                  | YES             |
| 40| a    |          | 462.56                       | 0.15073              | YES                  | YES             |
| 41| a    |          | 478.00                       | 0.30726              | YES                  | YES             |
| 42| a    |          | 484.74                       | 4.15259              | YES                  | YES             |
| 43| a    |          | 494.31                       | 0.50231              | YES                  | YES             |
| 44| a    |          | 508.46                       | 6.46553              | YES                  | YES             |
| 45| a    |          | 517.55                       | 3.38325              | YES                  | YES             |
| 46| a    |          | 532.07                       | 3.93291              | YES                  | YES             |
| 47| a    |          | 540.44                       | 7.63454              | YES                  | YES             |
| 48| a    |          | 550.21                       | 2.02811              | YES                  | YES             |
| 49| a    |          | 571.73                       | 3.60312              | YES                  | YES             |
| 50| a    |          | 584.40                       | 11.80876             | YES                  | YES             |
SCF Energy (au) BP86/SV(P) -2360.901282159
SCF Energy (au) PBE0/def2-TZVPP -2360.472310505
SCF Energy (au) PBE0/def2-TZVPP -2360.4790774360 (Toluene Correction)
Zero Point Energy (au) 0.4322002
Chemical Potential (kJ mol\(^{-1}\)) 964.24
Dispersion Correction (au) PBE0/def2-TZVPP -0.07607291

xyz coordinates
55

Mn  1.1113667  1.3348724  1.5861612
C  1.4699877  1.6516653  3.3555589
C  2.8218391  0.9509411  1.1861731
C  1.3330937  3.0123303  1.1264244
O  1.4398562  4.1363383  0.8073253
O  3.9285700  0.7046753  0.910342
O  1.7404877  1.8868693  4.4664707
C  -1.3153556  0.1806963  2.1987127
C  -1.8014961  2.4149834  1.6870746
C  -3.1674101  2.2149889  1.9303737
C  -3.6086731  0.9444533  2.3338820
C  -2.6600703 -0.0889149  2.4701893
C  -0.2103162 -0.8145822  2.334299
C  0.5835278 -1.2038861  1.2030727
C  1.5696859 -2.2093300  1.410756
C  1.7680680 -2.8008236  2.6650358
C  0.9733459 -2.4150911  3.7657916
C  -0.0059727 -1.4356985  3.5963081
H  -1.4013997  3.3956176  1.3832849
H  -3.8705058  3.0535141  1.8076860
H  -4.6756997  0.7575646  2.5365705
H  -2.9662670 -1.1038212  2.7735359
H  -2.1907749 -2.5199581  0.5601292
H  -2.5487827 -3.5692345  2.7908357
H  -1.1263528 -2.8744258  4.7539492
H  -0.6310610 -1.1247324  4.4495925
N  -0.9007362  1.4207614  1.8281105
C  0.5340973  1.4830152 -1.5717078
C  0.6101608  0.6849800 -0.2971277
C  0.3643061 -0.6479498 -0.1797845
C  -0.0538543 -1.6305026 -1.2656334
C  1.9156541  1.8340703 -2.1693745
H  -0.0592331  0.9432910 -2.3493952
H  -0.0129976  2.4375429 -1.3802344
H  0.6437644 -2.5030730 -1.2694781
H  0.0528994 -1.1530217 -2.2640702
C  -1.4947183 -2.1614023 -1.1072581
C  -1.8910644 -3.1959064 -2.1738244
H  -2.2024189 -1.2998908 -1.1401389
H  -1.6118991 -2.6166206 -0.0945834
H  -1.1802749 -4.0550810 -2.1326536
H  -1.7624382 -2.7453962 -3.1863849
C  -3.3279942 -3.7127451 -2.0228591
H  -3.5784653 -4.4590346 -2.8089909
H  -4.0672098 -2.8831574 -2.1005283
H  -3.4804237 -4.2028354 -1.0343510
H  2.5166168  2.3866163 -1.4115243
C  1.8301680  2.6701349 -3.4563536
H  2.4734648  0.8892167 -2.3710670
C  3.2025361  3.0100677 -4.0528118
H  1.2735884  3.6134453 -3.2424775
H  1.2206595  2.1220902 -4.2137046
### Vibrational Spectrum

| #  | Mode | Symmetry | Wave Number (cm\(^{-1}\)) | IR Intensity (km/mol) | Selection Rules |
|----|------|----------|-----------------------------|-----------------------|-----------------|
| 1  | a    |           | 0.00                        | 0.00000               | YES             |
| 2  | a    |           | 0.00                        | 0.00000               | YES             |
| 3  | a    |           | 0.00                        | 0.00000               | YES             |
| 4  | a    |           | 0.00                        | 0.00000               | YES             |
| 5  | a    |           | 0.00                        | 0.00000               | YES             |
| 6  | a    |           | 0.00                        | 0.00000               | YES             |
| 7  | a    | a         | 13.34                       | 0.11283               | YES             |
| 8  | a    | a         | 25.09                       | 0.03129               | YES             |
| 9  | a    | a         | 28.09                       | 0.18786               | YES             |
| 10 | a    | a         | 37.85                       | 0.64049               | YES             |
| 11 | a    | a         | 45.03                       | 0.03562               | YES             |
| 12 | a    | a         | 53.49                       | 0.24346               | YES             |
| 13 | a    | a         | 58.99                       | 0.36465               | YES             |
| 14 | a    | a         | 64.03                       | 0.04008               | YES             |
| 15 | a    | a         | 68.06                       | 0.24588               | YES             |
| 16 | a    | a         | 79.99                       | 0.05926               | YES             |
| 17 | a    | a         | 84.38                       | 0.19486               | YES             |
| 18 | a    | a         | 92.13                       | 0.18692               | YES             |
| 19 | a    | a         | 94.47                       | 0.83761               | YES             |
| 20 | a    | a         | 99.23                       | 0.48696               | YES             |
| 21 | a    | a         | 101.84                      | 0.42884               | YES             |
| 22 | a    | a         | 111.75                      | 0.05655               | YES             |
| 23 | a    | a         | 118.00                      | 0.13203               | YES             |
| 24 | a    | a         | 125.34                      | 0.16412               | YES             |
| 25 | a    | a         | 135.14                      | 0.13516               | YES             |
| 26 | a    | a         | 170.14                      | 1.02048               | YES             |
| 27 | a    | a         | 182.18                      | 0.33801               | YES             |
| 28 | a    | a         | 193.07                      | 0.50594               | YES             |
| 29 | a    | a         | 213.09                      | 0.22804               | YES             |
| 30 | a    | a         | 224.04                      | 0.17526               | YES             |
| 31 | a    | a         | 241.41                      | 0.41886               | YES             |
| 32 | a    | a         | 247.48                      | 0.21790               | YES             |
| 33 | a    | a         | 257.31                      | 0.63362               | YES             |
| 34 | a    | a         | 287.43                      | 0.63535               | YES             |
| 35 | a    | a         | 300.51                      | 0.52641               | YES             |
| 36 | a    | a         | 317.16                      | 1.48427               | YES             |
| 37 | a    | a         | 343.56                      | 0.72950               | YES             |
| 38 | a    | a         | 357.13                      | 0.08179               | YES             |
| 39 | a    | a         | 385.22                      | 0.44102               | YES             |
| 40 | a    | a         | 417.12                      | 1.89289               | YES             |
| 41 | a    | a         | 428.70                      | 4.60147               | YES             |
| 42 | a    | a         | 458.93                      | 0.22510               | YES             |
| 43 | a    | a         | 459.65                      | 0.88291               | YES             |
| 44 | a    | a         | 468.59                      | 4.26916               | YES             |
| 45 | a    | a         | 474.45                      | 0.45687               | YES             |
| 46 | a    | a         | 484.48                      | 1.64184               | YES             |
| 47 | a    | a         | 495.02                      | 5.00263               | YES             |
| 48 | a    | a         | 510.81                      | 8.03576               | YES             |
| 49 | a    | a         | 527.80                      | 4.57164               | YES             |
| 50 | a    | a         | 536.42                      | 0.97409               | YES             |
3ca

SCF Energy (au) BP86/SV(P) -2678.222750796
SCF Energy (au) PBE0/def2-TZVPP -2677.741199140
SCF Energy (au) PBE0/def2-TZVPP -2677.753621288 (Toluene Correction)
Zero Point Energy (au) 0.4177735
Chemical Potential (kJ mol⁻¹) 922.06
Dispersion Correction (au) PBE0/def2-TZVPP -0.08529995

xyz coordinates

Mn 0.0636696 1.6111328 -0.8491924
C 1.5305880 2.1895400 0.0801886
C 1.0436225 0.5324623 -1.9059389
C 0.1688237 2.9320425 -2.0074271
O 0.2269811 3.8343760 -2.7520615
O 1.6792676 -0.1601746 -2.5968114
O 2.4830343 2.5639964 0.6417431
C -1.4234957 1.7436940 1.4825916
C -1.9635197 3.6789869 0.2797856
C -2.8252705 4.1154596 1.2951276
C -2.9710718 3.3305480 2.4511613
C -2.2573617 2.1245152 2.5466284
C -0.6267010 0.4849612 1.4533082
C -0.8050618 -0.4633337 0.4197156
C -0.1193440 -1.7697392 0.5270746
N 0.7698340 -1.9465157 1.6357918
C 0.9516228 -0.9885818 2.6165126
C 0.2530664 0.2037401 2.5436844
H -1.8053058 4.2625049 -0.6407915
H -3.3701369 5.0646763 1.1751830
H -3.6377278 3.6509903 3.2679992
H -2.3495205 1.4696870 3.4267453
O -0.2933570 -2.6860680 -0.2781717
C 1.9011784 -1.2733206 3.7489853
H 0.4115791 0.9607065 3.3249143
N -1.2724795 2.5243810 0.3818916
C -2.5266545 0.9478085 -2.6966211
C -2.0482630 1.4007388 -3.9528735
C -2.9215011 1.6046010 -5.0314184
C -4.3021051 1.3820620 -4.8814423
C -4.7995416 0.9453821 -3.6404103
C -3.9253567 0.7288513 -2.5653109
H -0.9691196 1.5761126 -4.0850712
H -2.5192581 1.9452965 -6.0002335
H -4.9887656 1.5536703 -5.7270793
H -5.8814529 0.7740495 -3.5079285
H -4.3226421 0.3985879 -1.5910971
C -1.6271725 0.7047443 -1.5632998
C -1.7629983 -0.3443478 -0.7046295
H -2.4346265 -1.2097105 -0.8829210
H 1.9823365 -0.3844132 4.4063731
H 2.9174770 -1.5269463 3.3760077
H 1.5564095 -2.1285800 4.3740081
C 1.4697500 -3.2492764 1.6847932
H 1.4258115 -3.6430046 2.7199194
C 2.9070780 -3.2156046 1.1879399
H 0.8632975 -3.9110563 1.0317846
C 5.5741048 -3.2363148 0.2415008
C 5.2677551 -3.7893264 1.4956591
C 3.9427165 -3.7747900 1.9648590
C 3.2231298 -2.6724219 -0.0763338
C 4.5476388 -2.6785393 -0.5415754
| #  | mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules |
|----|------|----------|----------------------|---------------------|-----------------|
| 1  |      |          | 0.00                 | 0.00000             | -               |
| 2  |      |          | 0.00                 | 0.00000             | -               |
| 3  |      |          | 0.00                 | 0.00000             | -               |
| 4  |      |          | 0.00                 | 0.00000             | -               |
| 5  |      |          | 0.00                 | 0.00000             | -               |
| 6  |      |          | 0.00                 | 0.00000             | -               |
| 7  | a    |          | 18.61                | 0.45792             | YES             |
| 8  | a    |          | 20.78                | 0.19310             | YES             |
| 9  | a    |          | 29.85                | 0.31391             | YES             |
| 10 | a    |          | 32.25                | 0.44016             | YES             |
| 11 | a    |          | 39.02                | 0.66850             | YES             |
| 12 | a    |          | 45.99                | 0.33234             | YES             |
| 13 | a    |          | 50.47                | 0.19399             | YES             |
| 14 | a    |          | 56.23                | 1.74737             | YES             |
| 15 | a    |          | 68.28                | 1.39703             | YES             |
| 16 | a    |          | 69.73                | 0.36509             | YES             |
| 17 | a    |          | 84.03                | 1.01838             | YES             |
| 18 | a    |          | 85.80                | 0.48941             | YES             |
| 19 | a    |          | 96.54                | 1.61114             | YES             |
| 20 | a    |          | 98.74                | 0.20719             | YES             |
| 21 | a    |          | 102.86               | 0.31583             | YES             |
| 22 | a    |          | 107.00               | 0.56136             | YES             |
| 23 | a    |          | 138.11               | 0.28842             | YES             |
| 24 | a    |          | 144.37               | 0.21805             | YES             |
| 25 | a    |          | 157.74               | 0.97101             | YES             |
| 26 | a    |          | 163.60               | 1.04911             | YES             |
| 27 | a    |          | 185.47               | 0.24484             | YES             |
| 28 | a    |          | 201.82               | 1.54103             | YES             |
| 29 | a    |          | 207.76               | 1.05400             | YES             |
| 30 | a    |          | 233.47               | 0.65986             | YES             |
| 31 | a    |          | 245.35               | 1.21255             | YES             |
| 32 | a    |          | 258.57               | 1.52062             | YES             |
| 33 | a    |          | 272.27               | 1.59868             | YES             |
| 34 | a    |          | 289.99               | 0.13259             | YES             |
| 35 | a    |          | 311.62               | 4.20087             | YES             |
| 36 | a    |          | 329.43               | 1.98900             | YES             |
| 37 | a    |          | 362.92               | 2.40152             | YES             |
| 38 | a    |          | 377.48               | 2.46814             | YES             |
| 39 | a    |          | 395.04               | 12.41401            | YES             |
| 40 | a    |          | 403.33               | 0.34388             | YES             |
| 41 | a    |          | 407.17               | 0.15896             | YES             |
| 42 | a    |          | 426.10               | 2.97114             | YES             |
| 43 | a    |          | 440.77               | 1.24828             | YES             |
| 44 | a    |          | 452.05               | 1.61406             | YES             |
| 45 | a    |          | 459.30               | 0.36019             | YES             |
| 46 | a    |          | 463.85               | 1.07994             | YES             |
| 47 | a    |          | 479.01               | 2.34965             | YES             |
| 48 | a    |          | 485.60               | 1.09251             | YES             |
| 49 | a    |          | 490.13               | 4.05355             | YES             |
| 50 | a    |          | 497.90               | 6.21632             | YES             |
3ca'
SCF Energy (au) BP86/SV(P) -2678.218280289
SCF Energy (au) PBE0/def2-TZVPP -2677.737373921
SCF Energy (au) PBE0/def2-TZVPP -2677.7503837273 (Toluene Correction)
Zero Point Energy (au) 0.4178331
Chemical Potential (kJ mol⁻¹) 923.56
Dispersion Correction (au) PBE0/def2-TZVPP 0.08515989

xyz coordinates
57

Mn  0.2297979  2.1745138 -1.3347197
C  1.6171610  2.8370070 -0.3315315
C  1.2911652  1.0907227 -2.2971892
C  0.3343992  3.4203114 -2.5789391
O  0.3609910  4.2469473 -3.4069981
O  1.9707290  0.3987678 -2.9452103
O  2.5256098  3.2620245  0.2634741
C  -1.4768114  2.3038411  0.8307032
C  -1.8780000  4.2761384 -0.3609654
C  -2.8525899  4.6790307  0.5633144
C  -3.1316419  3.8533537  1.6646649
C  -2.4288200  2.6441698  1.8034043
C  -0.6369008  3.4203114 -2.5789391
C  -0.7131995  0.1374552 -0.2162608
C  0.1030264 -1.0946837 -0.1478118
N  0.9108383 -1.2652747  1.0291886
C  0.9564707 -0.3417857  2.0553849
C  0.1983591  0.8129073  1.9730585
H  -1.6156147  4.8907832 -1.2371658
H  -3.3824773  5.6283450  0.4151367
H  -3.8916590  4.6151546  2.4072869
H  -2.6179118  1.9615775  2.6460739
O  0.1013544 -1.9604783 -1.0212301
C  1.8320981 -0.6166457  3.2481219
O  0.2658504  1.5549755  2.7813309
N  -1.2054328  3.1165711 -0.2206989
H  -1.9357513  1.5131526 -3.1078177
C  -1.3585129  1.2726871 -2.1953513
C  -1.6781994  0.2414852 -1.3724655
C  -2.7915273 -0.7316675 -1.4904575
H  1.8106211  0.2490556  3.9400695
H  2.8864511 -0.8003277  2.9471307
H  1.4896528 -1.5130903  3.8135666
C  1.6729266 -2.5335254  1.0922998
H  1.5523006 -2.9724171  2.1030852
C  3.1473011 -2.4144786  0.7377724
H  1.1659724 -3.1938085  0.3581996
C  5.8898231 -2.2723622  0.0562233
C  5.4959697 -2.8570271  1.2710702
C  4.1330585 -2.9234494  1.6086874
C  3.5518096 -1.8408847 -0.4872837
C  4.9135787 -1.7658983 -0.8204193
H  6.9582646 -2.2136907 -0.2098935
H  6.2524496 -3.2618886  1.9637387
H  3.8306678 -3.3859600  2.5648116
H  2.7967394 -1.4638642 -1.1954814
H  5.2116198 -1.3127252 -1.7801833
C  -4.9711082 -2.5509902 -1.6925383
C  -4.3148150 -2.3649062 -0.4643236
C  -3.2400184 -1.4672536 -0.3665762
C  -3.4592078 -0.9391965 -2.7228957
C  -4.5351303 -1.8314917 -2.8212454
| #  | mode | symmetry | wave number | IR intensity | selection rules |
|----|------|----------|-------------|--------------|-----------------|
| 1  |      |          | 0.00        | 0.00000      | -               |
| 2  |      |          | 0.00        | 0.00000      | -               |
| 3  |      |          | 0.00        | 0.00000      | -               |
| 4  |      |          | 0.00        | 0.00000      | -               |
| 5  |      |          | 0.00        | 0.00000      | -               |
| 6  |      |          | 0.00        | 0.00000      | -               |
| 7  | a    | a        | 19.21       | 0.16432      | YES             |
| 8  | a    | a        | 23.47       | 0.45449      | YES             |
| 9  | a    | a        | 29.88       | 0.64780      | YES             |
| 10 | a    | a        | 39.48       | 0.08769      | YES             |
| 11 | a    | a        | 42.64       | 0.43937      | YES             |
| 12 | a    | a        | 44.77       | 2.00535      | YES             |
| 13 | a    | a        | 49.07       | 0.67123      | YES             |
| 14 | a    | a        | 55.87       | 0.47658      | YES             |
| 15 | a    | a        | 69.43       | 1.32303      | YES             |
| 16 | a    | a        | 73.15       | 0.50441      | YES             |
| 17 | a    | a        | 81.07       | 0.52119      | YES             |
| 18 | a    | a        | 90.08       | 0.21952      | YES             |
| 19 | a    | a        | 94.00       | 0.36477      | YES             |
| 20 | a    | a        | 97.20       | 1.86791      | YES             |
| 21 | a    | a        | 101.54      | 0.45680      | YES             |
| 22 | a    | a        | 109.42      | 0.68332      | YES             |
| 23 | a    | a        | 137.50      | 0.11320      | YES             |
| 24 | a    | a        | 144.65      | 2.13129      | YES             |
| 25 | a    | a        | 160.28      | 0.50306      | YES             |
| 26 | a    | a        | 181.46      | 0.53773      | YES             |
| 27 | a    | a        | 191.63      | 0.15253      | YES             |
| 28 | a    | a        | 197.91      | 1.11741      | YES             |
| 29 | a    | a        | 224.72      | 1.58425      | YES             |
| 30 | a    | a        | 233.22      | 0.59602      | YES             |
| 31 | a    | a        | 240.86      | 0.33051      | YES             |
| 32 | a    | a        | 257.01      | 0.35306      | YES             |
| 33 | a    | a        | 262.34      | 1.02785      | YES             |
| 34 | a    | a        | 295.93      | 0.90626      | YES             |
| 35 | a    | a        | 316.02      | 0.73711      | YES             |
| 36 | a    | a        | 319.52      | 4.67888      | YES             |
| 37 | a    | a        | 361.51      | 1.02386      | YES             |
| 38 | a    | a        | 378.85      | 1.70818      | YES             |
| 39 | a    | a        | 403.51      | 0.14089      | YES             |
| 40 | a    | a        | 404.39      | 0.54864      | YES             |
| 41 | a    | a        | 422.33      | 1.59328      | YES             |
| 42 | a    | a        | 428.18      | 1.08852      | YES             |
| 43 | a    | a        | 434.15      | 6.12589      | YES             |
| 44 | a    | a        | 455.16      | 4.69089      | YES             |
| 45 | a    | a        | 463.52      | 0.55268      | YES             |
| 46 | a    | a        | 466.18      | 0.63456      | YES             |
| 47 | a    | a        | 477.75      | 2.37488      | YES             |
| 48 | a    | a        | 489.32      | 1.31633      | YES             |
| 49 | a    | a        | 491.10      | 3.15360      | YES             |
| 50 | a    | a        | 507.95      | 6.32814      | YES             |
### SCF Energy (au)

- BP86/SV(P) -2409.037058188
- PBE0/def2-TZVPP -2408.578577113
- PBE0/def2-TZVPP (Toluene Correction) -2408.5876200366

### Zero Point Energy (au)
0.3203729

### Chemical Potential (kJ mol\(^{-1}\))
693.96

### Dispersion Correction (au)
- PBE0/def2-TZVPP 0.06859816

### xyz coordinates

#### 45 Molecules

- Mn: 1.1173719, 1.0312839, 0.3566833
- C: 1.5853652, 1.5750691, 2.0338526
- C: 2.7562093, 0.3798074, -0.0005427
- C: 1.4880160, 2.624045, -0.3098843
- O: 1.6808120, 3.7068467, -0.7146336
- O: 3.8142952, -0.0423134, -0.2474111
- O: 1.9234554, 1.9382031, 3.0908395
- N: 0.0460866, -0.7976603, 1.111016
- C: 0.0622448, -1.7181936, -0.0254837
- C: 0.2544036, -2.9977070, 0.4507647
- C: 0.3053010, -2.9554018, 1.8977565
- H: 1.4764482, 3.2355907, 0.1375581
- H: -2.736911, 0.2736911, 1.4376583
- C: 0.0947015, -1.1989255, 3.6301130
- H: 0.5895501, 0.8093864, -2.7920829
- C: 1.7257682, 1.5142081, -3.2664243
- C: 1.7502745, 2.0697311, -4.5537556
- C: 0.6308816, 1.9615782, -5.3988076
- C: -0.5109802, 1.2790708, -4.9444412
- C: 0.5287534, 0.7059350, -3.6634394
- H: 2.6131224, 1.6035099, -2.6204160
- H: 2.6539177, 2.5990724, -4.8995892
- H: 0.6476101, 2.4121817, -6.4050893
- H: -1.3988180, 1.1925165, -5.5935540
- H: -1.4314143, 0.1808745, -3.3093448
- C: 0.5521816, 0.1851989, -1.4555397
- C: 0.0988969, -1.108811, -1.3318299
- H: -0.1416297, -1.7453257, -2.2054555
- C: 0.2843591, -2.1930636, 4.6094536
- H: -0.0474494, -0.1445334, 3.9121403
- H: 0.2843663, -1.9096302, 5.6742443
- C: 0.4924938, -3.5405921, 4.2422694
- H: 0.6490521, -4.2965513, 5.0294823
- C: 0.5065170, -3.9343051, 2.8944337
- H: 0.6691984, -4.9887601, 2.6185332

### Vibrational Spectrum

| # | mode | symmetry | wave number (cm\(^{-1}\)) | IR intensity (km/mol) | selection rules |
|---|------|---------|---------------------------|----------------------|-----------------|
| 1 |      |         | 0.00                      | 0.00000              | -               |
| 2 |      |         | 0.00                      | 0.00000              | -               |
| 3 |      |         | 0.00                      | 0.00000              | -               |
|   |   |   |   |   |
|---|---|---|---|---|
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | a | 28.92 | 0.40565 | YES | YES |
| 8 | a | 37.26 | 0.06249 | YES | YES |
| 9 | a | 46.50 | 0.25372 | YES | YES |
| 10 | a | 54.32 | 0.01770 | YES | YES |
| 11 | a | 60.74 | 0.30107 | YES | YES |
| 12 | a | 69.85 | 1.24702 | YES | YES |
| 13 | a | 74.70 | 0.45702 | YES | YES |
| 14 | a | 81.89 | 0.81541 | YES | YES |
| 15 | a | 84.73 | 0.24313 | YES | YES |
| 16 | a | 95.20 | 0.25017 | YES | YES |
| 17 | a | 98.42 | 0.55231 | YES | YES |
| 18 | a | 109.24 | 0.18919 | YES | YES |
| 19 | a | 141.07 | 0.11060 | YES | YES |
| 20 | a | 152.17 | 1.49613 | YES | YES |
| 21 | a | 180.10 | 1.27728 | YES | YES |
| 22 | a | 189.89 | 0.05206 | YES | YES |
| 23 | a | 208.92 | 0.97205 | YES | YES |
| 24 | a | 223.73 | 0.79529 | YES | YES |
| 25 | a | 261.43 | 0.47915 | YES | YES |
| 26 | a | 268.90 | 2.74244 | YES | YES |
| 27 | a | 286.18 | 0.52435 | YES | YES |
| 28 | a | 325.79 | 2.71826 | YES | YES |
| 29 | a | 363.13 | 0.70236 | YES | YES |
| 30 | a | 396.44 | 2.80952 | YES | YES |
| 31 | a | 406.95 | 1.05324 | YES | YES |
| 32 | a | 423.82 | 1.01802 | YES | YES |
| 33 | a | 435.22 | 11.95528 | YES | YES |
| 34 | a | 448.51 | 2.81685 | YES | YES |
| 35 | a | 459.52 | 2.65076 | YES | YES |
| 36 | a | 471.73 | 0.78697 | YES | YES |
| 37 | a | 481.06 | 0.16180 | YES | YES |
| 38 | a | 490.42 | 1.12418 | YES | YES |
| 39 | a | 493.26 | 0.25020 | YES | YES |
| 40 | a | 507.66 | 6.69919 | YES | YES |
| 41 | a | 517.95 | 6.01909 | YES | YES |
| 42 | a | 523.84 | 3.06030 | YES | YES |
| 43 | a | 538.84 | 2.98628 | YES | YES |
| 44 | a | 557.16 | 6.48803 | YES | YES |
| 45 | a | 576.80 | 1.67949 | YES | YES |
| 46 | a | 590.09 | 2.39371 | YES | YES |
| 47 | a | 596.12 | 0.77841 | YES | YES |
| 48 | a | 613.34 | 0.49274 | YES | YES |
| 49 | a | 615.28 | 7.44090 | YES | YES |
| 50 | a | 629.75 | 37.33445 | YES | YES |
SCF Energy (au) BP86/SV(P) -2409.034407606
SCF Energy (au) PBE0/def2-TZVPP -2408.576885875
SCF Energy (au) PBE0/def2-TZVPP -2408.5859493044 (Toluene Correction)
Zero Point Energy (au) 0.3203032
Chemical Potential (kJ mol$^{-1}$) 693.18
Dispersion Correction (au) PBE0/def2-TZVPP -0.06741973

xyz coordinates

| Element | X (Å) | Y (Å) | Z (Å) |
|---------|-------|-------|-------|
| Mn      | 1.4340079 | 1.9877711 | 0.3062720 |
| C       | 1.8611104 | 2.6173755 | 1.9720891 |
| C       | 3.0597099 | 1.2662607 | 0.0417952 |
| C       | 1.8808437 | 3.4962167 | -0.4980946 |
| O       | 2.1288308 | 4.4943936 | -1.0556917 |
| O       | 4.1060042 | 0.7903219 | -0.1480240 |
| O       | 2.1753840 | 3.0340469 | 3.0164158 |

$\$vibrational spectrum

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|----------------|
| 1 |      |          | 0.00        | 0.000000     | -              |
| 2 |      |          | 0.00        | 0.000000     | -              |
| 3 |      |          | 0.00        | 0.000000     | -              |
|   |     |        |        |      |      |
|---|-----|--------|--------|------|------|
| 4 | 0.00| 0.00000| - | - |
| 5 | 0.00| 0.00000| - | - |
| 6 | 0.00| 0.00000| - | - |
| 7 | 30.85| 0.31969| YES | YES |
| 8 | 38.66| 0.26769| YES | YES |
| 9 | 44.03| 0.45409| YES | YES |
| 10 | 50.44| 0.46117| YES | YES |
| 11 | 58.79| 0.13910| YES | YES |
| 12 | 70.56| 0.77444| YES | YES |
| 13 | 73.15| 0.79337| YES | YES |
| 14 | 79.09| 0.77549| YES | YES |
| 15 | 85.25| 0.31938| YES | YES |
| 16 | 89.55| 0.27598| YES | YES |
| 17 | 96.42| 0.02125| YES | YES |
| 18 | 98.81| 0.32592| YES | YES |
| 19 | 143.17| 0.26355| YES | YES |
| 20 | 148.26| 1.57227| YES | YES |
| 21 | 186.79| 0.69674| YES | YES |
| 22 | 201.64| 0.61927| YES | YES |
| 23 | 213.25| 0.94402| YES | YES |
| 24 | 243.77| 0.81043| YES | YES |
| 25 | 254.48| 0.62309| YES | YES |
| 26 | 265.85| 1.47357| YES | YES |
| 27 | 284.54| 2.00587| YES | YES |
| 28 | 321.31| 0.94779| YES | YES |
| 29 | 355.83| 1.61262| YES | YES |
| 30 | 405.73| 0.07009| YES | YES |
| 31 | 409.56| 3.84672| YES | YES |
| 32 | 424.95| 1.86710| YES | YES |
| 33 | 428.29| 0.73869| YES | YES |
| 34 | 435.15| 11.43486| YES | YES |
| 35 | 456.30| 2.74287| YES | YES |
| 36 | 469.32| 1.54325| YES | YES |
| 37 | 479.73| 0.92292| YES | YES |
| 38 | 480.02| 2.45529| YES | YES |
| 39 | 490.24| 1.33349| YES | YES |
| 40 | 510.11| 1.02306| YES | YES |
| 41 | 517.63| 12.22340| YES | YES |
| 42 | 535.70| 3.25324| YES | YES |
| 43 | 544.60| 13.91874| YES | YES |
| 44 | 559.29| 0.84540| YES | YES |
| 45 | 586.19| 12.01317| YES | YES |
| 46 | 591.95| 7.84937| YES | YES |
| 47 | 612.80| 1.80156| YES | YES |
| 48 | 614.86| 8.34012| YES | YES |
| 49 | 623.92| 17.83804| YES | YES |
| 50 | 629.15| 19.67110| YES | YES |
### 3ea

| Property                              | Value                  |
|---------------------------------------|------------------------|
| SCF Energy (au) BP86/SV(P)            | -2583.785980288        |
| SCF Energy (au) PBE0/def2-TZVPP (P)   | -2583.33956677         |
| SCF Energy (au) PBE0/def2-TZVPP       | -2583.3503113936 (Toluene Correction) |
| Zero Point Energy (au)                | 0.3875299              |
| Chemical Potential (kJ mol\(^{-1}\))  | 845.24                 |
| Dispersion Correction (au)            | 0.07468328             |

### xyz coordinates

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Mn      | 1.9651695    | 1.7154598    | -0.0109753   |
| C       | 2.3480792    | 2.1006590    | 1.7392816    |
| C       | 3.6973241    | 1.7465730    | -0.5034005   |
| C       | 1.7741513    | 3.3973560    | -0.4504732   |
| O       | 1.6051695    | 4.5182711    | -0.7493858   |
| O       | 4.8192058    | 1.7633187    | -0.8235393   |
| O       | 2.6033358    | 2.3533202    | 2.8488849    |
| C       | -0.4596660   | 0.2929554    | 0.834070     |
| C       | -1.8865719   | 0.1335204    | 1.1967370    |
| C       | 0.5060078    | -0.8137106   | 1.0092949    |
| C       | 1.4409848    | -1.1567847   | -0.0335687   |
| C       | 2.3040319    | -2.2512157   | 0.2004136    |
| C       | 2.3043143    | -2.9730490   | 1.4097088    |
| C       | 1.3855560    | -2.6246036   | 2.4298631    |
| C       | 0.4961805    | -1.5686285   | 2.2040837    |
| H       | 3.0127941    | -2.5634002   | -0.5827856   |
| O       | 3.2069497    | -3.9838538   | 1.5007735    |
| H       | 1.3545968    | -3.1654988   | 3.3862966    |
| H       | -0.2292973   | -1.3047793   | 2.9906630    |
| N       | 0.0196209    | 1.4114102    | 0.3521336    |
| C       | 1.4688948    | 1.2072974    | -3.1371296   |
| C       | 2.2378999    | 2.2996925    | -3.6143953   |
| C       | 2.1892361    | 2.6901570    | -4.9601881   |
| C       | 1.3497766    | 2.0180364    | -5.8664389   |
| C       | 0.5608614    | 0.9467961    | -5.4106367   |
| C       | 0.6209091    | 0.5470609    | -4.0678958   |
| H       | 2.8950311    | 2.8414346    | -2.9166392   |
| H       | 2.8091079    | 3.5353018    | -5.3038577   |
| H       | 1.3020567    | 2.3353389    | -6.9215125   |
| C       | -0.1133541   | 0.4207023    | -6.1077445   |
| C       | -0.0163634   | -0.2805926   | -3.7138587   |
| C       | 1.5237799    | 0.7697178    | -1.7339513   |
| C       | 1.4568059    | -0.5578925   | -1.3974224   |
| H       | 1.5804506    | -1.3178251   | -2.1995321   |
| C       | -4.6486942   | -0.1440778   | 1.8216597    |
| C       | -3.8957116   | -1.2585711   | 1.3794449    |
| C       | -2.5409938   | -1.1210499   | 1.0794103    |
| C       | -2.6500765   | 1.2351825    | 1.6485544    |
| C       | -4.0110524   | 1.1102307    | 1.9590232    |
| O       | -5.9571818   | -0.3790843   | 2.0947564    |
| H       | -4.4092359   | -2.2272115   | 1.2753295    |
| H       | -1.9733789   | -1.9956395   | 0.7236929    |
| H       | -2.1637524   | 2.2140225    | 1.7981964    |
| H       | -4.5601925   | 1.9905313    | 2.3235603    |
| H       | -0.6890552   | 2.1269921    | 0.1307717    |
| C       | -6.7749949   | 0.6979217    | 2.5289010    |
| H       | -6.4171042   | 1.1218142    | 3.4963019    |
| H       | -7.7888033   | 0.2737619    | 2.6716324    |
| H       | -6.8227436   | 1.5107816    | 1.7666559    |
| C       | 3.2675396    | -4.7477234   | 2.6950863    |
| H       | 2.3081708    | -5.2818123   | 2.8928381    |
| H       | 3.5230979    | -4.1143063   | 3.5769682    |
| #  | mode | symmetry | wave number (cm\(^{-1}\)) | IR intensity (km/mol) | selection rules |
|----|------|----------|---------------------------|----------------------|----------------|
| 1  |      |          | 0.00                      | 0.00000              | -              |
| 2  |      |          | 0.00                      | 0.00000              | -              |
| 3  |      |          | 0.00                      | 0.00000              | -              |
| 4  |      |          | 0.00                      | 0.00000              | -              |
| 5  |      |          | 0.00                      | 0.00000              | -              |
| 6  |      |          | 0.00                      | 0.00000              | -              |
| 7  | a    |          | 14.51                     | 0.31178              | YES            |
| 8  | a    |          | 20.08                     | 0.83075              | YES            |
| 9  | a    |          | 25.76                     | 0.14120              | YES            |
| 10 | a    |          | 37.40                     | 0.41839              | YES            |
| 11 | a    |          | 41.74                     | 0.36272              | YES            |
| 12 | a    |          | 49.73                     | 0.66072              | YES            |
| 13 | a    |          | 55.73                     | 0.02701              | YES            |
| 14 | a    |          | 59.24                     | 0.47353              | YES            |
| 15 | a    |          | 72.72                     | 1.11749              | YES            |
| 16 | a    |          | 82.52                     | 2.52930              | YES            |
| 17 | a    |          | 85.90                     | 0.32333              | YES            |
| 18 | a    |          | 88.22                     | 0.71131              | YES            |
| 19 | a    |          | 96.11                     | 0.90403              | YES            |
| 20 | a    |          | 103.97                    | 1.16949              | YES            |
| 21 | a    |          | 114.15                    | 0.83859              | YES            |
| 22 | a    |          | 128.32                    | 0.20179              | YES            |
| 23 | a    |          | 146.83                    | 0.31438              | YES            |
| 24 | a    |          | 151.89                    | 1.29281              | YES            |
| 25 | a    |          | 168.11                    | 4.09408              | YES            |
| 26 | a    |          | 179.42                    | 1.14541              | YES            |
| 27 | a    |          | 200.02                    | 0.38012              | YES            |
| 28 | a    |          | 207.62                    | 1.66963              | YES            |
| 29 | a    |          | 226.15                    | 1.86463              | YES            |
| 30 | a    |          | 235.19                    | 0.92040              | YES            |
| 31 | a    |          | 239.41                    | 4.04946              | YES            |
| 32 | a    |          | 255.06                    | 2.65217              | YES            |
| 33 | a    |          | 269.98                    | 4.48469              | YES            |
| 34 | a    |          | 295.05                    | 0.80520              | YES            |
| 35 | a    |          | 302.33                    | 8.55660              | YES            |
| 36 | a    |          | 321.72                    | 4.90520              | YES            |
| 37 | a    |          | 332.49                    | 0.29942              | YES            |
| 38 | a    |          | 369.86                    | 2.17629              | YES            |
| 39 | a    |          | 406.94                    | 0.53710              | YES            |
| 40 | a    |          | 414.79                    | 0.71808              | YES            |
| 41 | a    |          | 423.67                    | 13.01661             | YES            |
| 42 | a    |          | 438.34                    | 2.17459              | YES            |
| 43 | a    |          | 443.47                    | 3.37086              | YES            |
| 44 | a    |          | 459.10                    | 0.73837              | YES            |
| 45 | a    |          | 466.53                    | 1.15636              | YES            |
| 46 | a    |          | 479.54                    | 5.36961              | YES            |
| 47 | a    |          | 486.06                    | 4.36720              | YES            |
| 48 | a    |          | 487.99                    | 0.66771              | YES            |
| 49 | a    |          | 508.96                    | 4.99059              | YES            |
| 50 | a    |          | 517.77                    | 16.82526             | YES            |
3ea'

SCF Energy (au) BP86/SV(P) -2583.783208244
SCF Energy (au) PBE0/def2-TZVPP -2583.33805995
SCF Energy (au) PBE0/def2-TZVPP -2583.349064570 (Toluene Correction)
Zero Point Energy (au) 0.3874885
Chemical Potential (kJ mol⁻¹) 845.08
Dispersion Correction (au) PBE0/def2-TZVPP -0.0765516

xyz coordinates

Mn    2.2974223    2.1044248    0.4369364
C     2.5307348    2.4894570    2.2189721
C     3.9961773    1.5489878    0.2111146
C     2.6950408    3.7214756 -0.1135425
O     2.9172068    4.8004252 -0.5113261
O     5.0878474    1.1750973    0.0386081
O     2.7266135    2.7509417    3.338771
C     3.3667679    1.2586260    0.8293903
C     0.5650690    0.0931635    1.0974360
C     1.4190804    -1.5631004    0.0796196
C     2.2164628    -2.1378792    1.6817671
C     1.3580732    -1.6084829    2.6786297
C     0.5452219    -0.5219353    2.3808379
O     2.9172068    -3.1913069    2.06243
H     1.3581999    -2.0726174    3.676043
H    -0.1263325    -0.1178035    3.155722
N     0.3099283    2.3397319    0.4920302
H     2.0412466    1.8893515    2.3888246
C     1.9315377    1.3882431    1.4079445
C     1.4722862    0.1082100    1.3263266
C    -0.0934724    -0.7792518    2.4587611
C     0.3152161    -2.4467361    4.6381530
C    -0.1268456    -2.7283626    3.3346308
C     0.2589812    -1.9081774    2.623096
C     1.5376021    -0.5183121    3.7808919
C     1.1510932    -1.3346910    4.8523306
H     0.0166338    -3.0916677    5.4811835
C    -0.7832348    -3.5953591    3.1483465
C    -0.1036392    -2.1414395    1.2473626
C     2.2121393    0.3334013    3.9649028
C     1.5166260    -1.0715088    5.8679953
C    -0.2535891    3.1571260    0.2143462
C    -1.8001614    1.1572467    0.9782788
C    -4.6305559    0.9519304    1.2004177
C    -3.9975071    2.2132014    1.3019330
C    -2.6042064    2.3022971    1.1927338
C    -2.4532462    -0.1014638    0.8965114
C    -3.8394319    -0.2047556    0.9993735
O     5.9688860    0.7507156    1.2899569
H    -4.5802896    3.1284535    1.4809860
H    -2.1331432    3.2929831    1.3085166
H    -1.8544808    -1.0106545    0.7282756
H    -4.3478546    -1.1784593    0.9226608
C    -6.8248518    1.8678565    1.4820771
H    -7.8555108    1.4617076    1.5106249
H    -6.7418905    2.5971653    0.6426280
H    -6.6108553    2.3890134    2.4446946
C     3.8940188    -3.7532632    1.1255572
H     4.6405768    -3.0004128    0.7809828
H     3.3628970    -4.1761989    0.2411378
vibrational spectrum

| #  | mode | symmetry | wave number (cm^-1) | IR intensity (km/mol) | selection rules |
|----|------|----------|--------------------|----------------------|-----------------|
|    |      |          |                    |                      | IR  | RAMAN |
| 1  |      |          | 0.00               | 0.00000              | -   | -     |
| 2  |      |          | 0.00               | 0.00000              | -   | -     |
| 3  |      |          | 0.00               | 0.00000              | -   | -     |
| 4  |      |          | 0.00               | 0.00000              | -   | -     |
| 5  |      |          | 0.00               | 0.00000              | -   | -     |
| 6  |      |          | 0.00               | 0.00000              | -   | -     |
| 7  | a    |          | 15.63              | 0.19309              | YES | YES   |
| 8  | a    |          | 21.60              | 0.77485              | YES | YES   |
| 9  | a    |          | 27.86              | 0.18949              | YES | YES   |
| 10 | a    |          | 35.39              | 0.38876              | YES | YES   |
| 11 | a    |          | 41.33              | 0.19663              | YES | YES   |
| 12 | a    |          | 44.02              | 0.29313              | YES | YES   |
| 13 | a    |          | 46.80              | 0.16734              | YES | YES   |
| 14 | a    |          | 56.38              | 0.54129              | YES | YES   |
| 15 | a    |          | 66.90              | 0.05337              | YES | YES   |
| 16 | a    |          | 79.52              | 0.12712              | YES | YES   |
| 17 | a    |          | 82.08              | 0.21891              | YES | YES   |
| 18 | a    |          | 91.71              | 0.53619              | YES | YES   |
| 19 | a    |          | 94.79              | 0.47801              | YES | YES   |
| 20 | a    |          | 104.40             | 2.24284              | YES | YES   |
| 21 | a    |          | 118.46             | 1.63451              | YES | YES   |
| 22 | a    |          | 134.87             | 1.59926              | YES | YES   |
| 23 | a    |          | 146.93             | 1.29975              | YES | YES   |
| 24 | a    |          | 160.54             | 2.27608              | YES | YES   |
| 25 | a    |          | 164.22             | 0.42093              | YES | YES   |
| 26 | a    |          | 178.65             | 1.05013              | YES | YES   |
| 27 | a    |          | 184.01             | 0.32613              | YES | YES   |
| 28 | a    |          | 208.70             | 2.55452              | YES | YES   |
| 29 | a    |          | 212.55             | 0.03873              | YES | YES   |
| 30 | a    |          | 239.72             | 0.04436              | YES | YES   |
| 31 | a    |          | 260.67             | 0.38034              | YES | YES   |
| 32 | a    |          | 270.38             | 1.24015              | YES | YES   |
| 33 | a    |          | 272.85             | 4.07023              | YES | YES   |
| 34 | a    |          | 298.06             | 9.95050              | YES | YES   |
| 35 | a    |          | 313.32             | 0.41120              | YES | YES   |
| 36 | a    |          | 318.07             | 1.89895              | YES | YES   |
| 37 | a    |          | 342.89             | 2.41294              | YES | YES   |
| 38 | a    |          | 403.82             | 0.05490              | YES | YES   |
| 39 | a    |          | 411.48             | 0.65777              | YES | YES   |
| 40 | a    |          | 417.18             | 2.58456              | YES | YES   |
| 41 | a    |          | 423.43             | 8.11935              | YES | YES   |
| 42 | a    |          | 439.84             | 3.47479              | YES | YES   |
| 43 | a    |          | 453.26             | 0.80939              | YES | YES   |
| 44 | a    |          | 454.51             | 2.07382              | YES | YES   |
| 45 | a    |          | 462.67             | 2.46979              | YES | YES   |
| 46 | a    |          | 473.90             | 0.79383              | YES | YES   |
| 47 | a    |          | 486.97             | 4.80856              | YES | YES   |
| 48 | a    |          | 491.01             | 1.88003              | YES | YES   |
| 49 | a    |          | 508.87             | 18.13092             | YES | YES   |
| 50 | a    |          | 515.17             | 21.25998             | YES | YES   |
xyz coordinates
63

Mn  1.8614852  1.8272271  0.7600694
C  2.1430144  2.1835792  2.5350904
C  3.6016826  1.4888772  0.4378122
C  2.0500388  3.5079382  0.2825505
O  2.1338044  4.6332195 -0.0284058
O  4.7256063  1.2775391  0.2046422
C  2.3623552  2.4227320  3.6562518
C -0.6663726  0.7692076  1.3127486
C -2.1059430  0.5460214  1.5349114
C  0.3567525 -0.2822895  1.5951215
C  1.2683272 -0.7312598  0.5727640
C  2.2161006 -1.7194815  0.9236190
C  2.3031394 -2.2513658  2.2233758
C  1.3933620 -1.8126449  3.2182310
C  0.4345636 -0.8518925  2.8895608
H  2.9102648 -2.1009480  0.1590779
O  3.2741955 -3.177885  2.4271941
H  1.4299679 -2.2109247  4.2423712
O -0.2749580 -0.5153012  3.6629406
N -0.1318268  1.8801622  0.8840006
C  1.3685189  1.7584076 -2.3716643
C  2.4382710  2.5544955 -2.8558632
C  2.3323582  3.2495815 -4.0700113
C  1.1444819  3.1943154 -4.8210521
C  0.0650148 -0.8518925  2.8895608
C  0.1764819  1.7142486 -3.1433719
H  3.3698502  2.6152232 -2.2702919
H  3.1851013  3.8506290 -4.4281487
H  1.0581312  3.7523870 -5.7681421
H -0.8747790  2.3805308 -4.9221699
H -0.6704910  1.1094425 -2.7804303
C  1.4573975  1.0464670 -1.0879726
C  1.1980761 -0.2803654 -0.8690963
C  0.9720158 -1.3465352 -1.8889216
C -4.8941321  0.1039928  1.9039173
C -4.0078525 -0.9885286  1.7460380
C -2.6427381 -0.7687003  1.5695352
C -3.0037724  1.6266523  1.7078248
C -4.3771537  1.4209155  1.8878551
O -6.2033108 -0.2092240  2.0707061
H -4.4261663 -2.0069376  1.7604853
H -1.9693135 -1.6301234  1.4357209
H -2.6227897  2.6613351  1.7321583
H -5.0348254  2.2906856  2.0302847
H -0.7729605  2.6285282  0.5818223
C -7.1518246  0.8383416  2.2158342
H -6.9520461  1.4508053  3.1261551
H -8.1385144  0.3447221  2.319327
H -7.1681416  1.5035833  3.1209379
C  3.4333409 -3.7393500  3.7213342
H  2.5244138 -4.3010910  4.0423651
H  3.6718864 -2.9596801  4.4819780
| #  | mode | symmetry | wave number | IR intensity (cm\(^{-1}\)) | IR intensity (km/mol) | selection rules |
|----|------|----------|-------------|-----------------------------|-----------------------|-----------------|
| 1  |      |          | 0.00        | 0.00000                     | -                     | -               |
| 2  |      |          | 0.00        | 0.00000                     | -                     | -               |
| 3  |      |          | 0.00        | 0.00000                     | -                     | -               |
| 4  |      |          | 0.00        | 0.00000                     | -                     | -               |
| 5  |      |          | 0.00        | 0.00000                     | -                     | -               |
| 6  |      |          | 0.00        | 0.00000                     | -                     | -               |
| 7  | a    |          | 16.39       | 0.11460                     | YES                   | YES             |
| 8  | a    |          | 21.37       | 0.06926                     | YES                   | YES             |
| 9  | a    |          | 27.70       | 0.35408                     | YES                   | YES             |
| 10 | a    |          | 34.81       | 0.58605                     | YES                   | YES             |
| 11 | a    |          | 36.88       | 0.42762                     | YES                   | YES             |
| 12 | a    |          | 45.70       | 0.11059                     | YES                   | YES             |
| 13 | a    |          | 47.61       | 0.39275                     | YES                   | YES             |
| 14 | a    |          | 50.03       | 0.43572                     | YES                   | YES             |
| 15 | a    |          | 54.24       | 0.47325                     | YES                   | YES             |
| 16 | a    |          | 56.72       | 0.23312                     | YES                   | YES             |
| 17 | a    |          | 66.85       | 0.24090                     | YES                   | YES             |
| 18 | a    |          | 73.98       | 0.70798                     | YES                   | YES             |
| 19 | a    |          | 83.56       | 0.35825                     | YES                   | YES             |
| 20 | a    |          | 86.20       | 0.95309                     | YES                   | YES             |
| 21 | a    |          | 89.67       | 0.50301                     | YES                   | YES             |
| 22 | a    |          | 98.55       | 0.80454                     | YES                   | YES             |
| 23 | a    |          | 103.82      | 1.38037                     | YES                   | YES             |
| 24 | a    |          | 117.97      | 0.55286                     | YES                   | YES             |
| 25 | a    |          | 130.79      | 1.31610                     | YES                   | YES             |
| 26 | a    |          | 146.21      | 0.78006                     | YES                   | YES             |
| 27 | a    |          | 149.50      | 0.24248                     | YES                   | YES             |
| 28 | a    |          | 154.90      | 1.76928                     | YES                   | YES             |
| 29 | a    |          | 174.48      | 1.03601                     | YES                   | YES             |
| 30 | a    |          | 188.27      | 0.72738                     | YES                   | YES             |
| 31 | a    |          | 204.30      | 1.41449                     | YES                   | YES             |
| 32 | a    |          | 216.12      | 0.28070                     | YES                   | YES             |
| 33 | a    |          | 229.06      | 0.17449                     | YES                   | YES             |
| 34 | a    |          | 232.97      | 1.30367                     | YES                   | YES             |
| 35 | a    |          | 241.26      | 1.73607                     | YES                   | YES             |
| 36 | a    |          | 250.95      | 1.60374                     | YES                   | YES             |
| 37 | a    |          | 253.42      | 1.45897                     | YES                   | YES             |
| 38 | a    |          | 260.82      | 1.45105                     | YES                   | YES             |
| 39 | a    |          | 295.61      | 3.47743                     | YES                   | YES             |
| 40 | a    |          | 296.85      | 2.88335                     | YES                   | YES             |
| 41 | a    |          | 319.22      | 3.17226                     | YES                   | YES             |
| 42 | a    |          | 346.77      | 0.76517                     | YES                   | YES             |
| 43 | a    |          | 401.35      | 0.73305                     | YES                   | YES             |
| 44 | a    |          | 403.69      | 0.30821                     | YES                   | YES             |
| 45 | a    |          | 406.71      | 0.54868                     | YES                   | YES             |
| 46 | a    |          | 413.00      | 0.48532                     | YES                   | YES             |
| 47 | a    |          | 432.96      | 2.64496                     | YES                   | YES             |
| 48 | a    |          | 436.95      | 11.61757                    | YES                   | YES             |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 49 | a | 445.85 | 6.05936 | YES | YES |
| 50 | a | 458.16 | 3.03188 | YES | YES |
### SCF Energy (au) BP86/SV(P)
-2391.992336901

### SCF Energy (au) PBE0/def2-TZVPP
-2391.554013615

### SCF Energy (au) PBE0/def2-TZVPP
-2391.5628786450 (Toluene Correction)

### Zero Point Energy (au)
0.3230498

### Chemical Potential (kJ mol⁻¹)
696.59

### Dispersion Correction (au) PBE0/def2-TZVPP
0.06995959

### xyz coordinates

|   |   |   |   |
|---|---|---|---|
| Mn | 1.3893256 | 0.0876337 | 0.7929616 |
| C  | 1.9375193 | 0.2572834 | 2.5295937 |
| C  | 2.9494388 | -0.6115109 | 0.2520024 |
| C  | 1.9693035 | 1.6982189 | 0.3876714 |
| O  | 2.3914858 | 2.7574452 | 0.0123627 |
| O  | 3.9613387 | -1.0608219 | -0.1172982 |
| O  | 2.3248523 | 0.3716485 | 3.6248438 |
| C  | -1.1604195 | -0.6563062 | 1.6342081 |
| C  | -1.2997661 | 1.6357765 | 1.1543460 |
| C  | -2.6639989 | 1.6633687 | 1.5209604 |
| C  | -3.2631552 | 0.4780593 | 1.9666187 |
| C  | -2.5078469 | -0.7036217 | 2.0277464 |
| C  | -0.2731292 | -1.8579394 | 1.6496923 |
| C  | 0.9424123 | -3.6500144 | 0.5190256 |
| C  | 1.0927035 | -4.3297003 | 1.7297636 |
| C  | 0.5719453 | -3.7794209 | 2.9200566 |
| C  | -0.1155225 | -2.5682225 | 2.8710743 |
| O  | -0.5978210 | 2.6959424 | 0.7265859 |
| H  | -3.2432555 | 2.5949506 | 1.4605104 |
| H  | -4.3259905 | 0.4779088 | 2.2582762 |
| H  | -2.9490841 | -1.6574740 | 2.3522989 |
| H  | 1.3483386 | -4.0826774 | -0.4104427 |
| H  | 1.6229371 | -5.2962157 | 1.7540469 |
| H  | 0.6957706 | -4.3060604 | 3.8800926 |
| H  | -0.5497869 | -2.1386511 | 3.7905391 |
| N  | -0.5745361 | 0.4961078 | 1.2257988 |
| C  | 0.5399501 | 0.2680166 | -2.3132376 |
| C  | 1.6306738 | 1.0208220 | -2.8181526 |
| C  | 1.5528546 | 1.6673793 | -4.0605371 |
| C  | 0.3748659 | 1.6006528 | -4.8265155 |
| C  | -0.7237283 | 0.8716036 | -4.3376641 |
| C  | -0.6410425 | 0.2119474 | -3.105705 |
| H  | 2.5602130 | 1.0809591 | -2.2308591 |
| H  | 2.4224991 | 2.2343528 | -4.4334197 |
| H  | 0.3123101 | 2.1192231 | -5.7977797 |
| H  | -1.6560547 | 0.8162619 | -4.9252319 |
| H  | -1.5090957 | -0.3495544 | -2.7178697 |
| C  | 0.6145950 | -0.4458345 | -1.0281940 |
| C  | 0.1482964 | -1.7181938 | -0.8798387 |
| H  | -0.1964605 | -2.3395073 | -1.7343853 |
| C  | -1.2373878 | 3.9568516 | 0.5722660 |
| H  | -2.0652377 | 3.9017843 | -0.1713883 |
| H  | -0.4521083 | 4.6418740 | 0.1979794 |
| H  | -1.6277885 | 4.3362318 | 1.5445606 |

### $\text{vibrational spectrum}$

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|-----------------|
| 1 |      |          | 0.00        | 0.00000      | -               |
| 2 |      |          | 0.00        | 0.00000      | -               |
| 3 |      |          | 0.00        | 0.00000      | -               |
|   |   |     |     |     |     |
|---|---|-----|-----|-----|-----|
| 4 |   | 0.00 | 0.00000 | -   | -   |
| 5 |   | 0.00 | 0.00000 | -   | -   |
| 6 |   | 0.00 | 0.00000 | -   | -   |
| 7 | a | 28.02 | 0.61831 | YES | YES |
| 8 | a | 35.88 | 0.12888 | YES | YES |
| 9 | a | 40.30 | 0.55568 | YES | YES |
| 10| a | 46.39 | 0.18241 | YES | YES |
|11| a | 54.16 | 0.21157 | YES | YES |
|12| a | 59.73 | 0.20736 | YES | YES |
|13| a | 71.76 | 1.45852 | YES | YES |
|14| a | 79.33 | 0.73701 | YES | YES |
|15| a | 86.90 | 0.34167 | YES | YES |
|16| a | 95.76 | 0.47929 | YES | YES |
|17| a | 102.86 | 0.18488 | YES | YES |
|18| a | 115.16 | 0.56838 | YES | YES |
|19| a | 116.40 | 1.09103 | YES | YES |
|20| a | 136.46 | 0.21938 | YES | YES |
|21| a | 145.56 | 1.21576 | YES | YES |
|22| a | 170.97 | 0.23423 | YES | YES |
|23| a | 183.55 | 0.65378 | YES | YES |
|24| a | 191.89 | 0.07650 | YES | YES |
|25| a | 207.95 | 0.58322 | YES | YES |
|26| a | 236.01 | 0.87400 | YES | YES |
|27| a | 261.57 | 0.19107 | YES | YES |
|28| a | 268.32 | 0.04572 | YES | YES |
|29| a | 293.06 | 1.07449 | YES | YES |
|30| a | 314.39 | 0.85664 | YES | YES |
|31| a | 326.70 | 1.24900 | YES | YES |
|32| a | 359.74 | 1.05307 | YES | YES |
|33| a | 407.02 | 0.18747 | YES | YES |
|34| a | 411.91 | 1.53031 | YES | YES |
|35| a | 443.70 | 2.15286 | YES | YES |
|36| a | 454.02 | 2.16238 | YES | YES |
|37| a | 464.43 | 3.10826 | YES | YES |
|38| a | 470.00 | 2.56835 | YES | YES |
|39| a | 475.86 | 2.54220 | YES | YES |
|40| a | 482.34 | 5.04952 | YES | YES |
|41| a | 498.98 | 1.16430 | YES | YES |
|42| a | 517.77 | 5.41991 | YES | YES |
|43| a | 526.65 | 3.00938 | YES | YES |
|44| a | 538.96 | 3.75754 | YES | YES |
|45| a | 546.71 | 2.40756 | YES | YES |
|46| a | 552.90 | 6.08976 | YES | YES |
|47| a | 562.03 | 1.58074 | YES | YES |
|48| a | 587.33 | 1.67984 | YES | YES |
|49| a | 613.53 | 0.81749 | YES | YES |
|50| a | 621.75 | 26.77573 | YES | YES |
### SCF Energy (au)
- BP86/SV(P) -2391.990036695
- PBE0/def2-TZVPP -2391.52440556
- PBE0/def2-TZVPP -2391.561837702 (Toluene Correction)

### Zero Point Energy (au)
- 0.3230933

### Chemical Potential (kJ mol⁻¹)
- 696.35

### Dispersion Correction (au)
- PBE0/def2-TZVPP -0.06902345

### xyz coordinates

| Element | X (Å) | Y (Å) | Z (Å) |
|---------|-------|-------|-------|
| Mn      | 1.5958874 | 1.2194711 | 0.8192433 |
| C       | 1.9119078 | 1.6502330 | 2.5727878 |
| C       | 3.2396413 | 0.5500429 | 0.5694944 |
| C       | 2.1294424 | 2.7816886 | 0.2114912 |
| O       | 2.5047679 | 3.7997952 | -0.2258318 |
| O       | 4.3043764 | 0.1080234 | 0.3896308 |
| O       | 2.1565181 | 1.9463207 | 3.6751769 |

| Element | X (Å) | Y (Å) | Z (Å) |
|---------|-------|-------|-------|
| C       | -0.9726965 | 0.3512824 | 1.3474514 |
| C       | -1.2238104 | 2.6135044 | 0.7817135 |
| C       | -3.1820694 | 1.3119655 | 1.3556269 |
| C       | -2.3514676 | 0.1968959 | 1.5560837 |
| C       | 0.0240809 | -0.7483572 | 1.5464177 |
| O       | 0.7453824 | -1.3160323 | 0.449884 |
| O       | 1.5727749 | -2.4420447 | 0.7078335 |
| O       | 1.7033937 | -2.950288 | 1.9919739 |
| O       | 0.9959331 | -2.408745 | 3.0721509 |
| O       | 0.1598273 | -1.3105294 | 2.8459492 |
| O       | -0.5535451 | 3.7193529 | 0.4183955 |
| H       | -3.2624194 | 3.4138406 | 0.9785656 |
| H       | -4.2714651 | 1.2304532 | 1.5015322 |
| H       | -2.7555639 | -0.7817643 | 1.8540149 |
| H       | -2.1196722 | -2.8922407 | -0.1363837 |
| H       | -2.3642676 | -3.8411970 | 2.1611832 |
| H       | -1.0999333 | -2.8189897 | 4.0880986 |
| H       | -0.4065927 | -0.8644197 | 3.6795261 |
| N       | -0.4311686 | 1.5383193 | 0.9824148 |
| H       | 1.1435329 | 1.0777133 | -1.9829699 |
| C       | 1.1108779 | 0.5381239 | -1.0164736 |
| C       | 0.6659029 | -0.7479829 | 0.9481779 |
| C       | 0.1936539 | -1.6064361 | -2.0644108 |
| C       | -0.7616451 | -3.2272995 | -4.2059009 |
| C       | -1.0822533 | -3.5470289 | -2.8759322 |
| C       | -0.6110365 | -2.7482870 | -1.8214930 |
| C       | 0.5126253 | -1.3050842 | -3.4133187 |
| C       | 0.0393637 | -2.0992962 | -4.4663745 |
| H       | -1.1272918 | -3.8553737 | -5.0351199 |
| H       | -1.7094212 | -4.4272095 | -2.6544714 |
| H       | -0.8813878 | -3.0085416 | -0.7844734 |
| H       | 1.1592413 | -0.4402662 | -3.6334657 |
| H       | 0.3090477 | -1.8425405 | -5.5048191 |
| C       | -1.2657020 | 4.929144 | 0.1631691 |
| H       | -1.9903366 | 4.7973859 | -0.6740308 |
| H       | -0.4972931 | 5.6669884 | -0.1255121 |
| H       | -1.8012224 | 5.2805898 | 1.0731657 |

### Vibrational spectrum

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|----------------|
| 1 | 0.00 | 0.00000 | - | - | - |
| 2 | 0.00 | 0.00000 | - | - | - |
| 3 | 0.00 | 0.00000 | - | - | - |
| Value | a | Value | a | Value | a | Value | a | Value | a |
|-------|---|-------|---|-------|---|-------|---|-------|---|
| 4     | 0.00 | 6     | 0.00 | 7     | 26.43 | 8     | 36.00 | 9     | 39.31 | 10 | 46.99 | 11 | 53.88 | 12 | 57.99 | 13 | 78.15 | 14 | 79.22 | 15 | 86.49 | 16 | 92.13 | 17 | 96.91 | 18 | 109.81 | 19 | 112.58 | 20 | 134.50 | 21 | 151.79 | 22 | 172.87 | 23 | 194.28 | 24 | 198.29 | 25 | 218.11 | 26 | 241.18 | 27 | 259.58 | 28 | 270.76 | 29 | 285.93 | 30 | 300.73 | 31 | 330.64 | 32 | 371.83 | 33 | 404.19 | 34 | 414.83 | 35 | 442.03 | 36 | 458.75 | 37 | 466.64 | 38 | 471.52 | 39 | 473.56 | 40 | 477.32 | 41 | 495.82 | 42 | 524.09 | 43 | 527.91 | 44 | 544.34 | 45 | 551.51 | 46 | 572.66 | 47 | 585.87 | 48 | 605.12 | 49 | 612.62 | 50 | 616.40 |
**SCF Energy (au) BP86/SV(P)**
-2508.432275552

**SCF Energy (au) PBE0/def2-TZVPP**
-2507.958331998

**SCF Energy (au) PBE0/def2-TZVPP**
-2507.9668305178 (Toluene Correction)

**Zero Point Energy (au)**
0.3699565

**Chemical Potential (kJ mol^-1)**
811.35

**Dispersion Correction (au) PBE0/def2-TZVPP**
-0.08488781

**xyz coordinates**

| Element | x     | y     | z     |
|---------|-------|-------|-------|
| Mn      | 1.2727708 | -0.4332971 | 0.8077556 |
| C       | 1.7707572  | -0.1092857  | 2.5352243  |
| C       | 2.7991138  | -1.2895947  | 0.4156375  |
| C       | 2.0107523  | 1.0823652   | 0.2975907  |
| O       | 2.5731236  | 2.0592395   | -0.0167825 |
| O       | 3.7865517  | -1.8502685  | 0.1476760  |
| O       | 2.1262832  | 0.1019435   | 3.6266265  |
| C       | 1.2039849  | -1.1041463  | 1.6676312  |
| C       | 1.4695332  | 1.1863673   | 1.1855316  |
| C       | 2.7829765  | 1.1473506   | 0.6963750  |
| C       | 2.0838516  | -0.0465461  | 2.1956206  |
| C       | 2.505134   | -1.1959060  | 2.1787170  |
| C       | 3.216629   | -2.2851359  | 1.7060502  |
| C       | 3.7821341  | -4.2238243  | 0.6584667  |
| O       | 2.9927149  | -4.8035228  | 1.9103597  |
| C       | 0.5920323  | -4.1259705  | 3.0824595  |
| C       | -0.0546454 | -2.8940219  | 2.973010   |
| C       | -0.9384016 | 2.4744860  | 0.6543132  |
| H       | -3.3838601 | 2.0688994  | 1.6725252  |
| H       | -4.3432384 | -0.0855125 | 2.5848200  |
| H       | -2.8746612 | -2.1647186 | 2.5513275  |
| H       | 1.1086373  | -4.7475062 | -0.2551866 |
| H       | 1.4833475  | -5.7883762 | 1.9831589  |
| H       | 0.7690507  | -4.5707846 | 4.0745333  |
| H       | -0.4056870 | -2.3746036 | 3.8804688  |
| N       | -0.6960826 | 0.0637399  | 1.1885210  |
| C       | 0.5422277  | -0.4556476 | -2.3450926 |
| C       | 1.6806026  | 0.2122683  | -2.8646464 |
| C       | 1.6670712  | 0.7770619  | -4.1489600 |
| C       | 0.5086847  | 0.7121400  | -4.9474528 |
| C       | -0.6353203 | 0.0661173  | -4.4435357 |
| C       | -0.6175203 | -0.5107555 | -3.1649267 |
| H       | 2.5954765  | 0.2701861  | -2.2546878 |
| H       | 2.5725715  | 1.2772438  | -4.5319369 |
| H       | 0.4969203  | 1.1670741  | -5.9491877 |
| H       | -1.5526615 | 0.0133452  | -5.0541335 |
| H       | -1.5208462 | -1.0092120 | -2.7729391 |
| C       | 0.5483680  | -1.0846884 | -1.0123511 |
| C       | 0.0500190  | -2.3411793 | -0.8280562 |
| H       | -0.2844929 | -2.9933694 | -1.6624084 |
| C       | -0.1022246 | 4.9745170  | -0.3583789 |
| C       | -0.5250942 | 4.8634252  | 0.9777925  |
| C       | -0.9495964 | 3.6232699  | 1.4789414  |
| C       | -0.5122545 | 2.5952404  | -0.6859912 |
| C       | -0.0998301 | 3.8397572  | -1.1866599 |
| H       | 0.2288094  | 5.9491154  | -0.7537595 |
| H       | -0.5213643 | 5.7475064  | 1.6364710  |
| H       | -1.2756174 | 3.5363344  | 2.5289025  |
| H       | -0.5093230 | 1.7116159  | -1.3418794 |
| H       | 0.2304268  | 3.9172061  | -2.2349916 |
| #  | mode | symmetry | wave number cm**(-1) | IR intensity km/mol | IR | RAMAN |
|----|------|----------|----------------------|---------------------|----|-------|
| 1  |      |          | 0.00                 | 0.00000             | -  | -     |
| 2  |      |          | 0.00                 | 0.00000             | -  | -     |
| 3  |      |          | 0.00                 | 0.00000             | -  | -     |
| 4  |      |          | 0.00                 | 0.00000             | -  | -     |
| 5  |      |          | 0.00                 | 0.00000             | -  | -     |
| 6  |      |          | 0.00                 | 0.00000             | -  | -     |
| 7  | a    |          | 25.84                | 0.04845             | YES| YES   |
| 8  | a    |          | 26.55                | 0.02052             | YES| YES   |
| 9  | a    |          | 35.80                | 0.32049             | YES| YES   |
| 10 | a    |          | 39.25                | 0.03499             | YES| YES   |
| 11 | a    |          | 50.44                | 0.01163             | YES| YES   |
| 12 | a    |          | 54.68                | 0.65930             | YES| YES   |
| 13 | a    |          | 62.61                | 0.01939             | YES| YES   |
| 14 | a    |          | 69.07                | 0.26530             | YES| YES   |
| 15 | a    |          | 80.18                | 1.09165             | YES| YES   |
| 16 | a    |          | 83.57                | 0.18719             | YES| YES   |
| 17 | a    |          | 91.28                | 0.07543             | YES| YES   |
| 18 | a    |          | 106.38               | 0.19122             | YES| YES   |
| 19 | a    |          | 107.60               | 0.29624             | YES| YES   |
| 20 | a    |          | 110.51               | 0.06144             | YES| YES   |
| 21 | a    |          | 125.01               | 1.02495             | YES| YES   |
| 22 | a    |          | 143.88               | 0.26257             | YES| YES   |
| 23 | a    |          | 154.72               | 0.83859             | YES| YES   |
| 24 | a    |          | 173.13               | 1.39150             | YES| YES   |
| 25 | a    |          | 190.08               | 0.40542             | YES| YES   |
| 26 | a    |          | 198.81               | 0.17350             | YES| YES   |
| 27 | a    |          | 230.09               | 0.74020             | YES| YES   |
| 28 | a    |          | 258.49               | 0.10339             | YES| YES   |
| 29 | a    |          | 265.26               | 0.79766             | YES| YES   |
| 30 | a    |          | 299.31               | 0.13424             | YES| YES   |
| 31 | a    |          | 320.51               | 1.06814             | YES| YES   |
| 32 | a    |          | 345.08               | 1.58179             | YES| YES   |
| 33 | a    |          | 372.24               | 0.09462             | YES| YES   |
| 34 | a    |          | 379.45               | 1.38213             | YES| YES   |
| 35 | a    |          | 400.84               | 0.39030             | YES| YES   |
| 36 | a    |          | 406.61               | 0.47180             | YES| YES   |
| 37 | a    |          | 418.10               | 1.20687             | YES| YES   |
| 38 | a    |          | 448.19               | 0.52402             | YES| YES   |
| 39 | a    |          | 455.32               | 0.83848             | YES| YES   |
| 40 | a    |          | 466.65               | 0.88780             | YES| YES   |
| 41 | a    |          | 474.11               | 0.33446             | YES| YES   |
| 42 | a    |          | 489.02               | 4.93957             | YES| YES   |
| 43 | a    |          | 501.61               | 1.47829             | YES| YES   |
| 44 | a    |          | 503.21               | 11.56780            | YES| YES   |
| 45 | a    |          | 523.20               | 2.12663             | YES| YES   |
| 46 | a    |          | 532.27               | 2.99148             | YES| YES   |
| 47 | a    |          | 540.69               | 5.81623             | YES| YES   |
| 48 | a    |          | 546.42               | 3.39454             | YES| YES   |
| 49 | a    |          | 556.83               | 2.45245             | YES| YES   |
| 50 | a    |          | 559.84               | 2.16353             | YES| YES   |
3ga' Energy (au) BP86/SV(P) -2508.431196130
SCF Energy (au) PBE0/def2-TZVPP -2507.957419935
SCF Energy (au) PBE0/def2-TZVPP -2507.966554808 (Toluene Correction)
Zero Point Energy (au) 0.3699454
Chemical Potential (kJ mol⁻¹) 810.86
Dispersion Correction (au) PBE0/def2-TZVPP -0.08233166
xyz coordinates

Mn 1.5028971  0.4619076  0.8244350
C  1.8610594  0.9959175  2.5377272
C  3.0723701 -0.3902685  0.6581873
C  2.2134124  1.8824475  0.0628351
O  2.7210324  2.7732632 -0.4990363
O  4.0913041 -0.9452745  0.5388870
O  2.1319073  1.3619097  3.619335
C -1.0799484 -0.2214387  1.2500738
C -1.2802869  2.0496447  0.6658923
C -2.890924  1.9284475 -0.2214387
C -3.2912878  0.7052950  0.9841893
C -2.4703122 -0.3910427  1.2953473
C -0.1231398 -1.3378904  1.556186
O  0.5226403 -2.0672512  0.5052292
O  2.2369224 -3.2447021  0.8533463
O  1.3388621 -3.6695889  2.180907
C  0.7224657 -2.9332044  3.2154580
C -0.0086079 -1.7861231  2.9021516
C -0.6547343  3.3735215  0.4001200
H  3.2976659  2.8196640  0.453923
H -4.3890445  0.6080301  0.9977374
H  2.8993230 -1.3749234  1.5560449
H  1.7260810 -3.8169703  0.0487384
H  1.9121756 -4.5804815  2.4201307
H  0.8104040 -3.2633623  4.2631026
H -0.5171513 -1.2181188  3.6987699
N  0.5033870  0.9675818  0.9360635
H  1.0805268  0.2185027 -1.9755761
C  0.9985047 -0.2854715 -0.9926964
C  0.5072780 -1.5551744 -0.9051413
C  0.0395398 -2.4266975 -2.0123330
C -0.9095803 -4.0676480 -4.1396019
C -1.3142116 -4.3163081 -2.8172489
C -0.8461257 -3.5069520 -1.7695609
C  0.4428470 -2.1974358 -3.3524435
C -0.0275756 -3.0017621 -4.393144
H  1.2735282 -4.7034473 -4.9636520
H -2.0055557 -5.1473674 -2.5972979
H  1.1830726 -3.7081036 -0.7387922
H  1.1530767 -1.3830656 -3.5690219
H  0.3076621 -2.8027175 -5.4312424
C  0.4275050  5.9411982 -0.0593172
C  0.7627062  5.2324467  1.1068621
C  0.2286643  3.9558823  1.3363159
C  0.9986846  4.0989691 -0.7624859
C  0.4540578  5.3716305 -0.9938517
H  0.8562097  6.9404445 -0.2417441
H  1.4492572  5.6761343  1.8462932
H  0.4867038  3.4108470  2.2577910
H -1.6816539  3.6493267 -1.5025631
H -0.7159876  5.9197807 -1.9139531
| # | mode | symmetry | wave number cm$^{-1}$ | IR intensity km/mol | IR | RAMAN |
|---|------|---------|----------------------|---------------------|----|-------|
| 1 | 0.00 | 0.00000 | -                    | -                   |   |       |
| 2 | 0.00 | 0.00000 | -                    | -                   |   |       |
| 3 | 0.00 | 0.00000 | -                    | -                   |   |       |
| 4 | 0.00 | 0.00000 | -                    | -                   |   |       |
| 5 | 0.00 | 0.00000 | -                    | -                   |   |       |
| 6 | 0.00 | 0.00000 | -                    | -                   |   |       |
| 7 | a    | 21.80   | 0.16220              | YES                 | YES|       |
| 8 | a    | 28.64   | 0.04894              | YES                 | YES|       |
| 9 | a    | 36.93   | 0.20170              | YES                 | YES|       |
| 10| a    | 41.81   | 0.24131              | YES                 | YES|       |
| 11| a    | 46.48   | 0.08780              | YES                 | YES|       |
| 12| a    | 56.43   | 0.06689              | YES                 | YES|       |
| 13| a    | 63.55   | 0.47475              | YES                 | YES|       |
| 14| a    | 69.71   | 0.08274              | YES                 | YES|       |
| 15| a    | 80.44   | 0.85743              | YES                 | YES|       |
| 16| a    | 83.10   | 0.29376              | YES                 | YES|       |
| 17| a    | 90.96   | 0.67737              | YES                 | YES|       |
| 18| a    | 97.65   | 0.51042              | YES                 | YES|       |
| 19| a    | 104.49  | 0.67564              | YES                 | YES|       |
| 20| a    | 109.49  | 0.09221              | YES                 | YES|       |
| 21| a    | 121.43  | 0.40199              | YES                 | YES|       |
| 22| a    | 144.90  | 1.16747              | YES                 | YES|       |
| 23| a    | 160.09  | 0.03778              | YES                 | YES|       |
| 24| a    | 175.91  | 0.87185              | YES                 | YES|       |
| 25| a    | 202.30  | 0.09861              | YES                 | YES|       |
| 26| a    | 209.00  | 1.87276              | YES                 | YES|       |
| 27| a    | 232.32  | 0.56181              | YES                 | YES|       |
| 28| a    | 247.26  | 0.89539              | YES                 | YES|       |
| 29| a    | 279.58  | 0.06946              | YES                 | YES|       |
| 30| a    | 291.77  | 0.24440              | YES                 | YES|       |
| 31| a    | 317.63  | 0.51329              | YES                 | YES|       |
| 32| a    | 332.98  | 1.35842              | YES                 | YES|       |
| 33| a    | 354.30  | 0.79297              | YES                 | YES|       |
| 34| a    | 401.06  | 0.13085              | YES                 | YES|       |
| 35| a    | 402.72  | 1.42056              | YES                 | YES|       |
| 36| a    | 404.75  | 0.25181              | YES                 | YES|       |
| 37| a    | 414.04  | 1.99353              | YES                 | YES|       |
| 38| a    | 456.26  | 2.32840              | YES                 | YES|       |
| 39| a    | 458.63  | 0.40697              | YES                 | YES|       |
| 40| a    | 466.41  | 1.26669              | YES                 | YES|       |
| 41| a    | 473.63  | 2.91763              | YES                 | YES|       |
| 42| a    | 475.99  | 0.58484              | YES                 | YES|       |
| 43| a    | 495.71  | 3.10966              | YES                 | YES|       |
| 44| a    | 507.57  | 5.64543              | YES                 | YES|       |
| 45| a    | 522.33  | 11.32701             | YES                 | YES|       |
| 46| a    | 530.23  | 5.55672              | YES                 | YES|       |
| 47| a    | 542.98  | 9.38660              | YES                 | YES|       |
| 48| a    | 555.30  | 2.52328              | YES                 | YES|       |
| 49| a    | 573.57  | 6.35314              | YES                 | YES|       |
| 50| a    | 604.68  | 6.94203              | YES                 | YES|       |
3ha

SCF Energy (au) BP86/SV(P) -2354.896525758
SCF Energy (au) PBE0/def2-TZVPP -2354.447582458
SCF Energy (au) PBE0/def2-TZVPP -2354.4561647301 (Toluene Correction)
Zero Point Energy (au) 0.3247184
Chemical Potential (kJ mol$^{-1}$) 698.72
Dispersion Correction (au) PBE0/def2-TZVPP -0.0673463

Mn 1.8497483    1.1028289    0.4584999
C  2.3962619    1.3587991    2.1905971
C  3.5333785    0.9238504    -0.1600726
C  1.8660182    2.8121141    0.0884741
O  1.8382320    3.9560846    -0.1641401
O  2.7520255    1.5276083    3.2875670
C  -0.7054563   -0.0098118   1.3823506
C  -2.1394295   -0.0003492   1.7665265
C  -0.1106602   -1.2432892   1.4872944
C  -0.9370762   -1.6414085   0.3886999
C  -1.6651054   -2.8726502   0.5552985
C  -1.6208297   -3.6127402   1.7405413
C  -0.8141070   -3.1633551   2.8134205
C  -0.0544973   -2.0172268   2.6716295
H  2.2822125   -3.2274646   -0.2869896
H  2.2163630   -4.5362864   1.8305783
H  0.7747562   -3.7599084   3.7515646
H  -0.5937026  -1.6784784   3.4963007
N  -0.0911736   1.0514123   0.9302620
C  -1.0975114   0.7866837   -2.6460164
C  -1.9569420   1.8049844   -3.1326176
C  -1.8791743   2.2488333   -4.4603469
C  -0.9228710   1.7061809   -5.3368813
C  -0.0454810   0.7109950   -4.8701619
C  -0.1322518   0.2579281   -3.5462639
H  2.7068543   -2.4571892   -2.4577649
H  2.5690828   -3.0340286   -4.8122970
H  0.8536291   -2.0605866   -6.3769160
H  -0.7189774   0.2877369   -5.5436486
H  -0.5735378   -0.5073957   -3.1825160
C  -1.1784931   0.2943742   -1.2632088
C  -0.9589983  -1.0244135   -0.9561433
H  -0.9396469  -1.7668659   -1.7838619
C  -4.8945020   0.0414844   2.4180097
C  -4.3029510  -1.1350330   1.9253431
C  -2.9367949  -1.1594302   1.6077318
C  -2.7462638   1.1766638   2.2726661
C  -4.1106720   1.1961662   2.5941723
H  -5.9670312   0.0575576   2.6722177
H  -4.9124069  -2.0426069   1.7835704
H  -2.4797178  -2.0799137   1.2112054
H  -2.1355333   2.0780554   2.4498845
H  -4.5635049   2.1166377   2.9976601
H  -0.7005380   1.8694253   0.7741796

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number (cm$^{-1}$) | IR intensity (km/mol) | selection rules |
|---|------|----------|--------------------------|-----------------------|-----------------|
| 1 | 0.00 | 0.00000  | -                        | -                     | -               |
| 2 | 0.00 | 0.00000  | -                        | -                     | -               |
| 3 | 0.00 | 0.00000  | -                        | -                     | -               |
| 4 | 0.00 | 0.00000  | -                        | -                     | -               |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | a | 18.81 | 0.42118 | YES | YES |
| 8 | a | 25.24 | 0.76632 | YES | YES |
| 9 | a | 32.01 | 0.00412 | YES | YES |
| 10 | a | 48.45 | 0.03318 | YES | YES |
| 11 | a | 51.30 | 0.16810 | YES | YES |
| 12 | a | 54.97 | 0.07239 | YES | YES |
| 13 | a | 63.80 | 0.33920 | YES | YES |
| 14 | a | 76.09 | 0.46646 | YES | YES |
| 15 | a | 82.01 | 0.53374 | YES | YES |
| 16 | a | 87.47 | 0.05751 | YES | YES |
| 17 | a | 95.81 | 0.15715 | YES | YES |
| 18 | a | 101.62 | 0.38770 | YES | YES |
| 19 | a | 121.65 | 0.62825 | YES | YES |
| 20 | a | 133.09 | 0.95562 | YES | YES |
| 21 | a | 158.91 | 0.65598 | YES | YES |
| 22 | a | 171.28 | 2.93053 | YES | YES |
| 23 | a | 204.45 | 8.52771 | YES | YES |
| 24 | a | 221.24 | 1.12574 | YES | YES |
| 25 | a | 225.57 | 2.57217 | YES | YES |
| 26 | a | 260.72 | 3.30447 | YES | YES |
| 27 | a | 262.54 | 0.90363 | YES | YES |
| 28 | a | 291.03 | 1.30239 | YES | YES |
| 29 | a | 312.22 | 11.28529 | YES | YES |
| 30 | a | 400.73 | 1.19342 | YES | YES |
| 31 | a | 405.42 | 0.45457 | YES | YES |
| 32 | a | 407.19 | 1.70779 | YES | YES |
| 33 | a | 420.52 | 2.13785 | YES | YES |
| 34 | a | 443.09 | 0.05262 | YES | YES |
| 35 | a | 445.72 | 2.31478 | YES | YES |
| 36 | a | 454.94 | 1.77653 | YES | YES |
| 37 | a | 468.28 | 3.39004 | YES | YES |
| 38 | a | 476.13 | 8.41032 | YES | YES |
| 39 | a | 481.68 | 2.49903 | YES | YES |
| 40 | a | 505.35 | 3.70312 | YES | YES |
| 41 | a | 515.80 | 16.83659 | YES | YES |
| 42 | a | 529.78 | 2.98947 | YES | YES |
| 43 | a | 534.51 | 2.41560 | YES | YES |
| 44 | a | 557.25 | 0.74365 | YES | YES |
| 45 | a | 569.79 | 5.61717 | YES | YES |
| 46 | a | 587.36 | 23.70126 | YES | YES |
| 47 | a | 610.02 | 1.28155 | YES | YES |
| 48 | a | 613.01 | 5.13310 | YES | YES |
| 49 | a | 618.55 | 45.97154 | YES | YES |
| 50 | a | 622.16 | 29.74323 | YES | YES |
3ha'

SCF Energy (au) BP86/SV(P) -2354.891997893
SCF Energy (au) PBE0/def2-TZVPP -2354.444420890
SCF Energy (au) PBE0/def2-TZVPP -2354.4536324230 (Toluene Correction)
Zero Point Energy (au) 0.3244849
Chemical Potential (kJ mol\(^{-1}\)) 697.48
Dispersion Correction (au) PBE0/def2-TZVPP -0.06855975

xyz coordinates
45

| Element | X      | Y      | Z      | X      | Y      | Z      |
|---------|--------|--------|--------|--------|--------|--------|
| Mn      | 2.1473163 | 1.8360644 | 0.6549980 |
| C       | 2.5134529  | 2.0827923  | 2.4407545  |
| C       | 3.8276642  | 1.3205676  | 0.2474063  |
| C       | 2.5110158  | 3.4912763  | 0.2106829  |
| O       | 2.7127039  | 4.5988164  | -0.1110798 |
| O       | 4.9051974  | 0.9874349  | -0.0456415 |
| O       | 2.7825573  | 2.2571479  | 3.5616359  |
| C       | -0.5045838 | 1.0098222  | 1.1597239  |
| C       | 0.3466433  | -0.2156809 | 1.2987456  |
| C       | 1.1533074  | -0.6772435 | 0.2074169  |
| C       | 1.9544921  | -1.8298941 | 0.4274221  |
| C       | 1.1679062  | -2.0335724 | 2.7208425  |
| C       | 0.3570502  | -0.9098951 | 2.5354940  |

$\text{vibrational spectrum}$

| #  | mode | symmetry | wave number | IR intensity | selection rules |
|----|------|----------|-------------|--------------|----------------|
| 1  |      |          | 0.00  | 0.00000 | - | - |
| 2  |      |          | 0.00  | 0.00000 | - | - |
| 3  |      |          | 0.00  | 0.00000 | - | - |
|   | a  | 19.54 | 0.06232 | YES | YES |
|---|----|-------|---------|-----|-----|
| 8 | a  | 30.72 | 0.02671 | YES | YES |
| 9 | a  | 33.19 | 0.15313 | YES | YES |
| 10| a  | 35.77 | 0.03630 | YES | YES |
| 11| a  | 45.96 | 0.10263 | YES | YES |
| 12| a  | 48.02 | 0.04022 | YES | YES |
| 13| a  | 50.48 | 0.39725 | YES | YES |
| 14| a  | 74.21 | 0.99841 | YES | YES |
| 15| a  | 80.25 | 0.36004 | YES | YES |
| 16| a  | 82.52 | 0.06077 | YES | YES |
| 17| a  | 88.33 | 0.24855 | YES | YES |
| 18| a  | 98.18 | 0.28632 | YES | YES |
| 19| a  | 118.70| 0.07417 | YES | YES |
| 20| a  | 139.85| 0.35431 | YES | YES |
| 21| a  | 159.69| 2.51650 | YES | YES |
| 22| a  | 180.91| 1.89325 | YES | YES |
| 23| a  | 188.41| 0.83797 | YES | YES |
| 24| a  | 202.24| 0.22099 | YES | YES |
| 25| a  | 238.03| 1.15483 | YES | YES |
| 26| a  | 272.89| 5.68818 | YES | YES |
| 27| a  | 279.98| 3.23812 | YES | YES |
| 28| a  | 299.79| 0.96235 | YES | YES |
| 29| a  | 311.67| 1.93608 | YES | YES |
| 30| a  | 399.61| 0.79350 | YES | YES |
| 31| a  | 401.93| 0.55369 | YES | YES |
| 32| a  | 405.62| 1.29219 | YES | YES |
| 33| a  | 411.42| 4.36505 | YES | YES |
| 34| a  | 448.49| 2.32542 | YES | YES |
| 35| a  | 454.57| 0.33329 | YES | YES |
| 36| a  | 462.84| 0.31148 | YES | YES |
| 37| a  | 464.29| 11.86901| YES | YES |
| 38| a  | 473.01| 1.22050 | YES | YES |
| 39| a  | 481.32| 7.29869 | YES | YES |
| 40| a  | 509.53| 3.69401 | YES | YES |
| 41| a  | 516.36| 36.11068| YES | YES |
| 42| a  | 528.45| 2.40935 | YES | YES |
| 43| a  | 551.04| 3.74614 | YES | YES |
| 44| a  | 572.47| 7.19075 | YES | YES |
| 45| a  | 576.98| 21.92925| YES | YES |
| 46| a  | 607.33| 4.65353 | YES | YES |
| 47| a  | 609.16| 12.77565| YES | YES |
| 48| a  | 611.63| 38.74875| YES | YES |
| 49| a  | 614.73| 0.08764 | YES | YES |
| 50| a  | 621.80| 51.19677| YES | YES |
The document contains data for a chemical system, including SCF energies, chemical potential, zero point energy, and vibrational spectrum. The xyz coordinates of the system's atoms are also presented. The vibrational spectrum includes several modes with their wave numbers and IR intensities. The document is a representation of quantum chemical calculations for a specific chemical compound.
|   | a | 60.67 | 0.24551 | YES | YES |
|---|---|-------|---------|-----|-----|
| 12| a | 72.56 | 0.62244 | YES | YES |
| 13| a | 79.27 | 0.63032 | YES | YES |
| 14| a | 90.97 | 0.49506 | YES | YES |
| 15| a | 95.26 | 0.11903 | YES | YES |
| 16| a | 101.74| 0.77547 | YES | YES |
| 17| a | 111.63| 1.15725 | YES | YES |
| 18| a | 125.72| 0.62482 | YES | YES |
| 19| a | 152.51| 0.33523 | YES | YES |
| 20| a | 169.52| 8.67190 | YES | YES |
| 21| a | 192.37| 0.29482 | YES | YES |
| 22| a | 216.20| 10.1299 | YES | YES |
| 23| a | 232.41| 0.24448 | YES | YES |
| 24| a | 241.88| 0.75526 | YES | YES |
| 25| a | 252.52| 6.68820 | YES | YES |
| 26| a | 293.90| 4.90373 | YES | YES |
| 27| a | 353.55| 2.36095 | YES | YES |
| 28| a | 392.82| 1.60206 | YES | YES |
| 29| a | 406.09| 0.60766 | YES | YES |
| 30| a | 416.38| 3.11805 | YES | YES |
| 31| a | 431.45| 0.83475 | YES | YES |
| 32| a | 452.00| 0.63243 | YES | YES |
| 33| a | 467.01| 0.40503 | YES | YES |
| 34| a | 474.57| 3.83516 | YES | YES |
| 35| a | 487.49| 12.9932 | YES | YES |
| 36| a | 493.95| 0.21123 | YES | YES |
| 37| a | 520.07| 1.81214 | YES | YES |
| 38| a | 527.15| 5.65477 | YES | YES |
| 39| a | 533.50| 0.52258 | YES | YES |
| 40| a | 564.99| 3.57873 | YES | YES |
| 41| a | 579.71| 0.36755 | YES | YES |
| 42| a | 600.52| 1.20567 | YES | YES |
| 43| a | 611.17| 1.41382 | YES | YES |
| 44| a | 612.98| 25.26251 | YES | YES |
| 45| a | 621.48| 7.53164 | YES | YES |
| 46| a | 629.58| 25.23277 | YES | YES |
| 47| a | 645.56| 30.57528 | YES | YES |
| 48| a | 688.43| 28.37147 | YES | YES |
| 49| a | 697.66| 30.34196 | YES | YES |
| 50| a | 717.08| 11.57712 | YES | YES |
### SCF Energy (au) BP86/SV(P)
-2183.136961706

### SCF Energy (au) PBE0/def2-TZVPP
-2182.727556389

### SCF Energy (au) PBE0/def2-TZVPP
-2182.7350096537 (Toluene Correction)

### Zero Point Energy (au)
0.2598973

### Chemical Potential (kJ mol⁻¹)
537.84

### Dispersion Correction (au) PBE0/def2-TZVPP
-0.05187819

### xyz coordinates

| # | Atomic Symbol | X            | Y            | Z            |
|---|--------------|--------------|--------------|--------------|
| 37 | Mn           | 1.1456731    | 2.4084287    | 1.0514434    |
|    | C            | 1.2843480    | 3.0374348    | 2.7773269    |
|    | C            | 2.8931301    | 2.1414828    | 0.8561337    |
|    | C            | 1.3131216    | 4.0054815    | 0.3609113    |
|    | O            | 1.3955239    | 5.0598688    | -0.1377030   |
|    | O            | 4.0299225    | 1.9255071    | 0.7060206    |
|    | O            | 1.4135291    | 3.4230247    | 3.8688410    |
|    | C            | -1.5463574   | 1.2579627    | 1.3745898    |
|    | C            | -3.0483446   | 1.3691686    | 1.4009870    |
|    | C            | -0.8895210   | -0.0592515   | 1.6022068    |
|    | O            | 0.0720327    | -0.5659509   | 0.6705188    |
|    | C            | 0.6462642    | -1.8285931   | 0.9599993    |
|    | C            | 0.3247948    | -2.5445601   | 2.1197813    |
|    | C            | -0.6257246   | -2.0367553   | 3.0241373    |
|    | C            | -1.2423982   | -0.8129867   | 2.7495235    |
|    | H            | 1.3697638    | -2.2486436   | 0.2426544    |
|    | H            | 0.8152544    | -3.5120111   | 2.3177643    |
|    | H            | -0.8882081   | -2.5966910   | 3.9362526    |
|    | H            | -1.9917681   | -0.4121785   | 3.4530209    |
|    | O            | -0.8668938   | 2.2793093    | 1.1438564    |
|    | H            | -1.1975253   | 1.7970538    | -1.6421925   |
|    | C            | 0.9189164    | 1.4000598    | -0.6460373   |
|    | C            | 0.4425086    | 0.1143609    | -0.6185621   |
|    | C            | 0.3414973    | -0.7211797   | -1.8562369   |
|    | H            | -3.3556380   | 2.4322364    | 1.3398434    |
|    | H            | -3.4756974   | 0.9006292    | 2.3143817    |
|    | H            | -3.4705582   | 0.8113526    | 0.5333939    |
|    | C            | 0.0811686    | -2.2377162   | -4.2519088   |
|    | C            | -0.8457575   | -2.3966710   | -3.2071173   |
|    | C            | -0.7134116   | -1.6537369   | -2.0239658   |
|    | C            | 1.2731481    | -0.5851976   | -2.9146930   |
|    | C            | 1.1430398    | -1.3293998   | -4.0968532   |
|    | H            | -0.0187059   | -2.8250778   | -5.1797095   |
|    | H            | -1.6839069   | -3.1057620   | -3.3152054   |
|    | H            | -1.4534085   | -1.7869382   | -1.2170713   |
|    | H            | 2.1270325    | 0.1014898    | -2.7953285   |
|    | H            | 1.8881048    | -1.2072921   | -4.9010036   |

### Vibrational Spectrum

| # | Mode | Symmetry | Wave Number (cm⁻¹) | IR Intensity (km/mol) | IR Selection Rules | RAMAN Selection Rules |
|---|------|----------|-------------------|-----------------------|-------------------|-----------------------|
| 1 |      |          | 0.00              | 0.00000               |                   |                       |
| 2 |      |          | 0.00              | 0.00000               |                   |                       |
| 3 |      |          | 0.00              | 0.00000               |                   |                       |
| 4 |      |          | 0.00              | 0.00000               |                   |                       |
| 5 |      |          | 0.00              | 0.00000               |                   |                       |
| 6 |      |          | 0.00              | 0.00000               |                   |                       |
| 7 | a    |          | 11.03             | 0.04299               | YES               | YES                   |
| 8 | a    |          | 29.88             | 0.03834               | YES               | YES                   |
| 9 | a    |          | 43.82             | 0.16594               | YES               | YES                   |
| 10 | a    |          | 51.24             | 0.15355               | YES               | YES                   |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 11| a | 61.74 | 0.30398 | YES | YES |
| 12| a | 69.23 | 1.44302 | YES | YES |
| 13| a | 79.86 | 0.04878 | YES | YES |
| 14| a | 85.57 | 0.38966 | YES | YES |
| 15| a | 88.81 | 0.11878 | YES | YES |
| 16| a | 97.83 | 0.27936 | YES | YES |
| 17| a | 106.39 | 0.50957 | YES | YES |
| 18| a | 110.87 | 0.22317 | YES | YES |
| 19| a | 146.59 | 2.94774 | YES | YES |
| 20| a | 157.49 | 1.94876 | YES | YES |
| 21| a | 204.75 | 0.39131 | YES | YES |
| 22| a | 218.92 | 2.28317 | YES | YES |
| 23| a | 231.59 | 0.37369 | YES | YES |
| 24| a | 252.43 | 0.43101 | YES | YES |
| 25| a | 289.71 | 0.21352 | YES | YES |
| 26| a | 309.83 | 0.54719 | YES | YES |
| 27| a | 358.37 | 0.71677 | YES | YES |
| 28| a | 374.94 | 1.21258 | YES | YES |
| 29| a | 404.39 | 0.02014 | YES | YES |
| 30| a | 417.18 | 2.72831 | YES | YES |
| 31| a | 427.00 | 1.39593 | YES | YES |
| 32| a | 445.95 | 1.88235 | YES | YES |
| 33| a | 457.11 | 1.40503 | YES | YES |
| 34| a | 465.73 | 7.32504 | YES | YES |
| 35| a | 486.02 | 2.33309 | YES | YES |
| 36| a | 521.44 | 4.72483 | YES | YES |
| 37| a | 523.49 | 5.61477 | YES | YES |
| 38| a | 527.41 | 4.31855 | YES | YES |
| 39| a | 547.92 | 4.01688 | YES | YES |
| 40| a | 577.62 | 2.23764 | YES | YES |
| 41| a | 598.63 | 2.96917 | YES | YES |
| 42| a | 599.31 | 11.79126 | YES | YES |
| 43| a | 612.20 | 1.68466 | YES | YES |
| 44| a | 614.93 | 32.37495 | YES | YES |
| 45| a | 618.76 | 29.53671 | YES | YES |
| 46| a | 630.83 | 8.60057 | YES | YES |
| 47| a | 657.53 | 6.90263 | YES | YES |
| 48| a | 695.80 | 27.47499 | YES | YES |
| 49| a | 696.46 | 8.46114 | YES | YES |
| 50| a | 704.54 | 39.55734 | YES | YES |
3ja
SCF Energy (au) BP86/SV(P) -2452.103080854
SCF Energy (au) PBE0/def2-TZVPP -2451.641880652
SCF Energy (au) PBE0/def2-TZVPP -2451.6499605316 (Toluene Correction)
Zero Point Energy (au) 0.3448731
Chemical Potential (kJ mol\(^{-1}\)) 740.54
Dispersion Correction (au) PBE0/def2-TZVPP -0.06861384

xyz coordinates
48

Mn  1.6497721  1.3358800  0.5377851
C  2.2607111  1.1039574  2.2578338
C  3.2884896  1.2193251 -0.1490047
C  1.7869671  3.0934275  0.5737376
O  1.8781603  4.2597576  0.5697864
O  4.3558709  1.1265886 -0.6172802
O  2.6536735  0.9511328  3.3429371
C -1.0368873  0.4731728  1.4794316
C -2.3887641  0.7350323  2.0440928
C -0.4926578 -0.8470109  1.3727270
C  0.4605652 -1.186026  0.3999303
C  1.0481149 -2.566603  0.4574499
O  0.3496116  1.4707664  1.0859053
C  1.427704  2.6775180 -2.8692160
C  3.1776742 -4.1690384
C  2.4529686 -5.1285574
C -0.2254333  1.2226328 -4.7807425
C -0.7547222  0.7160695 -3.4848411
H  1.7997466  3.2520937 -2.1120276
H  1.5514070  4.1454229 -4.437168
H  0.2445661  2.8532503 -6.1490767
H -0.8099279  0.6599920 -5.5274730
H -0.551777  -0.2390094 -3.2066295
C  0.8194577  0.9109833 -1.1540798
C  0.7721341 -0.4483760 -0.8194785
H  1.1284006 -1.1315150 -1.6198489
H -0.8315661 -1.6271544  2.0700320
C  2.2169575 -5.1499094  0.5825091
C  2.988023 -4.0412065  0.1967011
C  2.4100757 -2.7654005  0.1273000
C  0.2826793 -3.6927490  0.8410522
C  0.8598144 -4.9705594  0.8999324
H  2.6713797 -6.1531857  0.6332252
H  4.0574584 -4.1677738 -0.0476822
H  3.0296920 -1.8999209 -0.1607391
H -0.7895347 -3.5740838  1.0665908
H  0.2402736 -5.8351928  1.1902115
C -4.9417765  1.3110561  3.1085565
C -4.5833454 -0.0176796  2.8192199
C -3.3178408 -0.3043725  2.2870562
C -2.7625783  2.0690374  2.3354150
C -4.0287738  2.3534290  2.8623771
H -5.9378888  1.5353865  3.5250813
H -5.2993217 -0.8358795  3.0019444
H -3.0572988 -1.3454709  2.0391041
H -2.0348341  2.8714214  2.1397768
H -4.3079682  3.3959661  3.0875984
## Vibrational Spectrum

| # | Mode | Symmetry | Wave Number (cm\(^{-1}\)) | IR Intensity (km/mol) | IR | Raman |
|---|------|----------|-----------------------------|----------------------|----|-------|
| 1 | 1    |          | 0.00                        | 0.00000              | -  | -     |
| 2 | 1    |          | 0.00                        | 0.00000              | -  | -     |
| 3 | 1    |          | 0.00                        | 0.00000              | -  | -     |
| 4 | 1    |          | 0.00                        | 0.00000              | -  | -     |
| 5 | 1    |          | 0.00                        | 0.00000              | -  | -     |
| 6 | 1    |          | 0.00                        | 0.00000              | -  | -     |
| 7 | 1    | a        | 14.61                       | 0.38846              | YES | YES |
| 8 | 1    | a        | 22.13                       | 1.40826              | YES | YES |
| 9 | 1    | a        | 29.62                       | 0.58524              | YES | YES |
| 10| 1    | a        | 35.83                       | 0.11973              | YES | YES |
| 11| 1    | a        | 37.15                       | 1.03095              | YES | YES |
| 12| 1    | a        | 45.28                       | 0.39974              | YES | YES |
| 13| 1    | a        | 51.69                       | 0.80298              | YES | YES |
| 14| 1    | a        | 53.97                       | 0.16678              | YES | YES |
| 15| 1    | a        | 59.96                       | 0.19192              | YES | YES |
| 16| 1    | a        | 83.78                       | 0.20446              | YES | YES |
| 17| 1    | a        | 88.78                       | 0.11842              | YES | YES |
| 18| 1    | a        | 94.65                       | 0.05377              | YES | YES |
| 19| 1    | a        | 108.34                      | 1.43645              | YES | YES |
| 20| 1    | a        | 112.52                      | 0.66592              | YES | YES |
| 21| 1    | a        | 121.74                      | 2.50328              | YES | YES |
| 22| 1    | a        | 137.87                      | 2.51867              | YES | YES |
| 23| 1    | a        | 154.04                      | 1.13695              | YES | YES |
| 24| 1    | a        | 159.72                      | 19.21260             | YES | YES |
| 25| 1    | a        | 208.77                      | 5.50424              | YES | YES |
| 26| 1    | a        | 223.45                      | 5.51475              | YES | YES |
| 27| 1    | a        | 236.61                      | 6.29007              | YES | YES |
| 28| 1    | a        | 244.48                      | 0.51186              | YES | YES |
| 29| 1    | a        | 263.63                      | 0.36410              | YES | YES |
| 30| 1    | a        | 300.33                      | 15.23751             | YES | YES |
| 31| 1    | a        | 315.45                      | 2.35486              | YES | YES |
| 32| 1    | a        | 354.74                      | 4.40350              | YES | YES |
| 33| 1    | a        | 399.79                      | 0.34017              | YES | YES |
| 34| 1    | a        | 401.89                      | 0.37964              | YES | YES |
| 35| 1    | a        | 404.00                      | 0.99737              | YES | YES |
| 36| 1    | a        | 410.72                      | 1.43291              | YES | YES |
| 37| 1    | a        | 432.02                      | 13.66021             | YES | YES |
| 38| 1    | a        | 444.42                      | 0.94919              | YES | YES |
| 39| 1    | a        | 449.20                      | 0.88613              | YES | YES |
| 40| 1    | a        | 469.99                      | 3.80862              | YES | YES |
| 41| 1    | a        | 476.01                      | 1.14658              | YES | YES |
| 42| 1    | a        | 490.75                      | 5.89549              | YES | YES |
| 43| 1    | a        | 511.19                      | 3.28314              | YES | YES |
| 44| 1    | a        | 523.69                      | 2.96840              | YES | YES |
| 45| 1    | a        | 532.69                      | 13.34996             | YES | YES |
| 46| 1    | a        | 537.60                      | 6.45739              | YES | YES |
| 47| 1    | a        | 571.53                      | 10.37027             | YES | YES |
| 48| 1    | a        | 595.22                      | 21.30454             | YES | YES |
| 49| 1    | a        | 600.42                      | 1.13653              | YES | YES |
| 50| 1    | a        | 609.38                      | 0.96738              | YES | YES |
SCF Energy (au) BP86/SV(P)                              -2183.167100726
SCF Energy (au) PBE0/def2-TZVPP                         -2182.760093970
SCF Energy (au) PBE0/def2-TZVPP                         -2182.7673435546 (Toluene Correction)
Zero Point Energy (au)                                    0.262048
Chemical Potential (kJ mol^{-1})                           552.88
Dispersion Correction (au) PBE0/def2-TZVPP               -0.05528328

xyz coordinates
37
C   0.5519872  -2.6912867  -1.2913389
C   0.2840276  -0.7130500  -2.8426551
C  -0.3152585   0.3674579  -0.0427651
C   2.6292711  -1.3094929  -1.9255555
C  -1.1180588  -1.5613016   1.0385935
C   -1.8861600 -2.6710730   1.4213656
C   -0.5344483  -2.8386193   3.4524914
C   0.2436599  -1.7263580   3.0576751
C   -0.0589658  -1.0903227   1.8545506
C   0.6506036   0.0696267   1.1437708
C   1.0179321   1.2176860   2.0832109
Mn  1.0064560  -0.9825830  -1.2152724
O   1.7826055  -0.4273318   0.4228709
O   0.2895606  -3.8286872  -1.2814776
O  -0.1846590  -0.4983389   3.894827
C  -1.1895038  -0.7156615  -0.1640049
O   3.6722692  -1.5186156   2.3927036
C  -1.5874721  -3.3030468   2.6447767
C  -1.9587835  -0.8286218  -0.9438598
C  -0.2589714   1.5834644  -0.8799974
C  -0.2088766   3.9319931  -2.4783775
C   0.9676993   3.4679743  -1.8653119
C   0.9489654   2.3093202  -1.0758683
C  -1.4363562   2.0636611  -1.5112907
C  -1.4104639   3.2233530  -2.2967212
H  -0.1902141   4.8431914  -3.0984616
H   1.9172306   4.0091726  -2.0092557
H   1.8825905   1.9313140  -0.6341402
H  -2.3891518   1.5325110  -1.3564038
H  -2.3404965   3.5823853  -2.7675948
H   1.0743472  -1.3783058   3.6934000
H  -0.3103288  -3.3497958   4.4034055
H  -2.1830567  -4.1722517   2.9692037
H  -2.7093477  -3.0381332   0.7864306
H   1.4649868   2.0723840   1.5358923
H   1.7650006   0.8569529   2.8231957
H   0.1213801   1.5800935   2.6317052

$vibrational spectrum$

| #  | mode | symmetry | wave number | IR intensity | selection rules |
|----|------|----------|-------------|--------------|-----------------|
| 1  | 0    | 0.00     | 0.00000     | -            | -               |
| 2  | 0    | 0.00     | 0.00000     | -            | -               |
| 3  | 0    | 0.00     | 0.00000     | -            | -               |
| 4  | 0    | 0.00     | 0.00000     | -            | -               |
| 5  | 0    | 0.00     | 0.00000     | -            | -               |
| 6  | 0    | 0.00     | 0.00000     | -            | -               |
| 7  | a    | 20.11    | 0.20072     | YES          | YES             |
| 8  | a    | 43.70    | 0.18262     | YES          | YES             |
| 9  | a    | 55.91    | 0.39403     | YES          | YES             |
| 10 | a    | 72.01    | 0.02060     | YES          | YES             |
|   | a |    |        |        |       |   |   |
|---|---|----|--------|--------|-------|---|---|
| 11| a | 78.66 | 0.27668 | YES    | YES   |
| 12| a | 86.20 | 0.40743 | YES    | YES   |
| 13| a | 91.56 | 0.15210 | YES    | YES   |
| 14| a | 99.13 | 0.43175 | YES    | YES   |
| 15| a | 106.62| 0.83380 | YES    | YES   |
| 16| a | 108.75| 0.38617 | YES    | YES   |
| 17| a | 124.81| 0.80891 | YES    | YES   |
| 18| a | 173.83| 1.02082 | YES    | YES   |
| 19| a | 187.33| 0.44146 | YES    | YES   |
| 20| a | 208.12| 0.11055 | YES    | YES   |
| 21| a | 236.87| 0.28880 | YES    | YES   |
| 22| a | 250.26| 0.29553 | YES    | YES   |
| 23| a | 262.29| 2.69722 | YES    | YES   |
| 24| a | 276.55| 0.22091 | YES    | YES   |
| 25| a | 311.10| 7.63204 | YES    | YES   |
| 26| a | 335.74| 4.50892 | YES    | YES   |
| 27| a | 358.90| 3.92761 | YES    | YES   |
| 28| a | 409.49| 0.48452 | YES    | YES   |
| 29| a | 415.74| 1.38512 | YES    | YES   |
| 30| a | 441.65| 6.35928 | YES    | YES   |
| 31| a | 449.05| 0.51048 | YES    | YES   |
| 32| a | 464.02| 4.18320 | YES    | YES   |
| 33| a | 477.83| 10.23579| YES    | YES   |
| 34| a | 484.00| 5.78995 | YES    | YES   |
| 35| a | 503.35| 9.08164 | YES    | YES   |
| 36| a | 521.28| 8.94887 | YES    | YES   |
| 37| a | 532.86| 1.55631 | YES    | YES   |
| 38| a | 556.82| 8.49744 | YES    | YES   |
| 39| a | 560.73| 5.82532 | YES    | YES   |
| 40| a | 590.10| 10.15338| YES    | YES   |
| 41| a | 599.96| 27.22976| YES    | YES   |
| 42| a | 607.28| 14.07331| YES    | YES   |
| 43| a | 610.71| 3.00172 | YES    | YES   |
| 44| a | 638.06| 18.14658| YES    | YES   |
| 45| a | 648.93| 20.96493| YES    | YES   |
| 46| a | 670.45| 18.26347| YES    | YES   |
| 47| a | 692.11| 31.38006| YES    | YES   |
| 48| a | 697.96| 21.35305| YES    | YES   |
| 49| a | 704.56| 12.89033| YES    | YES   |
| 50| a | 746.65| 33.45622| YES    | YES   |
8ja
SCF Energy (au) BP86/SV(P) -2452.112960024
SCF Energy (au) PBE0/def2-TZVPP -2451.661992594
SCF Energy (au) PBE0/def2-TZVPP -2451.6706401152 (Toluene Correction)
Zero Point Energy (au) 0.3460163
Chemical Potential (kJ mol⁻¹) 747.33
Dispersion Correction (au) PBE0/def2-TZVPP -0.0730511

xyz coordinates
48

C  0.8108323  -2.5903869  -1.8551545
C  0.3540829  -0.6479745  -3.4094316
C  -0.0826625   0.4169862  -0.5404790
C   2.7762166  -1.1195163   -2.6223677
C  -0.8478166  -1.4866598   0.6328914
C  -1.7366531  -2.6171487   0.9565024
C   0.2389347  -1.0390112   1.3320947
C   0.9318723   0.0981200   0.5907915
C   1.3462114   1.2268378   1.5268983
Mn  1.1834611   0.8643311  -1.8247111
O   2.0238398   0.4190367  -0.1702391
O   0.6133847  -3.7407970  -1.8329725
O  -0.1845942  -0.4812006   4.4314630
C  -0.9733815  -0.6514769   0.5916826
O   3.8052897   1.2837979  -3.1362321
H  -1.7905066  -0.7560741   1.3207365
C  -0.0049395   1.6024817  -1.4098848
C   0.1173724   3.9102760  -3.0585552
C   1.2408968   3.5139527  -2.3143373
C   1.1863709   2.3767047  -1.4952047
C  -1.1333642   2.0200555  -2.1687061
C  -1.0715674   3.1590736  -2.9776495
H   0.1631612   4.8064150  -3.6988284
H   2.1747461   4.0968736  -2.3679992
H   2.0717122   2.0692665  -0.9211398
H  -2.0760080   1.4540942  -2.0993076
H  -1.9618472   3.4706015  -3.5482432
C  -3.4330047  -4.8051935   1.5919634
C  -2.6637013  -4.1884179   2.5962573
C  -1.8294188  -3.1077696   2.2832143
C  -2.5224466  -3.2442275  -0.0407170
C  -3.3575429  -4.3279362   0.2732583
H  -4.0918794  -5.6539004   1.8389797
H  -2.7208029  -4.5500213   3.6363777
H  -1.2500667  -2.6188642   3.0831149
H  -2.4615598  -2.9022017  -1.0859113
H  -3.9514708  -4.8057075  -0.5230304
C   2.1262996   3.2434620   3.3417805
C   3.0871860   2.3796812   2.7891985
C   2.7002511   1.3750198   1.8854352
C   0.3845893   2.0930841   2.0859939
C   0.7729370   3.0974656   2.9870120
H   2.4308740   4.0329286   4.0488730
H   4.1503046   2.4889089   3.0619363
H   3.4429536   0.6954052   1.4389028
H  -0.6785673   1.9830107   1.8118488
H   0.0129662   3.7725691   3.4145818
H   0.6770557  -1.4816048   2.2373501
| # | mode | symmetry | wave number (cm\(^{-1}\)) | IR intensity (km/mol) | selection rules |
|---|------|----------|-----------------------------|-----------------------|-----------------|
| 1 |      |          | 0.00                        | 0.00000               | -               |
| 2 |      |          | 0.00                        | 0.00000               | -               |
| 3 |      |          | 0.00                        | 0.00000               | -               |
| 4 |      |          | 0.00                        | 0.00000               | -               |
| 5 |      |          | 0.00                        | 0.00000               | -               |
| 6 |      |          | 0.00                        | 0.00000               | -               |
| 7 | a    |          | 9.39                        | 0.51363               | YES             |
| 8 | a    |          | 32.12                       | 0.20469               | YES             |
| 9 | a    |          | 34.81                       | 0.10117               | YES             |
| 10| a    |          | 37.44                       | 0.46825               | YES             |
| 11| a    |          | 40.24                       | 0.01493               | YES             |
| 12| a    |          | 45.91                       | 0.16691               | YES             |
| 13| a    |          | 51.66                       | 0.12131               | YES             |
| 14| a    |          | 67.30                       | 0.24290               | YES             |
| 15| a    |          | 73.61                       | 0.08827               | YES             |
| 16| a    |          | 82.74                       | 0.23275               | YES             |
| 17| a    |          | 90.31                       | 0.58714               | YES             |
| 18| a    |          | 96.41                       | 0.25560               | YES             |
| 19| a    |          | 106.21                      | 1.03310               | YES             |
| 20| a    |          | 122.44                      | 0.07124               | YES             |
| 21| a    |          | 135.04                      | 0.29045               | YES             |
| 22| a    |          | 159.90                      | 0.70650               | YES             |
| 23| a    |          | 171.85                      | 2.70924               | YES             |
| 24| a    |          | 202.85                      | 1.28940               | YES             |
| 25| a    |          | 216.36                      | 0.94684               | YES             |
| 26| a    |          | 226.97                      | 1.21257               | YES             |
| 27| a    |          | 240.13                      | 3.80695               | YES             |
| 28| a    |          | 258.11                      | 1.61148               | YES             |
| 29| a    |          | 265.91                      | 0.05346               | YES             |
| 30| a    |          | 335.01                      | 4.01898               | YES             |
| 31| a    |          | 383.95                      | 0.80238               | YES             |
| 32| a    |          | 401.10                      | 0.41059               | YES             |
| 33| a    |          | 401.14                      | 0.52167               | YES             |
| 34| a    |          | 404.62                      | 0.48174               | YES             |
| 35| a    |          | 412.48                      | 2.77429               | YES             |
| 36| a    |          | 420.42                      | 1.67771               | YES             |
| 37| a    |          | 443.53                      | 7.46887               | YES             |
| 38| a    |          | 450.80                      | 1.71787               | YES             |
| 39| a    |          | 466.08                      | 11.60292              | YES             |
| 40| a    |          | 472.43                      | 5.63197               | YES             |
| 41| a    |          | 480.54                      | 4.86212               | YES             |
| 42| a    |          | 497.71                      | 15.38443              | YES             |
| 43| a    |          | 512.43                      | 20.50597              | YES             |
| 44| a    |          | 531.11                      | 2.32273               | YES             |
| 45| a    |          | 542.35                      | 12.22692              | YES             |
| 46| a    |          | 563.25                      | 9.03231               | YES             |
| 47| a    |          | 599.68                      | 11.71928              | YES             |
| 48| a    |          | 604.55                      | 11.06808              | YES             |
| 49| a    |          | 609.38                      | 3.49552               | YES             |
| 50| a    |          | 610.81                      | 2.20605               | YES             |
**SCF Energy (au) BP86/SV(P)**
-2183.138380453

**SCF Energy (au) PBE0/def2-TZVPP**
-2182.724742562

**SCF Energy (au) PBE0/def2-TZVPP**
-2182.7310254792 (Toluene Correction)

Zero Point Energy (au) 0.2609739

Chemical Potential (kJ mol\(^{-1}\)) 548.90

Dispersion Correction (au) PBE0/def2-TZVPP -0.05007606

**xyz coordinates**

| #  | C    | C    | C    | C    | Mn  | O    | O    | O    | C    | C    | C    | C    | H    | H    | H    |
|----|------|------|------|------|-----|------|------|------|------|------|------|------|------|------|------|
| 1  | -0.4555222 | -1.0272451 | 3.0134137 |
| 2  | -2.2322748 | 0.4111283  | 1.9710883 |
| 3  | 0.0765045  | 0.6592913  | 0.2153566 |
| 4  | -2.0328828 | -2.2131014 | 1.3040033 |
| 5  | 0.6943673  | -1.7017693 | 0.2059772 |
| 6  | 1.4316334  | -2.8323304 | 0.7623819 |
| 7  | 1.3005899  | -4.0080826 | -1.3831930|
| 8  | 0.5988639  | -2.9877527 | -1.9733225|
| 9  | 0.2029760  | -1.8214566 | -1.2085885|
| 10 | -0.5734114 | -0.7912101 | 1.3497814 |
| 11 | -1.1030889 | -0.4177771 | -2.9922619|

**vibrational spectrum**

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|----------------|
| 1 | 0.00 | 0.00000  | 0.00000     | -            | -              |
| 2 | 0.00 | 0.00000  | 0.00000     | -            | -              |
| 3 | 0.00 | 0.00000  | 0.00000     | -            | -              |
| 4 | 0.00 | 0.00000  | 0.00000     | -            | -              |
| 5 | 0.00 | 0.00000  | 0.00000     | -            | -              |
| 6 | 0.00 | 0.00000  | 0.00000     | -            | -              |
| 7 | 32.09| 0.16433  | YES         | YES          |
| 8 | 41.04| 0.43457  | YES         | YES          |
| 9 | 43.30| 0.08549  | YES         | YES          |
| 10| 61.32| 0.14316  | YES         | YES          |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 11 | a | 70.63 | 0.24433 | YES | YES |
| 12 | a | 80.44 | 0.10310 | YES | YES |
| 13 | a | 88.72 | 0.56643 | YES | YES |
| 14 | a | 91.28 | 0.09064 | YES | YES |
| 15 | a | 101.03 | 0.17071 | YES | YES |
| 16 | a | 122.69 | 0.88529 | YES | YES |
| 17 | a | 137.08 | 0.61744 | YES | YES |
| 18 | a | 154.22 | 0.07845 | YES | YES |
| 19 | a | 160.24 | 2.97304 | YES | YES |
| 20 | a | 194.72 | 3.09354 | YES | YES |
| 21 | a | 210.73 | 1.39781 | YES | YES |
| 22 | a | 225.33 | 0.10436 | YES | YES |
| 23 | a | 264.83 | 0.46515 | YES | YES |
| 24 | a | 279.37 | 0.16220 | YES | YES |
| 25 | a | 328.31 | 2.31572 | YES | YES |
| 26 | a | 395.22 | 2.39126 | YES | YES |
| 27 | a | 401.33 | 1.58970 | YES | YES |
| 28 | a | 416.82 | 3.66140 | YES | YES |
| 29 | a | 423.99 | 7.52465 | YES | YES |
| 30 | a | 435.17 | 1.33824 | YES | YES |
| 31 | a | 461.94 | 5.83288 | YES | YES |
| 32 | a | 464.69 | 8.61675 | YES | YES |
| 33 | a | 473.03 | 2.00337 | YES | YES |
| 34 | a | 483.39 | 4.12031 | YES | YES |
| 35 | a | 485.54 | 1.74401 | YES | YES |
| 36 | a | 499.73 | 10.17819 | YES | YES |
| 37 | a | 505.07 | 2.18928 | YES | YES |
| 38 | a | 525.63 | 10.68491 | YES | YES |
| 39 | a | 528.37 | 6.68453 | YES | YES |
| 40 | a | 539.64 | 8.83679 | YES | YES |
| 41 | a | 569.83 | 17.33705 | YES | YES |
| 42 | a | 606.92 | 22.91671 | YES | YES |
| 43 | a | 609.38 | 19.50509 | YES | YES |
| 44 | a | 615.44 | 28.65066 | YES | YES |
| 45 | a | 639.94 | 47.13741 | YES | YES |
| 46 | a | 648.67 | 22.80887 | YES | YES |
| 47 | a | 677.37 | 47.26649 | YES | YES |
| 48 | a | 690.85 | 40.63817 | YES | YES |
| 49 | a | 700.88 | 5.60458 | YES | YES |
| 50 | a | 705.66 | 7.87861 | YES | YES |
9ja
SCF Energy (au) BP86/SV(P) -2452.123348709
SCF Energy (au) PBE0/def2-TZVPP -2451.669527954
SCF Energy (au) PBE0/def2-TZVPP -2451.6778817812 (Toluene Correction)
Zero Point Energy (au) 0.3465202
Chemical Potential (kJ mol\(^{-1}\)) 748.52
Dispersion Correction (au) PBE0/def2-TZVPP -0.06711919

xyz coordinates
48

C 2.3481734 2.2431881 1.1948046
C 0.1669204 2.3188157 2.429183
C -0.4497452 1.1219581 -0.1618083
C 1.7887959 0.1560994 2.6481949
C 1.5063152 -0.3478334 -0.2672712
C 2.9328444 -0.06229345 -0.5999385
C 0.594253 -1.4898840 -0.0218430
C -0.6543657 -1.2326713 0.4334046
C -1.8283792 -2.0885233 0.5937571
Mn 0.9803039 1.1277700 1.3506333
O -0.8371988 0.1422389 0.8244142
O 3.2417433 2.9837327 1.0599128
O -0.3559810 3.0919240 3.1280260
C 0.8256757 -0.7168583 0.4334046
O 2.3032906 -0.4872383 3.4703845
H 1.2711844 1.5624460 -1.4211007
C -1.4756507 2.0835584 -0.5975933
C -4.0855982 -3.7748885 0.9452271
C -2.9467578 -4.2450724 0.2634206
C -1.8353585 -3.4137417 0.0830389
C -2.908622 -1.6281341 1.2788312
C -4.0956897 -2.4630130 1.4475238
H -4.9620109 -4.4296990 1.0795436
H -2.9293074 -5.2697910 -0.1430840
H -0.9636572 -3.7922900 -0.4742328
H -2.9923089 -0.6067439 1.6857237
H -4.9814458 -2.0831672 1.9829698
H 0.8987698 -2.5058650 -0.3135795
C -3.4319440 3.9575317 -1.4261029
C -2.3158747 3.6924255 -2.2390909
C -1.3504676 2.7605723 -1.8347964
C -2.6048486 2.3545139 0.2113516
C -3.5729147 3.2799432 -0.2017181
H -4.1933155 4.6868346 -1.7478189
H -2.2010025 4.2109463 -3.2061260
H -0.4983866 2.5433499 -2.4980973
H -2.7102842 1.8425986 1.1795225
H -4.4441656 3.4791372 0.4434947
C 5.6523835 -1.2186915 -1.2127869
C 5.0527270 -0.0436213 -1.6970863
C 3.7148678 0.2504861 -1.3942853
C 3.5578032 -1.7978579 -0.1128142
C 4.8955628 -2.0926406 -0.4142897
H 6.7043340 -1.4473057 -1.4498788
H 5.6332163 0.6573574 -2.3196217
H 3.2815708 1.1826469 -1.7890620
H 2.9934402 -2.4831364 0.5401539
H 5.3521732 -3.0125058 -0.0126667
| # | mode | symmetry | wave number (cm⁻¹) | IR intensity (km/mol) | IR intensity (IR) | Raman intensity (RAMAN) | Selection rules |
|---|------|----------|-------------------|----------------------|------------------|-------------------------|----------------|
| 1 |      |          | 0.00              | 0.0000               | -                | -                       | YES            |
| 2 |      |          | 0.00              | 0.0000               | -                | -                       | YES            |
| 3 |      |          | 0.00              | 0.0000               | -                | -                       | YES            |
| 4 |      |          | 0.00              | 0.0000               | -                | -                       | YES            |
| 5 |      |          | 0.00              | 0.0000               | -                | -                       | YES            |
| 6 |      |          | 0.00              | 0.0000               | -                | -                       | YES            |
| 7 | a    |          | 10.18             | 0.33573              | YES              | YES                     |                |
| 8 | a    |          | 25.47             | 0.04866              | YES              | YES                     |                |
| 9 | a    |          | 28.98             | 0.47989              | YES              | YES                     |                |
| 10| a    |          | 37.98             | 0.33424              | YES              | YES                     |                |
| 11| a    |          | 40.14             | 0.15511              | YES              | YES                     |                |
| 12| a    |          | 43.28             | 0.33799              | YES              | YES                     |                |
| 13| a    |          | 47.51             | 0.07398              | YES              | YES                     |                |
| 14| a    |          | 64.19             | 0.02483              | YES              | YES                     |                |
| 15| a    |          | 65.43             | 0.04008              | YES              | YES                     |                |
| 16| a    |          | 85.18             | 0.26396              | YES              | YES                     |                |
| 17| a    |          | 86.74             | 0.47070              | YES              | YES                     |                |
| 18| a    |          | 99.55             | 0.10688              | YES              | YES                     |                |
| 19| a    |          | 112.34            | 0.21166              | YES              | YES                     |                |
| 20| a    |          | 133.07            | 0.22799              | YES              | YES                     |                |
| 21| a    |          | 156.64            | 0.23988              | YES              | YES                     |                |
| 22| a    |          | 176.24            | 0.31802              | YES              | YES                     |                |
| 23| a    |          | 178.08            | 5.06385              | YES              | YES                     |                |
| 24| a    |          | 201.08            | 1.21054              | YES              | YES                     |                |
| 25| a    |          | 224.13            | 0.38223              | YES              | YES                     |                |
| 26| a    |          | 231.65            | 0.53260              | YES              | YES                     |                |
| 27| a    |          | 253.66            | 0.13913              | YES              | YES                     |                |
| 28| a    |          | 283.75            | 0.39827              | YES              | YES                     |                |
| 29| a    |          | 339.79            | 1.84763              | YES              | YES                     |                |
| 30| a    |          | 370.05            | 0.66602              | YES              | YES                     |                |
| 31| a    |          | 397.59            | 0.44885              | YES              | YES                     |                |
| 32| a    |          | 399.17            | 1.01817              | YES              | YES                     |                |
| 33| a    |          | 400.76            | 0.01344              | YES              | YES                     |                |
| 34| a    |          | 409.24            | 6.36317              | YES              | YES                     |                |
| 35| a    |          | 419.18            | 9.63843              | YES              | YES                     |                |
| 36| a    |          | 429.06            | 3.29580              | YES              | YES                     |                |
| 37| a    |          | 446.88            | 0.94191              | YES              | YES                     |                |
| 38| a    |          | 454.75            | 2.00890              | YES              | YES                     |                |
| 39| a    |          | 471.78            | 6.65950              | YES              | YES                     |                |
| 40| a    |          | 475.15            | 4.60871              | YES              | YES                     |                |
| 41| a    |          | 491.20            | 5.83447              | YES              | YES                     |                |
| 42| a    |          | 497.32            | 7.85839              | YES              | YES                     |                |
| 43| a    |          | 505.28            | 16.47287             | YES              | YES                     |                |
| 44| a    |          | 529.69            | 11.38708             | YES              | YES                     |                |
| 45| a    |          | 542.19            | 1.29025              | YES              | YES                     |                |
| 46| a    |          | 556.07            | 1.17116              | YES              | YES                     |                |
| 47| a    |          | 577.70            | 32.51701             | YES              | YES                     |                |
| 48| a    |          | 594.52            | 11.60200             | YES              | YES                     |                |
| 49| a    |          | 610.95            | 9.31423              | YES              | YES                     |                |
| 50| a    |          | 611.61            | 15.19755             | YES              | YES                     |                |
SCF Energy (au) BP86/SV(P)  
SCF Energy (au) PBE0/def2-TZVPP  
SCF Energy (au) PBE0/def2-TZVPP  
(Toluene Correction)
Zero Point Energy (au)  
Chemical Potential (kJ mol^-1)  
Dispersion Correction (au) PBE0/def2-TZVPP
xyz coordinates

37

C 1.7416408 -0.3110429 2.6964122
C -0.8712760 0.4193370 2.4633608
C -0.1669048 0.7917484 -0.6034849
C -0.1250551 -2.0260195 2.8690518
C 1.2989200 -1.1605016 -0.1507975
C 2.5785955 -1.7819943 -0.2919384
C 1.5068238 -3.9769796 -0.2672980
C 0.1250551 -2.0260195 2.8690518
C -1.0938021 -1.1981647 0.2068743
Mn 0.2702500 -0.7301946 1.7199400
O -1.2283806 -0.0104199 -0.6625917
O 2.6724097 0.0000000 3.3308564
O -1.6464613 1.1574311 2.9338273
C 1.0636290 0.2867299 -0.0721054
O -0.3985336 -2.8882566 3.6132624
C 2.6744766 -3.1661645 -0.3522813
H 1.9213850 0.9676776 -0.0641243
C -0.4078879 2.1686693 -1.0679434
C -0.9215874 4.8009094 -1.9518210
C 0.4022624 4.3317557 -1.8682576
C 0.6593036 3.0255458 -1.4329481
C -1.7371538 2.6507631 -1.1584131
C -1.9892911 3.9564387 -1.5985609
H -1.1209938 5.8296381 -2.2948752
H 1.2405463 4.9881441 -2.1531103
H 1.6979338 2.6616762 -1.3974042
H -2.5646823 1.9881558 -0.8651030
H -3.0271132 4.3225561 -1.6596933
C -2.4511310 -1.8280817 0.3522992
H 3.4786001 -1.1497834 -0.3651810
H 3.6626138 -3.6431160 -0.4562814
H 1.6052489 -5.0741229 -0.3131083
H -0.6497154 -4.0382788 -0.0630405
H -3.1796535 -1.0938172 0.7576642
H -2.4062060 -2.6792928 1.0632910
H -2.8475492 -2.2028965 -0.6219486

$Vibrational spectrum

| # | mode | symmetry | wave number cm^-1 | IR intensity km/mol | selection rules |
|---|------|---------|------------------|---------------------|----------------|
| 1 | 0.00 | 0.00000 | 0.00000 | - | - |
| 2 | 0.00 | 0.00000 | 0.00000 | - | - |
| 3 | 0.00 | 0.00000 | 0.00000 | - | - |
| 4 | 0.00 | 0.00000 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | 0.00000 | - | - |
| 7 | a | 22.93 | 2.04808 | YES | YES |
| 8 | a | 35.63 | 0.05486 | YES | YES |
| 9 | a | 37.64 | 0.06628 | YES | YES |
| 10 | a | 67.71 | 1.08211 | YES | YES |
|   |   |   |   |   |
|---|---|---|---|---|
| 11 | a | 79.74 | 0.19435 | YES  | YES |
| 12 | a | 83.10 | 0.33410 | YES  | YES |
| 13 | a | 93.34 | 0.53032 | YES  | YES |
| 14 | a | 98.58 | 0.34548 | YES  | YES |
| 15 | a | 106.97 | 0.20771 | YES  | YES |
| 16 | a | 132.40 | 2.84990 | YES  | YES |
| 17 | a | 146.23 | 0.70162 | YES  | YES |
| 18 | a | 150.70 | 0.84470 | YES  | YES |
| 19 | a | 181.14 | 0.41538 | YES  | YES |
| 20 | a | 207.09 | 0.50058 | YES  | YES |
| 21 | a | 231.63 | 5.33756 | YES  | YES |
| 22 | a | 262.88 | 0.13112 | YES  | YES |
| 23 | a | 285.43 | 8.88123 | YES  | YES |
| 24 | a | 299.28 | 0.21116 | YES  | YES |
| 25 | a | 318.43 | 1.84098 | YES  | YES |
| 26 | a | 327.54 | 4.75623 | YES  | YES |
| 27 | a | 399.85 | 0.04054 | YES  | YES |
| 28 | a | 416.07 | 4.37544 | YES  | YES |
| 29 | a | 430.70 | 0.97133 | YES  | YES |
| 30 | a | 433.74 | 7.94172 | YES  | YES |
| 31 | a | 468.24 | 4.45534 | YES  | YES |
| 32 | a | 469.79 | 6.79562 | YES  | YES |
| 33 | a | 474.59 | 0.46909 | YES  | YES |
| 34 | a | 489.99 | 3.20937 | YES  | YES |
| 35 | a | 492.12 | 0.24457 | YES  | YES |
| 36 | a | 506.72 | 8.96440 | YES  | YES |
| 37 | a | 515.59 | 12.62066 | YES | YES |
| 38 | a | 527.61 | 7.60533 | YES  | YES |
| 39 | a | 531.09 | 6.41458 | YES  | YES |
| 40 | a | 559.16 | 2.49141 | YES  | YES |
| 41 | a | 589.33 | 2.07303 | YES  | YES |
| 42 | a | 607.23 | 29.54767 | YES | YES |
| 43 | a | 610.28 | 3.70786 | YES  | YES |
| 44 | a | 639.55 | 48.54657 | YES | YES |
| 45 | a | 656.40 | 12.12776 | YES | YES |
| 46 | a | 660.05 | 24.40755 | YES | YES |
| 47 | a | 677.96 | 60.85678 | YES  | YES |
| 48 | a | 686.84 | 36.23974 | YES  | YES |
| 49 | a | 713.28 | 1.40244 | YES  | YES |
| 50 | a | 728.90 | 69.19622 | YES  | YES |
SCF Energy (au) BP86/SV(P) -2452.145470468
SCF Energy (au) PBE0/def2-TZVPP -2451.692028912
SCF Energy (au) PBE0/def2-TZVPP -2451.7000699796 (Toluene Correction)
Zero Point Energy (au) 0.3474597
Chemical Potential (kJ mol^{-1}) 755.51
Dispersion Correction (au) PBE0/def2-TZVPP -0.06824413

xyz coordinates
48

C 1.6780743 1.2309898 1.9923960
C -0.9898958 1.2615352 1.9040674
C -0.0394979 1.1257232 -0.7683092
C 0.4310896 -0.8285674 2.7266545
C 1.3244149 -0.8822765 -0.2962105
C 0.0619896 -1.4838559 0.0472746
C -1.1331050 -0.7307102 -0.1021554
Mn 0.3600532 0.2340567 1.2849380
O -1.1312380 0.2895431 -1.0807702
O 2.5330402 1.8902683 2.436122
O -1.8603645 1.9235846 2.3016812
C 1.2333480 0.5092709 -0.6593866
O 0.4648208 -1.5390475 3.6535217
H 2.1524689 1.1048530 -0.7607071
C -0.2579604 2.5575621 -1.0564700
C -0.6966560 5.2882393 -1.6795272
C 0.5287824 4.874054 -1.1231468
C 0.7465173 3.5273047 -0.8115288
C -1.4886779 2.9853354 -1.6077039
C -1.7022905 4.3375931 -1.9170142
H -0.8671356 6.3509757 -1.9180002
H 1.3210578 5.6136787 -0.9187918
H 1.7011818 3.2340919 -0.3462086
H -2.2783306 2.2436561 -1.7939022
H -2.6684209 4.6501937 -2.3464741
C -2.4754089 -1.2349964 0.2527769
C 2.6058982 -1.6329494 -0.3207534
H 0.0287655 -2.4999361 0.4664834
C -5.0553649 -2.2494116 0.8431010
C -3.9315986 -2.7098572 1.5552067
C -2.6564172 -2.2072815 1.2680186
C -3.6124354 -0.7720371 -0.4502200
C -4.8861919 -1.2782083 -0.1573178
H -6.0586393 -2.6424943 1.0759038
H -4.0521713 -3.4610638 2.3530786
H -1.7964039 -2.5563690 1.8618409
H -3.4834345 -0.0170514 -1.2389274
H -5.7620081 -0.9074773 -0.7189706
C 5.0467166 -3.0764760 -0.4370671
C 4.8041327 -2.0249083 -1.3355181
C 3.5947439 -1.3125070 -1.2801693
C 2.8643005 -2.6954262 0.5781829
C 4.0694764 -3.4087702 0.5196244
H 5.9948251 -3.6371283 -0.4799334
H 5.5581945 -1.7596333 -2.0948183
H 3.4034500 -0.5111931 -2.0121849
H 2.1258729 -2.9471113 1.3563622
H 4.2529047 -4.2258964 1.2365219
| #  | mode | symmetry | wave number | IR intensity | selection rules |
|----|------|----------|-------------|--------------|-----------------|
| 1  |      |          | 0.00        | 0.00000      |                 |
| 2  |      |          | 0.00        | 0.00000      |                 |
| 3  |      |          | 0.00        | 0.00000      |                 |
| 4  |      |          | 0.00        | 0.00000      |                 |
| 5  |      |          | 0.00        | 0.00000      |                 |
| 6  |      |          | 0.00        | 0.00000      |                 |
| 7  | a    | a        | 23.29       | 0.10653      | YES             |
| 8  | a    | a        | 35.24       | 0.53647      | YES             |
| 9  | a    | a        | 38.30       | 0.24444      | YES             |
| 10 | a    | a        | 41.19       | 0.96698      | YES             |
| 11 | a    | a        | 44.55       | 0.52232      | YES             |
| 12 | a    | a        | 48.02       | 0.54913      | YES             |
| 13 | a    | a        | 49.84       | 0.29528      | YES             |
| 14 | a    | a        | 59.13       | 0.39726      | YES             |
| 15 | a    | a        | 66.22       | 0.40964      | YES             |
| 16 | a    | a        | 86.93       | 0.62262      | YES             |
| 17 | a    | a        | 89.10       | 0.71655      | YES             |
| 18 | a    | a        | 103.42      | 0.07471      | YES             |
| 19 | a    | a        | 126.51      | 0.15680      | YES             |
| 20 | a    | a        | 130.66      | 0.25646      | YES             |
| 21 | a    | a        | 147.29      | 0.78522      | YES             |
| 22 | a    | a        | 172.29      | 10.05456     | YES             |
| 23 | a    | a        | 180.03      | 7.32537      | YES             |
| 24 | a    | a        | 210.81      | 4.81705      | YES             |
| 25 | a    | a        | 214.90      | 2.33947      | YES             |
| 26 | a    | a        | 245.05      | 2.54091      | YES             |
| 27 | a    | a        | 256.36      | 1.31831      | YES             |
| 28 | a    | a        | 296.20      | 2.60722      | YES             |
| 29 | a    | a        | 343.61      | 21.91165     | YES             |
| 30 | a    | a        | 369.80      | 7.55395      | YES             |
| 31 | a    | a        | 381.75      | 7.18937      | YES             |
| 32 | a    | a        | 399.35      | 0.30002      | YES             |
| 33 | a    | a        | 401.85      | 0.56329      | YES             |
| 34 | a    | a        | 402.76      | 0.87591      | YES             |
| 35 | a    | a        | 409.32      | 7.61748      | YES             |
| 36 | a    | a        | 428.58      | 6.12174      | YES             |
| 37 | a    | a        | 443.00      | 0.49891      | YES             |
| 38 | a    | a        | 466.45      | 8.99863      | YES             |
| 39 | a    | a        | 473.38      | 2.05015      | YES             |
| 40 | a    | a        | 486.00      | 0.75574      | YES             |
| 41 | a    | a        | 488.36      | 1.35608      | YES             |
| 42 | a    | a        | 503.69      | 5.89648      | YES             |
| 43 | a    | a        | 515.51      | 29.07783     | YES             |
| 44 | a    | a        | 522.48      | 28.37979     | YES             |
| 45 | a    | a        | 544.90      | 4.36957      | YES             |
| 46 | a    | a        | 555.70      | 32.56046     | YES             |
| 47 | a    | a        | 563.22      | 1.88397      | YES             |
| 48 | a    | a        | 594.11      | 46.25290     | YES             |
| 49 | a    | a        | 608.59      | 1.40299      | YES             |
| 50 | a    | a        | 610.70      | 4.43086      | YES             |
### TS23aa

**SCF Energy (au)** BP86/SV(P)  
-2427.864609133

**SCF Energy (au)** PBE0/def2-TZVPP  
-2427.423479953

**SCF Energy (au)** PBE0/def2-TZVPP (Toluene Correction)  
-2427.433611029

**Zero Point Energy (au)**  
0.2961349

**Chemical Potential (kJ mol\(^{-1}\))**  
626.52

**Dispersion Correction (au)** PBE0/def2-TZVPP  
0.06311849

**xyz coordinates**  

|  | Mn  | C   | C   | C   | O   | O   | O   | C   | C   | C   | C   | O   | H   | H   | H   | H   | H   | H   |
|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
|  | 1.6788083 | 0.5413038 | 0.6660746 |
|  | 2.0503776  | 0.5296482  | 2.4309562 |
|  | 3.4054433  | 0.1742659  | 0.2830201 |
|  | 2.0529433  | 2.3065225  | 0.5143330 |
|  | 2.3294949  | 3.4417091  | 0.4733818 |
|  | 4.5278610  | 0.0167896  | 0.0295371 |
|  | 2.2814247  | 0.4988557  | 3.5712309 |
|  | -1.0926686 | -0.2583324 | 1.3776519 |
|  | -0.9973400 | 2.0490016  | 0.9698394 |
|  | -2.3651450 | 2.2050745  | 1.2189691 |
|  | -3.1234895 | 1.0695381  | 1.5546272 |
|  | -2.4812563 | -0.1687169 | 1.6297222 |
|  | -0.3111906 | -1.4899509 | 1.4194569 |
|  | 1.0201526  | -1.3705871 | 0.9948310 |
|  | 1.8629472  | -2.5728500 | 1.0052334 |
|  | 2.2739348  | -3.7544008 | 1.5323100 |
|  | -0.0161149 | -3.8397296 | 1.9367080 |
|  | -0.8418725 | -2.7488364 | 1.8724334 |
|  | 2.9976265  | -2.6790794 | 0.5829983 |
|  | -0.3753289 | -5.2043941 | 2.4389469 |
|  | -0.3659046 | 0.8571799  | 1.0459106 |
|  | 0.3346785  | 1.3859714  | -2.3672480 |
|  | 0.7595590  | 2.7269160  | -2.5583839 |
|  | 0.2076688  | 3.5125802  | -3.5802728 |
|  | -0.7871582 | 2.9913869  | -4.4262850 |
|  | -1.2257909 | 1.668207   | -4.2433593 |
|  | -0.6763379 | 0.8725536  | -3.2295837 |
|  | 0.8900099  | 0.5081948  | -1.3681614 |
|  | 1.2206952  | -0.6756461 | -0.9953258 |
|  | -0.3749161 | 2.9150525  | 0.6987359 |
|  | -2.8212774 | 3.2044537  | 1.1470848 |
|  | -4.2045597 | 1.1511865  | 1.7526742 |
|  | -3.0496866 | -1.0765220 | 1.8787698 |
|  | -1.8814572 | -2.8487494 | 2.2152355 |
|  | 1.5379814  | 3.1497117  | -1.9072265 |
|  | 0.5606496  | 4.5483909  | -3.7161426 |
|  | -1.2210490 | 3.6149772  | -5.2253032 |
|  | -2.0054478 | 1.2462192  | -4.9007374 |
|  | -1.0214133 | -0.1641280 | -3.0867825 |
|  | 1.6181458  | -1.6329900 | -1.3457148 |
|  | -1.4359054 | -5.2432596 | 2.7599516 |
|  | 0.2713780  | -5.4850809 | 3.3010068 |
|  | -0.2090293 | -5.9710504 | 1.6488693 |

$s$ vibrational spectrum

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|----------------|
| 1 | a    | -172.74  | 0.00000     | YES          | YES            |
| 2 | 0.00 | 0.00000  | -            | -            | -              |
| 3 | 0.00 | 0.00000  | -            | -            | -              |
| 4 | 0.00 | 0.00000  | -            | -            | -              |
| 5 | 0.00 | 0.00000  | -            | -            | -              |

S160
| 6 |   | 0.00 | 0.00000 |  -  |  -  |
|---|---|------|---------|-----|-----|
| 7 |   | 0.00 | 0.00000 |  -  |  -  |
| 8 | a | 17.15 | 0.19902 | YES | YES |
| 9 | a | 25.26 | 0.83606 | YES | YES |
| 10| a | 36.60 | 0.25361 | YES | YES |
| 11| a | 50.78 | 1.18797 | YES | YES |
| 12| a | 68.90 | 0.33269 | YES | YES |
| 13| a | 75.37 | 0.27528 | YES | YES |
| 14| a | 83.79 | 0.33993 | YES | YES |
| 15| a | 86.74 | 0.04327 | YES | YES |
| 16| a | 96.62 | 0.57822 | YES | YES |
| 17| a | 109.43| 0.42627 | YES | YES |
| 18| a | 114.10| 0.77591 | YES | YES |
| 19| a | 125.09| 0.29870 | YES | YES |
| 20| a | 139.91| 0.23751 | YES | YES |
| 21| a | 147.81| 0.17597 | YES | YES |
| 22| a | 157.72| 0.40932 | YES | YES |
| 23| a | 160.75| 0.93429 | YES | YES |
| 24| a | 166.63| 0.17092 | YES | YES |
| 25| a | 197.22| 0.23595 | YES | YES |
| 26| a | 218.08| 0.19371 | YES | YES |
| 27| a | 240.38| 0.46477 | YES | YES |
| 28| a | 253.84| 0.64059 | YES | YES |
| 29| a | 263.01| 0.61563 | YES | YES |
| 30| a | 296.72| 2.08692 | YES | YES |
| 31| a | 326.39| 1.40105 | YES | YES |
| 32| a | 358.07| 7.40260 | YES | YES |
| 33| a | 400.87| 3.17185 | YES | YES |
| 34| a | 401.88| 0.60941 | YES | YES |
| 35| a | 413.51| 2.56676 | YES | YES |
| 36| a | 428.75| 2.81648 | YES | YES |
| 37| a | 445.21| 21.76269| YES | YES |
| 38| a | 452.26| 1.83643 | YES | YES |
| 39| a | 464.49| 7.14943 | YES | YES |
| 40| a | 476.70| 0.11278 | YES | YES |
| 41| a | 488.43| 2.37409 | YES | YES |
| 42| a | 500.20| 9.44866 | YES | YES |
| 43| a | 518.27| 3.03466 | YES | YES |
| 44| a | 529.63| 23.82817| YES | YES |
| 45| a | 541.63| 1.06373 | YES | YES |
| 46| a | 544.47| 13.48474| YES | YES |
| 47| a | 549.76| 9.80746 | YES | YES |
| 48| a | 557.70| 1.89472 | YES | YES |
| 49| a | 578.36| 4.12900 | YES | YES |
| 50| a | 595.17| 0.22690 | YES | YES |
TS23aa'

SCF Energy (au) BP86/SV(P) -2427.853649810
SCF Energy (au) PBE0/def2-TZVPP -2427.411853990
SCF Energy (au) PBE0/def2-TZVPP -2427.4224059121 (Toluene Correction)
Zero Point Energy (au) 0.2956693
Chemical Potential (kJ mol\(^{-1}\)) 626.31
Dispersion Correction (au) PBE0/def2-TZVPP 0.06517125

xyz coordinates
43

Mn  1.0604984  1.9929986  0.6823022
C   1.1926923  1.9710117  2.4887800
C   2.8402352  1.7610039  0.5343487
C   1.3031491  3.7726719  0.5343487
O   1.4575616  4.9226638  0.4009624
O   3.9979345  1.6996050  0.4251379
O   1.2638844  1.9542238  3.6513366
C   -1.7427753  0.9781922  0.9238369
C   -1.7520834  3.3143000  0.7426142
C   -3.1498270  3.3684228  0.7892244
C   -3.8676255  2.1628212  0.8860943
O   -0.8901215  0.0135517  0.9731314
O   -1.414444   -2.3394707  1.3652037
C   -0.4883289  2.5283980  1.5730719
C   -1.3770827  1.4975889  1.4105772
O   -2.6192985  1.0743837  0.8711519
C   -0.8132012  3.9205660  1.1998310
N   -1.0561467  2.1591024  0.8084151
H   0.5555830  2.6948941  0.6524449
C   -3.6603325  4.3429790  0.7462084
H   -4.9694859  2.1626073  0.9105492
H   -3.6911847  0.0015311  1.0122905
H   -2.4402450  1.6718158  1.6303188
C   1.1039835  0.5017176  -1.8602694
H   -1.9022736  4.0486906  2.1688486
H   -0.2713592  4.1858413  2.9365708
H   -0.4852060  4.6580329  1.2257502
C   1.7790484  2.7511502  3.4308975
C   0.5012548  2.6531301  2.8533448
C   0.1673545  1.5412404  2.0635187
C   2.3883301  0.6096707  2.4425055
H   2.7209197  1.7283106  3.2208056
H   2.0437175  3.6285309  4.0436556
H   -0.2420134  3.4504317  3.0172470
H   -0.8337747  1.4639422  1.6100762
H   3.1263228  0.1883341  2.2657896
H   3.7275781  1.8025624  3.6644467

$vibrational spectrum$

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|-----------------|
| 1 | a    | -288.74  | 0.00000     | YES          | YES             |
| 2 | 0.00 | 0.00000  | -             | -            | -               |
| 3 | 0.00 | 0.00000  | -             | -            | -               |
| 4 | 0.00 | 0.00000  | -             | -            | -               |
| 5 | 0.00 | 0.00000  | -             | -            | -               |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 6 | 0.00 | 0.00000 | - | - |
| 7 | 0.00 | 0.00000 | - | - |
| 8 | a | 21.46 | 0.39886 | YES | YES |
| 9 | a | 30.55 | 0.36529 | YES | YES |
| 10 | a | 45.61 | 0.14736 | YES | YES |
| 11 | a | 48.26 | 1.22449 | YES | YES |
| 12 | a | 61.67 | 1.09460 | YES | YES |
| 13 | a | 78.38 | 0.44833 | YES | YES |
| 14 | a | 80.46 | 0.36741 | YES | YES |
| 15 | a | 86.87 | 0.15774 | YES | YES |
| 16 | a | 87.52 | 0.03196 | YES | YES |
| 17 | a | 102.02 | 0.56412 | YES | YES |
| 18 | a | 117.64 | 0.72443 | YES | YES |
| 19 | a | 128.81 | 0.28060 | YES | YES |
| 20 | a | 139.44 | 0.17071 | YES | YES |
| 21 | a | 151.48 | 0.37273 | YES | YES |
| 22 | a | 154.69 | 1.64005 | YES | YES |
| 23 | a | 163.17 | 0.10362 | YES | YES |
| 24 | a | 183.63 | 4.33893 | YES | YES |
| 25 | a | 193.95 | 0.97564 | YES | YES |
| 26 | a | 205.28 | 1.95662 | YES | YES |
| 27 | a | 217.80 | 0.71034 | YES | YES |
| 28 | a | 241.30 | 0.10665 | YES | YES |
| 29 | a | 260.18 | 0.11090 | YES | YES |
| 30 | a | 294.13 | 2.09385 | YES | YES |
| 31 | a | 318.15 | 4.59114 | YES | YES |
| 32 | a | 336.13 | 5.10675 | YES | YES |
| 33 | a | 393.18 | 3.92944 | YES | YES |
| 34 | a | 401.13 | 0.22347 | YES | YES |
| 35 | a | 424.46 | 2.13993 | YES | YES |
| 36 | a | 430.37 | 0.36767 | YES | YES |
| 37 | a | 455.80 | 1.51566 | YES | YES |
| 38 | a | 461.35 | 3.17289 | YES | YES |
| 39 | a | 478.45 | 0.81725 | YES | YES |
| 40 | a | 486.10 | 4.10302 | YES | YES |
| 41 | a | 497.65 | 8.36675 | YES | YES |
| 42 | a | 504.82 | 14.06983 | YES | YES |
| 43 | a | 519.59 | 6.15730 | YES | YES |
| 44 | a | 527.76 | 18.80972 | YES | YES |
| 45 | a | 539.96 | 1.42932 | YES | YES |
| 46 | a | 550.42 | 22.84540 | YES | YES |
| 47 | a | 556.16 | 4.99382 | YES | YES |
| 48 | a | 559.43 | 1.35728 | YES | YES |
| 49 | a | 577.03 | 5.35828 | YES | YES |
| 50 | a | 595.77 | 4.13113 | YES | YES |
TS23ba

SCF Energy (au) BP86/SV(P) -2277.50841284
SCF Energy (au) PBE0/def2-TZVPP -2277.05921476
SCF Energy (au) PBE0/def2-TZVPP -2277.0663116709 (Toluene Correction)
Zero Point Energy (au) 0.2893905
Chemical Potential (kJ mol⁻¹) 617.01
Dispersion Correction (au) PBE0/def2-TZVPP 0.06065985

xyz coordinates
41
Mn    1.5462735    0.3705217    0.7753154
C     1.9074785    0.6310002    2.5277213
C     3.2407096 -0.1119005    0.4629426
C     1.9480722    2.0777093    0.3447596
O     2.2410160    3.1806368    0.0936545
O     4.3448104 -0.4362008    0.2648014
O     2.1292592    0.7906648    3.6591366

h   1.-2537830 -0.2555350    1.5959263
C    -1.0996745    1.9697746    0.8633464
C    -2.4649227    2.1924425    1.0617323
C    -3.2557673    1.1294770    1.5353928
C    -2.6464858 -0.0988281    1.7968796
C    -0.5014315 -1.4808271    1.8581717
C     0.8516553 -1.5011387    1.3910424
C     1.6375491 -2.6423727    1.7084079
C     1.1063609 -3.7167233    2.4268538
C    -0.2425309 -3.7004240    2.8496778
C    -1.0364875 -2.5874485    2.5642042
H     -0.4503635    2.7714576    0.4801914
H     -2.8950271    3.1812287    0.8405819
H     -4.3388895    1.2594921    1.6936461
H     -3.2441323 -0.9503939    2.1538562
H      2.6862936 -2.6887826    1.3693071
H      1.7476473 -4.5817195    2.6667466
H     -0.6612248 -4.5507498    3.4116467
H    -2.0786672 -2.5634039    2.9225327
N     -0.5004788    0.7858067    1.1211501
C     0.3494049    0.6612376 -2.3782613
C     0.9745764    1.8354334 -2.8740594
C     0.5652123    2.4058176 -4.0878125
C    -0.4881425    1.8378149 -4.8263467
C    -1.1277044    0.6820037 -4.3411795
C    -0.7159981    0.0978621 -3.1365469
H      1.7966554    2.2946711 -2.3060925
H      1.0739469    3.3109476 -4.4593641
H     -0.8125999    2.2955245 -5.7753977
H     -1.9568402    0.2282210 -4.9096864
H     -2.183045 -0.8065564 -2.7569113
C     0.7583943    0.0048373 -1.1586284
C     0.9391618 -1.1406739 -0.5838789
H     1.1481747 -2.1808689 -0.8504819

$vibrational spectrum

#  mode  symmetry  wave number  IR intensity  selection rules
#  cm**(-1)  km/mol
1   a  -230.16    0.00000  YES     YES
2   0.00  0.00000  -  -
3   0.00  0.00000  -  -
4   0.00  0.00000  -  -
5   0.00  0.00000  -  -
6   0.00  0.00000  -  -
7   0.00  0.00000  -  -
|   |   |  |   |   |   |   |
|---|---|---|---|---|---|---|
| 8 | a | 15.33 | 0.05488 | YES | YES |
| 9 | a | 25.28 | 0.19576 | YES | YES |
| 10| a | 45.61 | 0.05019 | YES | YES |
| 11| a | 58.66 | 0.11086 | YES | YES |
| 12| a | 71.59 | 0.08026 | YES | YES |
| 13| a | 82.53 | 0.01510 | YES | YES |
| 14| a | 89.55 | 0.28337 | YES | YES |
| 15| a | 92.92 | 1.09647 | YES | YES |
| 16| a | 100.46| 0.46379 | YES | YES |
| 17| a | 109.98| 0.06435 | YES | YES |
| 18| a | 116.38| 0.03637 | YES | YES |
| 19| a | 132.51| 0.35585 | YES | YES |
| 20| a | 162.15| 1.17092 | YES | YES |
| 21| a | 182.00| 0.54087 | YES | YES |
| 22| a | 187.25| 0.55331 | YES | YES |
| 23| a | 217.10| 0.99499 | YES | YES |
| 24| a | 233.54| 0.82810 | YES | YES |
| 25| a | 259.73| 0.63802 | YES | YES |
| 26| a | 278.83| 0.12353 | YES | YES |
| 27| a | 343.57| 8.45214 | YES | YES |
| 28| a | 359.38| 1.36759 | YES | YES |
| 29| a | 385.36| 2.37851 | YES | YES |
| 30| a | 402.36| 0.07350 | YES | YES |
| 31| a | 415.74| 3.16983 | YES | YES |
| 32| a | 430.74| 1.25286 | YES | YES |
| 33| a | 447.29| 0.41322 | YES | YES |
| 34| a | 453.95| 8.13841 | YES | YES |
| 35| a | 463.51| 5.86149 | YES | YES |
| 36| a | 474.07| 1.00384 | YES | YES |
| 37| a | 488.83| 0.36260 | YES | YES |
| 38| a | 496.72| 7.61252 | YES | YES |
| 39| a | 503.64| 5.23803 | YES | YES |
| 40| a | 522.87| 0.37797 | YES | YES |
| 41| a | 544.04| 13.92394| YES | YES |
| 42| a | 546.27| 13.93147| YES | YES |
| 43| a | 553.19| 0.61857 | YES | YES |
| 44| a | 583.04| 24.49030| YES | YES |
| 45| a | 610.29| 10.92190| YES | YES |
| 46| a | 614.19| 12.97094| YES | YES |
| 47| a | 620.33| 1.05024 | YES | YES |
| 48| a | 625.80| 33.87210| YES | YES |
| 49| a | 639.10| 0.33601 | YES | YES |
| 50| a | 656.26| 9.87788 | YES | YES |
TS23Ba

SCF Energy (au) BP86/SV(P) -2277.498753669
SCF Energy (au) PBE0/def2-TZVPP -2277.050675757
SCF Energy (au) PBE0/def2-TZVPP -2277.05793890 (Toluene Correction)
Zero Point Energy (au) 0.2891519
Chemical Potential (kJ mol\(^{-1}\)) 617.56
Dispersion Correction (au) PBE0/def2-TZVPP -0.06291758

xyz coordinates
41

Mn  1.1693515  1.7942172  0.3501382
C   1.3530807  2.1824100  2.1120978
C   2.8984100  1.3543494  0.2491536
C   1.5418946  3.4606063 -0.2139974
O   1.7908638  4.5248368 -0.6268932
O   4.0275882  1.0587937  0.1914371
O   1.4670734  2.4424552  3.2421069
C   1.6743451  1.0921558  0.9437799
C   1.5381688  3.2923065  0.1440870
C   -2.9237216  3.4672754  0.2150309
C   -3.7137545  2.3901122  0.6558466
C   -3.0839075 -1.2000501  1.3628840
C   -0.9017448 -0.0900528  1.3304482
C   -0.1133275  0.9201197
C   -0.6142475 -1.2177803  2.5683531
C   -4.1316588 -1.1289586  2.1356710
C   -0.8861808  4.1064820 -0.2083692
H   -3.3692387  4.4305340 -0.0775210
H   -4.8108328  2.4810647  0.7124324
H   -3.6776879  0.3285333  1.3496471
H   -2.3226434 -1.2577098  1.0512727
H   -1.4009614 -3.0169031  2.5362660
H   -1.0266261 -2.9709426  3.2128557
H   -2.4836241 -1.0931220  2.4637971
N   -0.9209399  2.1431123  0.4957934
H   -0.6386519  1.8377141 -2.5520672
C   -0.6896772  1.3458523 -1.5751871
C   -0.6556402  0.1490567 -1.0778296
C   -0.8042723 -1.2237752 -1.5915096
C   -1.0787431 -3.7779246 -2.7828737
C   -2.0089812 -2.7639563 -3.0681654
C   -1.8725870 -1.4960946 -2.4811888
C   -0.1193572 -2.2559564 -1.3035661
C   -0.0135775 -3.5173396 -1.9016755
H   -1.1842179 -4.7734357 -3.2452973
H   -2.8502730 -2.9600918 -3.7535367
H   -2.6014809 -0.6992120 -2.6983808
H   -0.9537246 -2.0579155 -0.6121681
H   -0.7225716 -4.3068894 -1.6765880

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|-----------------|
|   |      |          | cm**(-1)    | km/mol       | IR   | RAMAN |
| 1 | a    |          | -281.20     | 0.00000      | YES  | YES   |
| 2 | 0.00 | 0.00000  |             |              |      |       |
| 3 | 0.00 | 0.00000  |             |              |      |       |
| 4 | 0.00 | 0.00000  |             |              |      |       |
| 5 | 0.00 | 0.00000  |             |              |      |       |
| 6 | 0.00 | 0.00000  |             |              |      |       |
| 7 | 0.00 | 0.00000  |             |              |      |       |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 8 | a | 24.93 | 0.17999 | YES | YES |
| 9 | a | 27.66 | 0.48622 | YES | YES |
|10 | a | 45.67 | 0.02077 | YES | YES |
|11 | a | 62.41 | 0.22472 | YES | YES |
|12 | a | 65.71 | 0.29527 | YES | YES |
|13 | a | 78.12 | 0.03628 | YES | YES |
|14 | a | 88.38 | 0.19623 | YES | YES |
|15 | a | 91.74 | 0.15481 | YES | YES |
|16 | a | 100.11 | 0.55229 | YES | YES |
|17 | a | 104.64 | 0.31790 | YES | YES |
|18 | a | 117.99 | 0.09532 | YES | YES |
|19 | a | 140.73 | 0.44197 | YES | YES |
|20 | a | 163.87 | 0.86445 | YES | YES |
|21 | a | 173.92 | 2.70349 | YES | YES |
|22 | a | 194.82 | 1.83630 | YES | YES |
|23 | a | 215.19 | 2.41823 | YES | YES |
|24 | a | 221.11 | 2.12687 | YES | YES |
|25 | a | 248.39 | 0.85224 | YES | YES |
|26 | a | 282.00 | 0.34236 | YES | YES |
|27 | a | 311.11 | 3.32284 | YES | YES |
|28 | a | 357.00 | 1.24876 | YES | YES |
|29 | a | 402.97 | 0.19811 | YES | YES |
|30 | a | 405.95 | 4.72270 | YES | YES |
|31 | a | 412.17 | 4.75989 | YES | YES |
|32 | a | 438.81 | 1.52677 | YES | YES |
|33 | a | 459.78 | 0.38930 | YES | YES |
|34 | a | 464.82 | 0.37031 | YES | YES |
|35 | a | 476.22 | 0.84671 | YES | YES |
|36 | a | 488.03 | 1.90597 | YES | YES |
|37 | a | 495.73 | 1.86045 | YES | YES |
|38 | a | 503.95 | 1.64839 | YES | YES |
|39 | a | 508.14 | 20.16433 | YES | YES |
|40 | a | 530.44 | 4.19986 | YES | YES |
|41 | a | 536.50 | 13.61825 | YES | YES |
|42 | a | 551.86 | 3.52941 | YES | YES |
|43 | a | 558.62 | 18.82493 | YES | YES |
|44 | a | 563.39 | 4.96911 | YES | YES |
|45 | a | 607.86 | 39.79700 | YES | YES |
|46 | a | 613.27 | 0.66942 | YES | YES |
|47 | a | 619.75 | 1.86931 | YES | YES |
|48 | a | 625.45 | 41.97016 | YES | YES |
|49 | a | 639.98 | 3.75850 | YES | YES |
|50 | a | 655.90 | 36.17631 | YES | YES |
SCF Energy (au) BP86/SV(P) -2505.228414752
SCF Energy (au) PBE0/def2-TZVPP -2504.778820226
SCF Energy (au) PBE0/def2-TZVPP -2504.7885430275 (Toluene Correction)
Zero Point Energy (au) 0.3313323
Chemical Potential (kJ mol\(^{-1}\)) 705.79
Dispersion Correction (au) PBE0/def2-TZVPP -0.06493997

xyz coordinates
47

Mn    1.5438696    0.9121769    1.8459137
C     2.0798231    0.9719827    3.5736955
C     3.1974123    0.4569030    1.3335957
C     1.9102005    2.6474432    1.5317027
O     2.1536748    3.7650521    1.2941777
O     4.2787058    0.1493930    1.0206017
O     2.4160219    1.0083613    4.6878982
C-1.1654630    0.1794923    2.8715540
C-1.0519913    2.4881328    2.4653612
C-2.3845969    2.6819223    2.8412507
C-3.1387447    1.5606357    3.2329710
C-2.5215322    0.3067525    3.2499353
C-0.4090617    -1.0728692    2.8813346
C 0.8736495    -1.0406434    2.2486695
C 1.6714458    -2.2132932    2.3163424
C 1.2170099    -3.3654072    2.9657126
C -0.0642883    -3.3954557    3.5605320
C -0.8684506    -2.2533241    3.5161742
H -0.4291977    3.3392628    2.1480412
H -2.8179453    3.6938075    2.8222620
H -4.1964514    1.6646260    3.5247371
H -3.0947039    -0.5874665    3.5376316
H 2.6647491    -2.2217370    1.8373571
H 1.8666377    -4.2555965    3.0141119
H -0.4225746    -4.3057289    4.0675956
H -1.8534569    -2.2681725    4.0106361
N -0.4512635    1.2776419    2.4717770
C 0.3693367    1.7188046    -1.1444068
C 0.6498899    0.8052351    -0.0221054
C 0.7090328    -0.4233841    0.3630955
H 0.6788933    -1.4385500    -0.0426014
O -0.1688441    1.0330044    -2.3015015
H -0.4003790    2.4718013    -0.8668055
H 1.2983409    2.2526720    -1.4426764
C 0.7049208    0.7742823    -3.3204458
O 1.8753878    1.1155984    -3.311180
C 0.0472152    0.0363104    -4.4440085
H -1.0840302    -1.3458045    -6.6194205
C -1.8713107    -1.0393509    -5.4947766
C -1.3103816    -0.3504427    -4.4085130
C 0.8333988    -0.2740593    -5.5746196
C 0.2691938    -0.9621104    -6.6578499
H -1.5277977    -1.8874805    -7.4714750
H -2.9315905    -1.3403637    -5.4649314
H -1.9178860    -0.1074050    -3.5239907
H 1.8897097    0.0374432    -5.5794971
H 0.8870432    -1.2018104    -7.5389247

$\text{vibrational spectrum}$

\[
\begin{array}{cccccc}
\text{mode} & \text{symmetry} & \text{wave number} & \text{IR intensity} & \text{selection rules} \\
1 & a & -244.44 & 0.00000 & \text{YES} & \text{YES} \\
\end{array}
\]
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 2 | 0.00 | 0.00000 | - | - |
| 3 | 0.00 | 0.00000 | - | - |
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | 0.00 | 0.00000 | - | - |
| 8 | a | 10.09 | 0.14991 | YES | YES |
| 9 | a | 12.41 | 0.42334 | YES | YES |
| 10 | a | 19.22 | 0.07028 | YES | YES |
| 11 | a | 36.42 | 0.34341 | YES | YES |
| 12 | a | 49.37 | 0.00449 | YES | YES |
| 13 | a | 53.56 | 1.03068 | YES | YES |
| 14 | a | 63.81 | 0.10861 | YES | YES |
| 15 | a | 68.11 | 0.21311 | YES | YES |
| 16 | a | 81.72 | 0.07782 | YES | YES |
| 17 | a | 91.80 | 0.56193 | YES | YES |
| 18 | a | 94.63 | 0.43159 | YES | YES |
| 19 | a | 101.38 | 0.53503 | YES | YES |
| 20 | a | 106.77 | 0.28635 | YES | YES |
| 21 | a | 122.46 | 0.47390 | YES | YES |
| 22 | a | 144.26 | 0.30543 | YES | YES |
| 23 | a | 165.36 | 0.72460 | YES | YES |
| 24 | a | 171.49 | 0.24320 | YES | YES |
| 25 | a | 185.89 | 0.55184 | YES | YES |
| 26 | a | 213.01 | 0.47639 | YES | YES |
| 27 | a | 230.75 | 3.89429 | YES | YES |
| 28 | a | 239.47 | 1.28996 | YES | YES |
| 29 | a | 248.79 | 3.55678 | YES | YES |
| 30 | a | 275.42 | 0.73147 | YES | YES |
| 31 | a | 280.32 | 1.12081 | YES | YES |
| 32 | a | 328.93 | 26.14672 | YES | YES |
| 33 | a | 358.46 | 1.92623 | YES | YES |
| 34 | a | 362.92 | 3.07572 | YES | YES |
| 35 | a | 404.07 | 0.86355 | YES | YES |
| 36 | a | 404.41 | 2.01337 | YES | YES |
| 37 | a | 417.15 | 1.67101 | YES | YES |
| 38 | a | 431.57 | 5.04544 | YES | YES |
| 39 | a | 439.66 | 0.34171 | YES | YES |
| 40 | a | 446.69 | 1.08182 | YES | YES |
| 41 | a | 461.13 | 0.75367 | YES | YES |
| 42 | a | 471.59 | 3.36562 | YES | YES |
| 43 | a | 483.05 | 4.85382 | YES | YES |
| 44 | a | 487.66 | 0.99726 | YES | YES |
| 45 | a | 495.49 | 1.19401 | YES | YES |
| 46 | a | 503.25 | 1.96319 | YES | YES |
| 47 | a | 538.01 | 10.91463 | YES | YES |
| 48 | a | 541.54 | 18.16062 | YES | YES |
| 49 | a | 555.44 | 1.04452 | YES | YES |
| 50 | a | 608.16 | 29.89436 | YES | YES |
TS2

SCF Energy (au) BP86/SV(P)  -2505.224054475
SCF Energy (au) PBE0/def2-TZVPP -2504.774662695
SCF Energy (au) PBE0/def2-TZVPP -2504.7841905779 (Toluene Correction)
Zero Point Energy (au) 0.3314439
Chemical Potential (kJ mol\(^{-1}\)) 709.37
Dispersion Correction (au) PBE0/def2-TZVP-P 0.06628063

xyz coordinates

47

Mn 1.2176947 1.8127312 1.4456319
C 1.4666299 2.4182820 3.1346110
C 2.8893178 1.1728893 1.4137244
C 1.7679512 3.3323829 0.6551328
O 2.1268865 4.2962021 0.1018704
O 3.9807488 0.7592320 1.4167611
O 1.6187517 2.8163816 4.2189751

C -1.6838173 1.5142621 2.1055525
C -1.2983862 3.5883820 1.0814943
C -2.6544880 3.9279053 1.1212621
C -3.5615029 3.0007085 1.6654012
C -3.0715137 1.7883817 2.5576600
C -1.0522464 0.3000024 2.6278138
O 0.9900761 -1.0164614 2.8399414
C 0.3403405 -1.8804578 3.7303729
C -1.0174117 -1.6817832 4.0587049
C -1.7050384 -0.5940762 3.5088041
H -0.5586526 4.2812524 0.6514182
H -2.9875741 4.8995658 0.7252030
H -4.6407100 3.2219184 1.7026697
H -3.7603152 1.0398129 2.5746974
H 2.0494275 -1.1997610 2.5938167
H 0.8985435 -2.7185790 4.1805668
H -1.5292451 -2.3650339 4.7553365
H -2.7527021 -0.4154062 3.8017342
N -0.8163498 2.4183728 1.5543468
H 0.6856472 1.5157013 -1.4528148
C 0.6638975 1.1671894 -0.4162421
C 0.4808754 0.0959589 0.2799620
C 0.2934903 -1.3751688 0.0287064
H 1.1764943 -1.9454385 0.3875599
O 0.1108113 -1.6183489 -1.3743703
H -0.6198903 -1.7588766 0.5291987
C 1.2148822 -2.0214416 -2.0778786
C 0.9116156 -2.2027878 -3.5308409
O 2.3038448 -2.2167652 -1.5675274
C 0.4570424 -2.5830452 -6.2818126
C -0.5934419 -2.1600732 -5.4474376
C -0.3701491 -1.9689868 -4.0754074
C 1.9629695 -2.6268606 -4.3723148
C 1.7357560 -2.8156257 -5.7425261
H 0.2779652 -2.7320770 -7.3598355
H -1.5950647 -1.9776276 -5.8706516
H -1.1845808 -1.6372763 -3.4145553
H 2.9540616 -2.8025317 -3.9254058
H 2.5594795 -3.1462033 -6.3964612

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|----------------|
| 1 | a    |          | -278.19     | 0.000000     | YES YES        |

S170
| a | Time   | Distance | All_Yes | All_Yes |
|---|--------|----------|---------|---------|
| 0.00 | 0.00000 | 0       | 0       | 0       |
| 0.00 | 0.00000 | 0       | 0       | 0       |
| 0.00 | 0.00000 | 0       | 0       | 0       |
| 0.00 | 0.00000 | 0       | 0       | 0       |
| 0.00 | 0.00000 | 0       | 0       | 0       |
| 0.00 | 0.00000 | 0       | 0       | 0       |
| 0.00 | 0.00000 | 0       | 0       | 0       |
| 14.29 | 0.20383 | YES     | YES     |         |
| 18.08 | 0.34253 | YES     | YES     |         |
| 22.29 | 0.24399 | YES     | YES     |         |
| 44.01 | 0.53700 | YES     | YES     |         |
| 48.83 | 0.03663 | YES     | YES     |         |
| 55.33 | 0.76764 | YES     | YES     |         |
| 62.75 | 0.67513 | YES     | YES     |         |
| 72.87 | 0.20665 | YES     | YES     |         |
| 81.93 | 0.03362 | YES     | YES     |         |
| 91.19 | 0.30181 | YES     | YES     |         |
| 97.97 | 0.10896 | YES     | YES     |         |
| 100.80 | 0.65510 | YES     | YES     |         |
| 104.64 | 0.37368 | YES     | YES     |         |
| 131.83 | 0.49765 | YES     | YES     |         |
| 143.99 | 0.40575 | YES     | YES     |         |
| 153.64 | 0.20252 | YES     | YES     |         |
| 174.60 | 0.14773 | YES     | YES     |         |
| 189.03 | 0.20652 | YES     | YES     |         |
| 212.84 | 2.82187 | YES     | YES     |         |
| 221.80 | 0.80722 | YES     | YES     |         |
| 240.53 | 0.72260 | YES     | YES     |         |
| 261.29 | 0.28153 | YES     | YES     |         |
| 281.46 | 0.06689 | YES     | YES     |         |
| 337.95 | 6.76754 | YES     | YES     |         |
| 345.86 | 3.26526 | YES     | YES     |         |
| 370.77 | 4.72662 | YES     | YES     |         |
| 372.63 | 8.73134 | YES     | YES     |         |
| 404.28 | 0.00737 | YES     | YES     |         |
| 416.30 | 4.57346 | YES     | YES     |         |
| 428.03 | 2.77797 | YES     | YES     |         |
| 438.60 | 0.63452 | YES     | YES     |         |
| 447.54 | 4.17340 | YES     | YES     |         |
| 457.06 | 1.37976 | YES     | YES     |         |
| 464.31 | 0.81569 | YES     | YES     |         |
| 474.49 | 7.60730 | YES     | YES     |         |
| 486.49 | 5.48000 | YES     | YES     |         |
| 492.07 | 3.12404 | YES     | YES     |         |
| 497.16 | 0.53026 | YES     | YES     |         |
| 520.26 | 8.99771 | YES     | YES     |         |
| 536.66 | 8.13746 | YES     | YES     |         |
| 539.91 | 7.75461 | YES     | YES     |         |
| 557.69 | 1.52783 | YES     | YES     |         |
| 594.61 | 14.24688 | YES     | YES     |         |
## TS23bc

| SCF Energy (au) BP86/SV(P) | -2281.108277972 |
|---------------------------|------------------|
| SCF Energy (au) PBE0/def2-TZVPP | -2280.675226907 |
| SCF Energy (au) PBE0/def2-TZVPP (Toluene Correction) | -2280.6812177349 |
| Zero Point Energy (au) | 0.3569715 |
| Chemical Potential (kJ mol\(^{-1}\)) | 792.89 |
| Dispersion Correction (au) PBE0/def2-TZVPP | -0.06589746 |

### xyz coordinates

47

|  |  |  |  |
|---|---|---|---|
| Mn | 1.2409727 | 0.0904313 | 1.1054278 |
| C | 1.7311248 | 0.3069725 | 2.8341453 |
| C | 2.9349362 | -0.2493845 | 0.6484351 |
| C | 1.4660984 | 1.8319250 | 0.7125130 |
| O | 1.6364875 | 2.9606134 | 0.4571049 |
| O | 4.0432610 | -0.4834398 | 0.3624492 |
| O | 2.0488129 | 0.4436701 | 3.9464924 |
| C | -1.4110895 | -0.8149669 | 2.1472777 |
| C | -1.4941407 | 1.4652372 | 1.6033007 |
| C | -2.8401766 | 1.5663166 | 1.9674951 |
| C | -3.4994615 | 0.4091231 | 2.4211488 |
| O | -2.7800988 | -0.7837775 | 2.5083186 |
| C | -0.5475761 | -1.9909043 | 2.2519126 |
| C | 0.7415510 | -1.8796710 | 1.6418711 |
| C | 1.6440474 | -2.9638656 | 1.8098994 |
| C | 1.2824482 | -4.1071377 | 2.5287496 |
| C | -0.0064634 | -4.2200319 | 3.0972038 |
| C | -0.9113734 | -3.1642600 | 2.9579791 |
| H | -0.9461394 | 2.3464649 | 1.236120 |
| H | -3.3574921 | 2.5350863 | 1.8893364 |
| H | -4.5644064 | 0.4401332 | 2.7038671 |
| H | -3.2718994 | -1.7047943 | 2.8544300 |
| H | 2.6470104 | -2.9102543 | 1.3538155 |
| H | 2.0115115 | -4.9257753 | 2.6532134 |
| H | -0.2919077 | -5.1243727 | 3.6582021 |
| H | -1.9036072 | -3.2389523 | 3.4322280 |
| N | -0.7912019 | 0.3135281 | 1.6784625 |
| C | 0.2036167 | 0.4229103 | -2.1177340 |
| C | 0.4513932 | -0.2496748 | -0.8076748 |
| C | 0.5544724 | -1.4233179 | -0.2809152 |
| H | 0.5633337 | -2.4760312 | -0.5790808 |
| C | 1.5251228 | 0.9180030 | -2.7641032 |
| H | -0.2221469 | -0.3552697 | -2.7995672 |
| C | -0.8249443 | 1.5785412 | -2.0498146 |
| H | 1.9931170 | 1.6754389 | -2.0945966 |
| C | 1.2743359 | 1.5382902 | -4.1498764 |
| H | 2.2434790 | 0.0717299 | -2.8390196 |
| C | -1.0745684 | 2.1931968 | -3.4382736 |
| H | -0.4370484 | 2.3638521 | -1.3613850 |
| H | -1.7785201 | 1.2070255 | -1.6127079 |
| H | 2.2338584 | 1.9152600 | -4.5702918 |
| C | 0.2347654 | 2.6710113 | -4.0898355 |
| H | 0.9156396 | 0.7455923 | -4.8492349 |
| H | -1.7966169 | 3.0368433 | -3.3533072 |
| H | -1.5580063 | 1.4319299 | -4.0963259 |
| H | 0.0361840 | 3.0674924 | -5.113184 |
| H | 0.6509482 | 3.5192177 | -3.4963377 |
| # | mode | symmetry | wave number \( \text{cm}^{-1} \) | IR intensity \( \text{km/mol} \) | selection rules |
|---|---|---|---|---|---|
| 1 | a | -233.32 | 0.00000 | YES | YES |
| 2 | 0.00 | 0.00000 | - | - |
| 3 | 0.00 | 0.00000 | - | - |
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | 0.00 | 0.00000 | - | - |
| 8 | a | 25.44 | 0.27019 | YES | YES |
| 9 | a | 35.20 | 0.13176 | YES | YES |
| 10 | a | 46.20 | 0.02342 | YES | YES |
| 11 | a | 53.63 | 0.13003 | YES | YES |
| 12 | a | 66.66 | 0.05869 | YES | YES |
| 13 | a | 78.23 | 0.40040 | YES | YES |
| 14 | a | 89.32 | 0.15455 | YES | YES |
| 15 | a | 92.83 | 0.72234 | YES | YES |
| 16 | a | 100.02 | 0.31098 | YES | YES |
| 17 | a | 107.64 | 0.22848 | YES | YES |
| 18 | a | 111.47 | 0.08287 | YES | YES |
| 19 | a | 118.84 | 0.19875 | YES | YES |
| 20 | a | 139.08 | 0.70360 | YES | YES |
| 21 | a | 164.03 | 0.45277 | YES | YES |
| 22 | a | 178.62 | 0.17963 | YES | YES |
| 23 | a | 203.50 | 0.48532 | YES | YES |
| 24 | a | 222.28 | 0.01933 | YES | YES |
| 25 | a | 230.18 | 2.70261 | YES | YES |
| 26 | a | 252.56 | 0.24883 | YES | YES |
| 27 | a | 275.88 | 0.27280 | YES | YES |
| 28 | a | 297.12 | 0.59696 | YES | YES |
| 29 | a | 350.68 | 0.94622 | YES | YES |
| 30 | a | 357.11 | 3.26921 | YES | YES |
| 31 | a | 369.95 | 2.21091 | YES | YES |
| 32 | a | 406.80 | 5.59754 | YES | YES |
| 33 | a | 420.17 | 1.06675 | YES | YES |
| 34 | a | 426.52 | 2.17763 | YES | YES |
| 35 | a | 438.74 | 0.84404 | YES | YES |
| 36 | a | 454.19 | 11.41550 | YES | YES |
| 37 | a | 459.39 | 1.23093 | YES | YES |
| 38 | a | 471.27 | 2.01419 | YES | YES |
| 39 | a | 471.95 | 3.22404 | YES | YES |
| 40 | a | 489.54 | 1.07058 | YES | YES |
| 41 | a | 497.71 | 3.64178 | YES | YES |
| 42 | a | 501.29 | 0.55328 | YES | YES |
| 43 | a | 512.85 | 3.57526 | YES | YES |
| 44 | a | 538.43 | 8.95694 | YES | YES |
| 45 | a | 546.38 | 13.34263 | YES | YES |
| 46 | a | 554.60 | 0.78629 | YES | YES |
| 47 | a | 575.01 | 5.02399 | YES | YES |
| 48 | a | 608.92 | 30.54046 | YES | YES |
| 49 | a | 620.85 | 1.38396 | YES | YES |
| 50 | a | 626.27 | 27.58342 | YES | YES |
TS_{23bc}'

SCF Energy (au) BP86/SV(P) -2281.103977722
SCF Energy (au) PBE0/def2-TZVPP -2280.671218205
SCF Energy (au) PBE0/def2-TZVPP -2280.6773988784 (Toluene Correction)
Zero Point Energy (au) 0.3568424
Chemical Potential (kJ mol\(^{-1}\)) 797.65
Dispersion Correction (au) PBE0/def2-TZVPP -0.06661635

xyz coordinates

47

Mn 1.0584974  2.0075745  0.8636094
C  1.4065610  2.2963033  2.6176727
C  2.7788548  1.6425535  0.5573960
C  1.3205956  3.7147665  0.3651363
O  1.4974053  4.8097286 -0.0032252
O  3.9057319  1.3940366  0.3681308
O  1.6234799  2.4911867  3.7462495
C  1.7061683  1.1522758  1.6243631
C  1.6886102  3.4310935  1.0701333
C  3.0684950  1.0701333  1.2626764
C  3.7950418  2.4032639  1.6319445
C  1.089848  1.2000770  1.806790
C -0.0319920  2.1236832  2.4369192
C -0.4377380 -2.2114362  2.8578647
C -1.3174290 -1.1648302  2.5617230
H -1.0871356  4.3015186  0.7649208
H -3.5595699  4.5246115  1.1173136
H -4.8867356  2.4495819  1.7772479
H -3.6530995  0.2847545  2.0850452
H  2.4021464 -0.9837975  1.3745237
H  1.6198810 -2.9228353  2.7019266
H  0.7867523 -3.0815597  3.4369294
H -2.3524705 -1.2085626  2.9388834
N -1.0173060  2.2713703  1.2407304
H  0.2052153  2.1992758 -1.9447688
C  0.3697731  1.6399617 -1.0188688
C  0.4261576  0.4189076 -0.5900383
C  0.4748275 -0.9544359 -1.2231924
C  0.5425282 -1.0274437 -2.3907468
H  0.1864101 -1.7265873 -0.4769103
C  1.8966294 -1.2981526 -1.7380544
C  1.9297454 -2.6760491 -2.4233278
H  2.6279615 -1.2662767 -0.9017107
H  2.2091946 -0.5067970 -2.4582144
H -1.5643380 -0.8028396 -2.0120097
C -0.5107904 -2.4069750 -3.0738193
H -0.2949055 -0.2366847 -3.1362682
H -0.8600705 -3.1820754 -2.3511143
H -1.2319186 -2.4215374 -3.9225519
H  1.7134871 -3.4671955 -1.6670317
H  2.9551625 -2.8796649 -2.8066906
C  0.9019421 -2.7681382 -3.5641145
H  0.9073472 -3.7886735 -4.0097542
H  1.1970819 -2.0659092 -4.3799218
| # | mode | symmetry | wave number cm\(^{-1}\) | IR intensity km/mol | IR | RAMAN |
|---|------|---------|-------------------------|---------------------|----|-------|
| 1 | a    |         | -292.01                 | 0.00000             | YES| YES   |
| 2 | a    |         | -3.78                   | 0.00000             | YES| YES   |
| 3 |      |         | 0.00                    | 0.00000             | -  | -     |
| 4 |      |         | 0.00                    | 0.00000             | -  | -     |
| 5 |      |         | 0.00                    | 0.00000             | -  | -     |
| 6 |      |         | 0.00                    | 0.00000             | -  | -     |
| 7 |      |         | 0.00                    | 0.00000             | -  | -     |
| 8 |      |         | 0.00                    | 0.00000             | -  | -     |
| 9 | a    |         | 28.49                   | 0.43330             | YES| YES   |
| 10| a    |         | 46.44                   | 0.00067             | YES| YES   |
| 11| a    |         | 51.71                   | 0.11284             | YES| YES   |
| 12| a    |         | 64.85                   | 0.27708             | YES| YES   |
| 13| a    |         | 79.34                   | 0.02072             | YES| YES   |
| 14| a    |         | 89.33                   | 0.29511             | YES| YES   |
| 15| a    |         | 92.02                   | 0.20021             | YES| YES   |
| 16| a    |         | 101.05                  | 0.72661             | YES| YES   |
| 17| a    |         | 104.97                  | 0.29552             | YES| YES   |
| 18| a    |         | 111.48                  | 0.11726             | YES| YES   |
| 19| a    |         | 127.74                  | 0.14195             | YES| YES   |
| 20| a    |         | 163.52                  | 1.93071             | YES| YES   |
| 21| a    |         | 168.19                  | 0.28006             | YES| YES   |
| 22| a    |         | 171.57                  | 0.06476             | YES| YES   |
| 23| a    |         | 201.66                  | 2.28831             | YES| YES   |
| 24| a    |         | 221.68                  | 0.90382             | YES| YES   |
| 25| a    |         | 228.11                  | 0.13987             | YES| YES   |
| 26| a    |         | 240.12                  | 0.50932             | YES| YES   |
| 27| a    |         | 263.48                  | 0.36210             | YES| YES   |
| 28| a    |         | 281.08                  | 0.10385             | YES| YES   |
| 29| a    |         | 342.96                  | 0.25244             | YES| YES   |
| 30| a    |         | 356.62                  | 1.72735             | YES| YES   |
| 31| a    |         | 407.65                  | 3.82895             | YES| YES   |
| 32| a    |         | 413.53                  | 1.94417             | YES| YES   |
| 33| a    |         | 420.48                  | 4.32053             | YES| YES   |
| 34| a    |         | 430.59                  | 1.93295             | YES| YES   |
| 35| a    |         | 441.75                  | 1.74368             | YES| YES   |
| 36| a    |         | 460.81                  | 2.24741             | YES| YES   |
| 37| a    |         | 463.86                  | 0.83593             | YES| YES   |
| 38| a    |         | 483.58                  | 1.45069             | YES| YES   |
| 39| a    |         | 486.62                  | 1.58686             | YES| YES   |
| 40| a    |         | 495.34                  | 0.90332             | YES| YES   |
| 41| a    |         | 501.19                  | 0.27970             | YES| YES   |
| 42| a    |         | 520.05                  | 2.89286             | YES| YES   |
| 43| a    |         | 523.61                  | 6.81593             | YES| YES   |
| 44| a    |         | 539.03                  | 12.66528            | YES| YES   |
| 45| a    |         | 548.96                  | 4.06695             | YES| YES   |
| 46| a    |         | 559.92                  | 3.76532             | YES| YES   |
| 47| a    |         | 587.65                  | 7.96722             | YES| YES   |
| 48| a    |         | 609.87                  | 30.76435            | YES| YES   |
| 49| a    |         | 621.24                  | 4.29310             | YES| YES   |
| 50| a    |         | 627.98                  | 39.61848            | YES| YES   |
TS23bd
SCF Energy (au) BP86/SV(P)  
-2411.377999102
SCF Energy (au) PBE0/def2-TZVPP  
-2410.917172120
SCF Energy (au) PBE0/def2-TZVPP  
-2410.9254826611 (Toluene Correction)
Zero Point Energy (au)  
0.3599214
Chemical Potential (kJ mol\(^{-1}\))  
787.62
Dispersion Correction (au) PBE0/def2-TZVPP  
0.06897874

xyz coordinates
49
Mn  1.6834630  -0.0525723  1.9499502
C   2.0090554   0.2577901  3.6992573
C   3.3713646  -0.5845235  1.6926125
C   2.1363629   1.6313506  1.4813795
O   2.4693042   2.7221616  1.2215237
O   4.4707655  -0.9441518  1.5293227
O   2.2100084   0.4495467  4.8302512
C   -1.1470986  -0.5976926  2.7197754
C   -0.9324977  1.5925442  1.9007414
C   -2.2982368  1.8471218  2.0506641
C   -3.1213617  0.8185427  2.5459622
C   -2.5420504  -0.4077008  2.8750646
C   -0.4262491  -1.8243502  3.9470872
C    1.6931261  -3.0281449  2.9933610
C    1.1210401  -4.0697105  3.7279511
C    -0.2386122  -4.0167145  4.1126819
C    -1.0019301  -2.8981569  3.7716426
H    -0.2574610  2.3661431  1.5045454
H    -2.7036819  2.8331761  1.7769299
H    -4.2059321  0.9735543  2.6683121
H    -3.1647403  -1.2331882  3.2502307
H    -2.7509778  -3.1042007  2.6890843
H     1.7393524  -4.9380311  4.0129915
H    -0.6882753  -4.8412553  4.6890756
H    -2.0532278  -2.8431750  4.0993138
N    -0.3613988  0.4102460  2.2236019
C    -0.5722182  0.1518922  -0.4529288
C     1.1001983  1.3865545  -1.7046310
C     0.7455663  1.9262172  -2.9429411
C     -0.1863450  1.2707796  -3.8004005
C     -0.7356187  0.0382648  -3.3340738
C     -0.3620324  -0.4981225  -2.1018884
H     1.8215642  1.939246  -1.0809394
H     1.2023613  2.8797746  -3.2433579
N     -0.5456798  1.8075638  -5.0264299
H     -1.4654832  -0.5137298  -3.9434549
H     -0.8068323  -1.4520759  -1.7746075
C     0.9425459  -0.4725647  -0.0024645
C     1.0810974  -1.5992534  0.6214019
H     1.3031505  -2.6483348  0.4068866
H     -1.4962568  1.1107966  -5.8749848
C     0.0455147  3.0575437  -5.4719449
H     -0.1894395  3.9030832  -4.7811889
H     -0.3548213  3.3171793  -6.4718110
H     1.1569677  2.9896755  -5.5569684
H     -1.1337429  0.0962807  -6.1692087
H     -1.6569254  1.6947161  -6.8027670
H    -2.4882151  0.9841219  -5.3774916
| #  | mode | symmetry | wave number | IR intensity | selection rules |
|----|------|----------|-------------|--------------|----------------|
|    |      | cm**(-1) | km/mol       |              | IR            | RAMAN         |
| 1  | a    | -232.90  | 0.00000     | YES          | YES           |
| 2  | a    | 0.00     | 0.00000     | -            | -             |
| 3  | a    | 0.00     | 0.00000     | -            | -             |
| 4  | a    | 0.00     | 0.00000     | -            | -             |
| 5  | a    | 0.00     | 0.00000     | -            | -             |
| 6  | a    | 0.00     | 0.00000     | -            | -             |
| 7  | a    | 0.00     | 0.00000     | -            | -             |
| 8  | a    | 17.63    | 0.42854     | YES          | YES           |
| 9  | a    | 23.50    | 0.02888     | YES          | YES           |
| 10 | a    | 39.27    | 0.17692     | YES          | YES           |
| 11 | a    | 52.61    | 0.70633     | YES          | YES           |
| 12 | a    | 60.93    | 0.75764     | YES          | YES           |
| 13 | a    | 69.86    | 0.00642     | YES          | YES           |
| 14 | a    | 73.50    | 0.05396     | YES          | YES           |
| 15 | a    | 79.07    | 0.32040     | YES          | YES           |
| 16 | a    | 87.05    | 0.20507     | YES          | YES           |
| 17 | a    | 91.02    | 0.05740     | YES          | YES           |
| 18 | a    | 93.52    | 1.26300     | YES          | YES           |
| 19 | a    | 102.25   | 0.54171     | YES          | YES           |
| 20 | a    | 109.71   | 0.09419     | YES          | YES           |
| 21 | a    | 113.69   | 0.14201     | YES          | YES           |
| 22 | a    | 133.88   | 0.09814     | YES          | YES           |
| 23 | a    | 172.62   | 0.27658     | YES          | YES           |
| 24 | a    | 173.33   | 0.33520     | YES          | YES           |
| 25 | a    | 192.99   | 0.53918     | YES          | YES           |
| 26 | a    | 203.92   | 0.52000     | YES          | YES           |
| 27 | a    | 211.52   | 0.00193     | YES          | YES           |
| 28 | a    | 232.77   | 1.06116     | YES          | YES           |
| 29 | a    | 249.78   | 0.59980     | YES          | YES           |
| 30 | a    | 259.75   | 0.23298     | YES          | YES           |
| 31 | a    | 279.20   | 0.33588     | YES          | YES           |
| 32 | a    | 294.51   | 4.85642     | YES          | YES           |
| 33 | a    | 341.09   | 0.32281     | YES          | YES           |
| 34 | a    | 358.51   | 3.22369     | YES          | YES           |
| 35 | a    | 396.61   | 1.95742     | YES          | YES           |
| 36 | a    | 412.41   | 1.72339     | YES          | YES           |
| 37 | a    | 419.20   | 0.32576     | YES          | YES           |
| 38 | a    | 428.07   | 21.42381    | YES          | YES           |
| 39 | a    | 434.00   | 1.48273     | YES          | YES           |
| 40 | a    | 443.83   | 5.47313     | YES          | YES           |
| 41 | a    | 459.17   | 0.37495     | YES          | YES           |
| 42 | a    | 467.34   | 6.59154     | YES          | YES           |
| 43 | a    | 473.89   | 0.79606     | YES          | YES           |
| 44 | a    | 481.82   | 2.47340     | YES          | YES           |
| 45 | a    | 494.42   | 3.20775     | YES          | YES           |
| 46 | a    | 502.22   | 4.26468     | YES          | YES           |
| 47 | a    | 507.05   | 10.25813    | YES          | YES           |
| 48 | a    | 526.69   | 7.26318     | YES          | YES           |
| 49 | a    | 543.84   | 16.93748    | YES          | YES           |
| 50 | a    | 545.01   | 27.45832    | YES          | YES           |
TS23bd'

SCF Energy (au) BP86/SV(P) -2411.368746066
SCF Energy (au) PBE0/def2-TZVPP -2410.909311614
SCF Energy (au) PBE0/def2-TZVPP -2410.9178265345 (Toluene Correction)
Zero Point Energy (au) 0.3597223
Chemical Potential (kJ mol\(^{-1}\)) 787.33
Dispersion Correction (au) PBE0/def2-TZVPP -0.07129753

xyz coordinates

49

Mn  0.8765013  2.7963850  0.9256197
C  0.9665915  3.2424892  2.6802605
C  2.6063238  2.3530971  0.9199746
C  1.2790913  4.4416824  0.3257752
O  1.5517344  5.4917965 -0.1099508
O  3.7367907  2.0547615  0.9224713
O  1.0198641  3.5439671  3.8052743
O  1.9912887  2.1018574  1.3960254
C  1.8177428  4.2754438  0.5328868
C  3.2051678  4.4498593  0.9656546
C  4.0151754  3.3853344  0.9656546
C  3.4030226  2.2059291  1.3950251
C  1.2377681  0.9352140  1.8589081
C -1.0078131 -1.1055827  3.1834053
C -1.8056209 -0.0770676  2.6726767
H -1.1489615  5.0789482  0.1874558
H -3.6362272  5.4026418  0.1861606
H -5.1138208  3.4754524  0.9651434
H -4.0118098 -1.658238  2.0340893
C  0.3691824 -1.1376972  2.8695996
C -1.0078131 -1.1055827  3.1834053
C -1.8056209 -0.0770676  2.6726767
H -1.1489615  5.0789482  0.1874558
H -3.6362272  5.4026418  0.1861606
H -5.1138208  3.4754524  0.9651434
H -4.0118098 -1.658238  2.0340893
N  1.1945533 -4.1852326  2.5914633
H  2.7696160 -2.0099100  3.0174565
H  2.4214364  0.2297555 -2.0624777
H -1.1018264 -1.1757743  0.0361319
H -0.7974877 -3.4146339 -0.9115329
C  0.2833252 -5.2604066  2.2400371
C  2.3290919 -4.4509679  3.4588670
H  3.3052120 -4.2826688  2.9419781
H  2.3149097 -3.8095463  4.3723163
H  2.2986772 -5.5081616 -3.7892528
H -0.7685960 -5.0289145  2.5330402
H  0.2886267 -5.4784424  1.1443368
H  0.5848459 -6.1851661 -2.7709595
| #  | mode | symmetry | wave number (cm\(^{-1}\)) | IR intensity (km/mol) | selection rules |
|----|------|----------|-----------------------------|-----------------------|-----------------|
| 1  | a    |          | -281.14                     | 0.00000               | YES             |
| 2  | a    |          | 0.00                         | 0.00000               | -               |
| 3  | a    |          | 0.00                         | 0.00000               | -               |
| 4  | a    |          | 0.00                         | 0.00000               | -               |
| 5  | a    |          | 0.00                         | 0.00000               | -               |
| 6  | a    |          | 0.00                         | 0.00000               | -               |
| 7  | a    |          | 0.00                         | 0.00000               | -               |
| 8  | a    |          | 20.19                        | 0.87179               | YES             |
| 9  | a    |          | 27.26                        | 0.34281               | YES             |
| 10 | a    |          | 38.91                        | 0.12241               | YES             |
| 11 | a    |          | 48.94                        | 0.33750               | YES             |
| 12 | a    |          | 62.05                        | 0.55669               | YES             |
| 13 | a    |          | 65.23                        | 0.13583               | YES             |
| 14 | a    |          | 73.20                        | 0.38913               | YES             |
| 15 | a    |          | 80.39                        | 0.02581               | YES             |
| 16 | a    |          | 83.34                        | 0.07330               | YES             |
| 17 | a    |          | 89.03                        | 0.82535               | YES             |
| 18 | a    |          | 98.01                        | 0.35279               | YES             |
| 19 | a    |          | 103.39                       | 0.62865               | YES             |
| 20 | a    |          | 103.76                       | 0.08370               | YES             |
| 21 | a    |          | 128.54                       | 0.82791               | YES             |
| 22 | a    |          | 136.25                       | 0.50399               | YES             |
| 23 | a    |          | 151.00                       | 8.53754               | YES             |
| 24 | a    |          | 172.53                       | 1.79403               | YES             |
| 25 | a    |          | 173.86                       | 0.17583               | YES             |
| 26 | a    |          | 205.54                       | 2.72256               | YES             |
| 27 | a    |          | 208.09                       | 0.60019               | YES             |
| 28 | a    |          | 220.35                       | 1.63172               | YES             |
| 29 | a    |          | 243.30                       | 0.79741               | YES             |
| 30 | a    |          | 264.70                       | 1.09374               | YES             |
| 31 | a    |          | 280.06                       | 1.21745               | YES             |
| 32 | a    |          | 283.52                       | 4.52251               | YES             |
| 33 | a    |          | 355.23                       | 1.65612               | YES             |
| 34 | a    |          | 368.43                       | 10.41136              | YES             |
| 35 | a    |          | 371.16                       | 17.81186              | YES             |
| 36 | a    |          | 409.54                       | 9.00014               | YES             |
| 37 | a    |          | 420.83                       | 0.00760               | YES             |
| 38 | a    |          | 432.92                       | 1.90686               | YES             |
| 39 | a    |          | 448.63                       | 5.06107               | YES             |
| 40 | a    |          | 458.25                       | 0.05615               | YES             |
| 41 | a    |          | 464.84                       | 0.40177               | YES             |
| 42 | a    |          | 476.00                       | 5.71754               | YES             |
| 43 | a    |          | 482.29                       | 1.90114               | YES             |
| 44 | a    |          | 493.30                       | 1.86918               | YES             |
| 45 | a    |          | 498.67                       | 1.51402               | YES             |
| 46 | a    |          | 505.43                       | 25.56968              | YES             |
| 47 | a    |          | 512.67                       | 8.91216               | YES             |
| 48 | a    |          | 534.45                       | 2.22502               | YES             |
| 49 | a    |          | 538.22                       | 10.33803              | YES             |
| 50 | a    |          | 548.54                       | 5.78802               | YES             |
TS23Be

SCF Energy (au) BP86/SV(P)   -2391.942812015
SCF Energy (au) PBE0/def2-TZVPP -2391.495806536
SCF Energy (au) PBE0/def2-TZVPP -2391.5041329799 (Toluene Correction)
Zero Point Energy (au)         0.3207053
Chemical Potential (kJ mol⁻¹)  692.34
Dispersion Correction (au) PBE0/def2-TZVPP -0.06659232

xyz coordinates
45

Mn  0.8603316  2.3382340  0.6760216
C  0.9379708  2.8134409  2.4240064
C  2.5972322  1.9219831  0.6837214
C  1.2383753  3.9807492  0.0509475
O  1.4943236  5.0284896 -0.3993022
O  3.7314917  1.6393026  0.6929300
O  0.9821245  3.1300685  3.5447706
C  2.0001052  1.6116006  1.1448314
C  1.8528766  3.7743982  0.2505319
C  3.2462132  3.9286207  0.0230344
C  4.0396691  2.8590150  0.6846638
C  3.4130628  1.6950717  1.1349044
C  1.2323193  0.4638250  1.6312906
C  0.1593725  0.4460522  1.2975217
C  0.9491070  0.6005383  1.8421360
C  0.3982303  1.5675800  2.6885341
C  0.9812609  1.5513558  2.990768
C  1.7903207  0.5429819  2.4581476
H  1.1942219  4.5826265 -0.1032778
H  3.6853800  4.8699977 -0.1221602
H  5.1394155  2.9332059  0.6768765
H  4.0114237  0.837251  1.4749357
H  2.017462  -0.6538559  1.5932197
H  1.0465926 -2.3497724  3.1180270
H  1.4162982 -2.3185221  3.6519113
H  2.8597754 -0.5109985  2.7242278
N  1.2390138  2.6535486  0.6889858
H  0.4719437  2.2253396 -2.2449167
C  0.4880967  1.7815788 -1.9240234
C  0.4524668  0.6049359 -0.6992029
C  0.6761080 -0.7825776 1.1266604
C  1.1038637 -3.3947654 -2.1684267
C  2.0076121 -2.3538623 -2.4722466
C  1.7857646 -1.0670649 -1.9553061
C  0.2132866  1.8449432 -0.8213911
C  0.0108466 -3.1234504 -1.3391414
O  1.2167345  4.6758329  2.6162467
H  2.8885494  2.5306660 -3.1066706
H  2.4926790  0.2586425 -2.1904050
H  1.0849297  1.6524542 -0.1762487
H  0.7078168 -3.9463402 -1.1155303
C  2.3137170 -5.0144689 -3.4480481
H  2.1995729  6.0916702 -3.6844566
H  3.2895722 -4.8568574  2.9300167
H  2.3074563 -4.4300586 -4.3986280

$\text{vibrational spectrum}$

| mode | symmetry | wave number (cm⁻¹) | IR intensity (km/mol) | selection rules |
|------|----------|------------------|----------------------|-----------------|
| 1    | a        | -282.68          | 0.00000              | YES YES         |
| 2    |          | 0.00             | 0.00000              | - -             |
| 3    |          | 0.00             | 0.00000              | - -             |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | 0.00 | 0.00000 | - | - |
| 8 | a | 20.94 | 0.84604 | YES | YES |
| 9 | a | 29.19 | 0.79127 | YES | YES |
| 10 | a | 45.47 | 0.13936 | YES | YES |
| 11 | a | 54.95 | 0.03365 | YES | YES |
| 12 | a | 65.46 | 0.30469 | YES | YES |
| 13 | a | 69.54 | 0.04339 | YES | YES |
| 14 | a | 82.63 | 0.10799 | YES | YES |
| 15 | a | 89.06 | 0.48148 | YES | YES |
| 16 | a | 96.18 | 0.65098 | YES | YES |
| 17 | a | 100.10 | 0.89539 | YES | YES |
| 18 | a | 104.29 | 0.41734 | YES | YES |
| 19 | a | 119.76 | 1.61318 | YES | YES |
| 20 | a | 133.23 | 0.66472 | YES | YES |
| 21 | a | 151.62 | 0.52672 | YES | YES |
| 22 | a | 160.18 | 5.85576 | YES | YES |
| 23 | a | 176.79 | 0.15200 | YES | YES |
| 24 | a | 190.84 | 1.83338 | YES | YES |
| 25 | a | 217.29 | 0.68853 | YES | YES |
| 26 | a | 229.68 | 2.61832 | YES | YES |
| 27 | a | 245.29 | 0.45810 | YES | YES |
| 28 | a | 266.00 | 0.50973 | YES | YES |
| 29 | a | 274.25 | 4.73900 | YES | YES |
| 30 | a | 282.77 | 0.36243 | YES | YES |
| 31 | a | 356.37 | 1.42389 | YES | YES |
| 32 | a | 367.34 | 4.02929 | YES | YES |
| 33 | a | 410.21 | 3.71430 | YES | YES |
| 34 | a | 411.57 | 16.17621 | YES | YES |
| 35 | a | 414.46 | 0.20458 | YES | YES |
| 36 | a | 433.24 | 4.05431 | YES | YES |
| 37 | a | 447.79 | 3.75264 | YES | YES |
| 38 | a | 461.59 | 0.27501 | YES | YES |
| 39 | a | 476.88 | 7.40511 | YES | YES |
| 40 | a | 481.37 | 0.22403 | YES | YES |
| 41 | a | 490.38 | 1.44038 | YES | YES |
| 42 | a | 496.63 | 4.12182 | YES | YES |
| 43 | a | 503.13 | 10.48972 | YES | YES |
| 44 | a | 521.41 | 27.61373 | YES | YES |
| 45 | a | 533.34 | 2.49739 | YES | YES |
| 46 | a | 537.21 | 9.83007 | YES | YES |
| 47 | a | 546.83 | 10.77086 | YES | YES |
| 48 | a | 552.96 | 7.48015 | YES | YES |
| 49 | a | 559.28 | 19.86247 | YES | YES |
| 50 | a | 608.71 | 41.44731 | YES | YES |
**TS23be**

SCF Energy (au) BP86/SV(P) -2391.952065529

SCF Energy (au) PBE0/def2-TZVPP -2391.503796793

SCF Energy (au) PBE0/def2-TZVPP -2391.511922258 (Toluene Correction)

Zero Point Energy (au) 0.3209337

Chemical Potential (kJ mol⁻¹) 692.54

Dispersion Correction (au) PBE0/def2-TZVPP -0.06432154

**xyz coordinates**

|   |   |   |
|---|---|---|
| 1 | Mn | 0.8621936 -1.7437725 0.792015 |
| 2 | C  | 2.0691026 -2.3221484 2.0057398 |
| 3 | C  | 0.3354707 -3.4232205 0.4714875 |
| 4 | C  | 2.0477510 -1.8564604 -0.5663307 |
| 5 | O  | 2.8360809 -1.9745973 -1.4217577 |
| 6 | O  | -0.0127487 -4.5200114 0.2724205 |
| 7 | C  | 2.8397678 -2.6915675 2.7970921 |
| 8 | C  | 0.7186338 0.8031975 2.3400358 |
| 9 | C  | 2.1364778 1.0577432 0.4859888 |
|10 | C  | 2.3787566 2.4023179 0.7796241 |
|11 | C  | 1.7428917 2.9681817 1.8998988 |
|12 | C  | 0.9075607 2.1655473 2.6776365 |
|13 | C  | -0.1123756 -0.1382387 3.0862403 |
|14 | C  | -0.3468487 -1.4032020 4.4074671 |
|15 | C  | -0.5781318 -2.0972743 5.0635798 |
|16 | C  | -0.3719378 -0.8308322 4.3711397 |
|17 | C  | -0.6428491 0.1382771 4.3711397 |
|18 | H  | 2.6030517 0.5818446 -0.3896668 |
|19 | H  | 3.0483642 2.9911698 0.1341671 |
|20 | H  | 1.8951081 4.0295186 2.1584286 |
|21 | H  | 0.3867636 2.5872098 3.5498997 |
|22 | H  | -1.2721714 -3.3628597 2.7460214 |
|23 | H  | -2.1328733 -2.8773296 5.0191101 |
|24 | H  | -1.7684895 -0.6134081 6.0684463 |
|25 | H  | -0.4549848 1.1142585 4.8487020 |
|26 | N  | 1.3329404 0.2712019 1.2367404 |
|27 | C  | -0.7281873 -0.0738313 -1.6978335 |
|28 | C  | 0.0682062 -0.3455665 -2.8377042 |
|29 | C  | 0.1602890 0.2987836 -4.0637801 |
|30 | C  | -1.1912045 1.2563263 -4.1786851 |
|31 | C  | -1.9875578 1.5500737 -3.0454890 |
|32 | C  | -1.7625880 0.8964494 -1.8360872 |
|33 | H  | 0.8807869 -1.0823544 -2.7715149 |
|34 | H  | 0.4793908 0.0469182 -4.9224714 |
|35 | O  | -1.4906495 1.9459369 -5.3146853 |
|36 | H  | -2.7851059 2.3030503 -3.1476681 |
|37 | H  | -2.3898731 1.1356930 -0.9621762 |
|38 | C  | -0.5628082 -0.7472342 -0.4310331 |
|39 | C  | -1.1738842 -1.1609112 0.6325697 |
|40 | H  | -2.1688995 -1.4811356 0.9544857 |
|41 | C  | -0.7396093 1.6854028 -6.4882063 |
|42 | H  | -1.1636778 2.3394228 -7.2766994 |
|43 | H  | -0.8310382 0.6206259 -6.8093990 |
|44 | H  | 0.3402008 1.9319926 -6.3518091 |

$vibrational spectrum$

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|-----------------|
|   |      |          | cm⁻¹(-1)    | km/mol       | IR | RAMAN |
| 1 | a    | -227.33  | 0.00000     | YES | YES |
| 2 | 0.00  | 0.00000  | - | - |
| 3 | 0.00  | 0.00000  | - | - |
|   | a  |     |          |     |      |     |     |
|---|----|-----|--------|-----|------|-----|-----|
| 4 | 0.00 | 0.00000 | -    | -   |      |    |    |
| 5 | 0.00 | 0.00000 | -    | -   |      |    |    |
| 6 | 0.00 | 0.00000 | -    | -   |      |    |    |
| 7 | 0.00 | 0.00000 | -    | -   |      |    |    |
| 8 | a  | 19.41 | 0.41189 | YES | YES |    |    |
| 9 | a  | 27.78 | 0.54285 | YES | YES |    |    |
|10 | a  | 40.10 | 0.12463 | YES | YES |    |    |
|11 | a  | 54.50 | 0.43267 | YES | YES |    |    |
|12 | a  | 67.65 | 0.31805 | YES | YES |    |    |
|13 | a  | 70.24 | 0.07862 | YES | YES |    |    |
|14 | a  | 86.69 | 0.50336 | YES | YES |    |    |
|15 | a  | 90.08 | 0.47264 | YES | YES |    |    |
|16 | a  | 91.94 | 1.11787 | YES | YES |    |    |
|17 | a  | 100.97 | 0.83703 | YES | YES |    |    |
|18 | a  | 109.03 | 0.03787 | YES | YES |    |    |
|19 | a  | 113.63 | 0.02923 | YES | YES |    |    |
|20 | a  | 123.87 | 0.95877 | YES | YES |    |    |
|21 | a  | 148.01 | 0.67670 | YES | YES |    |    |
|22 | a  | 176.03 | 0.53732 | YES | YES |    |    |
|23 | a  | 181.06 | 1.33249 | YES | YES |    |    |
|24 | a  | 202.81 | 0.52002 | YES | YES |    |    |
|25 | a  | 232.05 | 0.65903 | YES | YES |    |    |
|26 | a  | 233.23 | 0.92839 | YES | YES |    |    |
|27 | a  | 249.69 | 3.09180 | YES | YES |    |    |
|28 | a  | 259.35 | 0.42038 | YES | YES |    |    |
|29 | a  | 278.91 | 0.18843 | YES | YES |    |    |
|30 | a  | 287.88 | 3.04993 | YES | YES |    |    |
|31 | a  | 357.46 | 1.85353 | YES | YES |    |    |
|32 | a  | 367.87 | 5.71411 | YES | YES |    |    |
|33 | a  | 404.64 | 1.03540 | YES | YES |    |    |
|34 | a  | 413.15 | 1.34921 | YES | YES |    |    |
|35 | a  | 422.17 | 1.05395 | YES | YES |    |    |
|36 | a  | 428.34 | 9.27362 | YES | YES |    |    |
|37 | a  | 438.19 | 0.18566 | YES | YES |    |    |
|38 | a  | 449.62 | 3.72182 | YES | YES |    |    |
|39 | a  | 461.50 | 0.42404 | YES | YES |    |    |
|40 | a  | 472.12 | 2.83535 | YES | YES |    |    |
|41 | a  | 479.94 | 1.51383 | YES | YES |    |    |
|42 | a  | 486.82 | 0.41372 | YES | YES |    |    |
|43 | a  | 498.30 | 1.84853 | YES | YES |    |    |
|44 | a  | 507.44 | 9.78614 | YES | YES |    |    |
|45 | a  | 529.46 | 6.30823 | YES | YES |    |    |
|46 | a  | 544.91 | 28.96894 | YES | YES |    |    |
|47 | a  | 545.21 | 18.42229 | YES | YES |    |    |
|48 | a  | 553.60 | 0.31762 | YES | YES |    |    |
|49 | a  | 568.43 | 45.03624 | YES | YES |    |    |
|50 | a  | 610.58 | 21.48888 | YES | YES |    |    |
SCF Energy (au) BP86/SV(P) -2376.678364254
SCF Energy (au) PBE0/def2-TZVPP -2376.251797975
SCF Energy (au) PBE0/def2-TZVPP -2376.2588756073 (Toluene Correction)
Zero Point Energy (au) 0.2815138
Chemical Potential (kJ mol\(^{-1}\)) 593.78
Dispersion Correction (au) PBE0/def2-TZVPP -0.06085022

xyz coordinates

|   |   |   |
|---|---|---|
| Mn | 1.5619780 | 0.3660655 | 0.7861690 |
| C  | 1.9208386 | 0.6208485 | 2.5406451 |
| C  | 3.2541360 | -0.1276676 | 0.4770720 |
| C  | 1.9785849 | 2.0697894 | 0.3569203 |
| O  | 2.2835054 | 3.1695638 | 0.1046869 |
| O  | 4.3562761 | -0.4595864 | 0.281469 |
| O  | 2.1400928 | 0.7768074 | 3.6726748 |
| C  | -1.2440467 | -0.2454675 | 1.5945022 |
| C  | -1.0702898 | 1.9843787 | 0.8796638 |
| C  | -2.4384866 | 2.2155314 | 1.0724391 |
| C  | -3.2360103 | 1.1542217 | 1.5324193 |
| C  | -2.6368801 | -0.0802475 | 1.7882012 |
| C  | -0.5011196 | -1.4767078 | 1.8553073 |
| C  | 0.8563183 | -1.5017281 | 1.4009004 |
| C  | 1.6332937 | -2.6484384 | 1.7196354 |
| C  | 1.0885552 | -3.7252870 | 2.4242352 |
| C  | -0.2647148 | -3.7051008 | 2.8323911 |
| C  | -1.0494699 | -2.5854594 | 2.5475681 |
| H  | -0.4127089 | 2.7847534 | 0.5080550 |
| H  | -2.8564114 | 3.2094672 | 0.8580455 |
| H  | -4.3190959 | 1.2907115 | 1.6852720 |
| H  | -3.2426676 | -0.9298586 | 2.1358996 |
| H  | 2.6853571 | -2.6982887 | 1.3913901 |
| H  | 1.7225618 | -4.5955856 | 2.6642926 |
| H  | -0.6941026 | -4.5576641 | 3.3827492 |
| H  | -2.0952652 | -2.5585120 | 2.8949469 |
| N  | -0.4812431 | 0.7936973 | 1.1302499 |
| C  | 0.3501391 | 0.6559185 | -2.3668529 |
| C  | 0.9112785 | 1.8710060 | -2.8413999 |
| C  | 0.4926697 | 2.4378441 | -4.0527881 |
| C  | -0.5125640 | 1.8032486 | -4.7954455 |
| C  | -1.1025882 | 0.6096096 | -4.3535508 |
| C  | -0.6698862 | 0.0429080 | -3.1497629 |
| H  | 1.6958594 | 2.3738398 | -2.2531371 |
| H  | 0.9341938 | 3.3739313 | -4.4286426 |
| F  | -0.9275114 | 2.3519564 | -5.9545333 |
| F  | -1.8929051 | 0.1390941 | -4.9592008 |
| H  | -1.1268168 | -0.8930985 | -2.7913662 |
| C  | 0.7735382 | 0.0070599 | -1.1487214 |
| C  | 0.9568754 | -1.1398979 | -0.5775206 |
| H  | 1.1704449 | -2.1796208 | -0.8418947 |

$vibrational spectrum$

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|----------------|
|   |      |          | cm\(^{-1}\) | km/mol       | IR  | RAMAN |
| 1 | a    | -227.53  | 0.0000000  | YES | YES |
| 2 | 0.00 | 0.0000000 | - | - | - |
| 3 | 0.00 | 0.0000000 | - | - | - |
| 4 | 0.00 | 0.0000000 | - | - | - |
| 5 | 0.00 | 0.0000000 | - | - | - |
| 6 | 0.00 | 0.0000000 | - | - | - |
| 7 | 0.00 | 0.0000000 | - | - | - |
|   |   |   |   |
|---|---|---|---|
| 8 | a | 19.21 | 0.24348 | YES | YES |
| 9 | a | 23.75 | 0.12982 | YES | YES |
|10 | a | 42.92 | 0.09885 | YES | YES |
|11 | a | 56.70 | 0.11916 | YES | YES |
|12 | a | 70.27 | 0.09686 | YES | YES |
|13 | a | 76.59 | 0.08731 | YES | YES |
|14 | a | 88.98 | 0.27995 | YES | YES |
|15 | a | 92.03 | 0.96432 | YES | YES |
|16 | a | 97.86 | 0.53452 | YES | YES |
|17 | a | 108.76 | 0.12355 | YES | YES |
|18 | a | 110.28 | 0.02049 | YES | YES |
|19 | a | 116.73 | 0.06153 | YES | YES |
|20 | a | 146.46 | 0.79840 | YES | YES |
|21 | a | 177.78 | 0.27680 | YES | YES |
|22 | a | 182.39 | 1.18811 | YES | YES |
|23 | a | 205.49 | 1.46760 | YES | YES |
|24 | a | 233.38 | 0.72356 | YES | YES |
|25 | a | 258.43 | 0.38635 | YES | YES |
|26 | a | 275.64 | 2.52772 | YES | YES |
|27 | a | 278.75 | 0.07715 | YES | YES |
|28 | a | 355.94 | 2.58164 | YES | YES |
|29 | a | 363.22 | 3.60620 | YES | YES |
|30 | a | 388.27 | 5.12682 | YES | YES |
|31 | a | 406.29 | 2.57962 | YES | YES |
|32 | a | 411.37 | 0.41426 | YES | YES |
|33 | a | 423.31 | 3.72845 | YES | YES |
|34 | a | 428.92 | 4.46412 | YES | YES |
|35 | a | 445.07 | 0.06098 | YES | YES |
|36 | a | 456.35 | 2.81889 | YES | YES |
|37 | a | 466.29 | 6.63396 | YES | YES |
|38 | a | 475.36 | 1.39436 | YES | YES |
|39 | a | 486.90 | 0.50086 | YES | YES |
|40 | a | 497.88 | 4.81588 | YES | YES |
|41 | a | 504.43 | 12.18303 | YES | YES |
|42 | a | 516.93 | 6.22702 | YES | YES |
|43 | a | 540.83 | 14.84431 | YES | YES |
|44 | a | 543.79 | 23.93456 | YES | YES |
|45 | a | 553.24 | 0.35600 | YES | YES |
|46 | a | 561.21 | 22.34925 | YES | YES |
|47 | a | 611.02 | 24.09647 | YES | YES |
|48 | a | 620.17 | 2.09154 | YES | YES |
|49 | a | 623.93 | 31.33547 | YES | YES |
|50 | a | 628.11 | 10.34672 | YES | YES |
SCF Energy (au) BP86/SV(P) -2376.669021186
SCF Energy (au) PBE0/def2-TZVPP -2376.243801851
SCF Energy (au) PBE0/def2-TZVPP -2376.2510386261 (Toluene Correction)
Zero Point Energy (au) 0.2813228
Chemical Potential (kJ mol$^{-1}$) 594.57
Dispersion Correction (au) PBE0/def2-TZVPP -0.06310967

$\text{TS}_2\text{Br}^-$

xyz coordinates

Mn 1.1679605 1.7937775 0.3566876
C 1.3550067 2.1748786 2.1202758
C 2.8948304 1.3467086 0.2513224
C 1.5482691 3.4604883 -0.2019107
O 1.8028072 4.5246093 -0.6113293
O 4.0222238 1.0452474 0.1892069
O 1.4715723 2.4296359 3.2510797
C -1.6803990 1.1013854 0.9435919
C -1.5330810 3.3042479 0.1537376
C -2.9181923 2.4080422 0.6542685
C -3.0897143 1.2110733 1.0121351
C -0.9131107 -0.0848258 1.3288097
C -0.4585613 -0.1118585 0.9211469
C 1.2528511 -1.2010783 1.3662344
C -0.7256611 -2.2017573 2.1886064
C -0.6352314 -2.1751473 2.5649013
C -1.4485718 -1.1236896 2.1304586
H -0.8768868 4.1173775 -0.1931761
H -3.3590507 4.4503817 -0.0685604
H -4.8107081 2.5029422 0.7075116
H -3.6879218 0.3476784 1.3392749
H 2.3096177 -1.2610650 1.0582935
H 1.3785562 -3.0180279 2.5406817
H -1.0517775 -2.9678258 3.2072608
H -2.5015099 -1.0854712 2.4550728
N -0.9214283 2.1511209 0.5024351
H 0.6243956 1.8451641 -2.5424786
C 0.6810058 1.3514882 -1.5667166
C 0.6470050 0.1528502 -1.0719944
C 0.8050998 -1.2154115 -1.5896971
C 1.1005693 -3.7481923 -2.7710760
C 2.0104261 -2.7370103 -3.0964077
C 1.8558790 -1.4713673 -2.5055919
C -0.0902993 -2.2668373 -1.2791782
C 0.0471259 -3.5285723 -1.8715097
F 1.2421296 -4.9643436 -3.3325375
H 2.8286622 -2.9435393 -3.8026004
H 2.5658972 -0.6638700 -2.7434700
H -0.9133767 -2.0872068 -0.5704353
H -0.6510337 -4.3494144 -1.6453449

$vibrational$ $spectrum$

| # | mode | symmetry | wave number cm$^{-1}$ | IR intensity km/mol | selection rules |
|---|------|----------|----------------------|---------------------|-----------------|
| 1 | a    | -281.12  | 0.00000              | YES                 | YES             |
| 2 |      | 0.00     | 0.00000              | -                   | -               |
| 3 |      | 0.00     | 0.00000              | -                   | -               |
| 4 |      | 0.00     | 0.00000              | -                   | -               |
| 5 |      | 0.00     | 0.00000              | -                   | -               |
| 6 |      | 0.00     | 0.00000              | -                   | -               |
| 7 |      | 0.00     | 0.00000              | -                   | -               |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 8 | a | 23.06 | 0.43019 | YES | YES |
| 9 | a | 33.28 | 0.22086 | YES | YES |
| 10 | a | 45.13 | 0.06902 | YES | YES |
| 11 | a | 57.85 | 0.03442 | YES | YES |
| 12 | a | 65.73 | 0.24950 | YES | YES |
| 13 | a | 74.52 | 0.20522 | YES | YES |
| 14 | a | 85.64 | 0.15124 | YES | YES |
| 15 | a | 90.27 | 0.39165 | YES | YES |
| 16 | a | 99.81 | 0.62535 | YES | YES |
| 17 | a | 104.52 | 0.34564 | YES | YES |
| 18 | a | 110.26 | 0.08384 | YES | YES |
| 19 | a | 136.48 | 0.24950 | YES | YES |
| 20 | a | 154.01 | 0.08206 | YES | YES |
| 21 | a | 167.10 | 3.25609 | YES | YES |
| 22 | a | 181.48 | 0.60014 | YES | YES |
| 23 | a | 205.28 | 1.40959 | YES | YES |
| 24 | a | 218.29 | 0.72221 | YES | YES |
| 25 | a | 245.32 | 1.21865 | YES | YES |
| 26 | a | 258.04 | 2.84291 | YES | YES |
| 27 | a | 281.62 | 0.30776 | YES | YES |
| 28 | a | 356.45 | 1.45448 | YES | YES |
| 29 | a | 359.88 | 1.62025 | YES | YES |
| 30 | a | 403.54 | 8.10795 | YES | YES |
| 31 | a | 412.41 | 1.13305 | YES | YES |
| 32 | a | 413.93 | 0.24644 | YES | YES |
| 33 | a | 430.46 | 0.39448 | YES | YES |
| 34 | a | 444.28 | 12.65374 | YES | YES |
| 35 | a | 449.03 | 11.34976 | YES | YES |
| 36 | a | 460.93 | 0.31257 | YES | YES |
| 37 | a | 478.37 | 8.32081 | YES | YES |
| 38 | a | 486.58 | 11.15331 | YES | YES |
| 39 | a | 492.15 | 10.15353 | YES | YES |
| 40 | a | 496.96 | 1.50645 | YES | YES |
| 41 | a | 507.24 | 2.14471 | YES | YES |
| 42 | a | 531.58 | 2.35931 | YES | YES |
| 43 | a | 536.44 | 13.07556 | YES | YES |
| 44 | a | 545.62 | 3.08104 | YES | YES |
| 45 | a | 552.27 | 11.54518 | YES | YES |
| 46 | a | 557.93 | 12.44836 | YES | YES |
| 47 | a | 607.80 | 42.28800 | YES | YES |
| 48 | a | 619.49 | 1.47328 | YES | YES |
| 49 | a | 624.35 | 37.81025 | YES | YES |
| 50 | a | 629.46 | 2.75821 | YES | YES |
TS_{23bg}

SCF Energy (au) BP86/SV(P) -2614.32191435
SCF Energy (au) PBE0/def2-TZVPP -2613.93838064
SCF Energy (au) PBE0/def2-TZVPP -2613.945634346 (Toluene Correction)
Zero Point Energy (au) 0.2938786
Chemical Potential (kJ mol\(^{-1}\)) 609.72
Dispersion Correction (au) PBE0/def2-TZVPP -0.06429204

xyz coordinates
44

Mn 1.619926 0.1839127 1.2244550
C 1.9703585 0.4585406 2.9778204
C 3.3203503 -0.2897316 0.9266841
C 2.0127327 1.8912149 0.7828043
O 2.2972423 2.9875574 0.5179697
O 4.4275292 -0.6078570 0.7384601
O 2.1853940 0.6268440 4.1086720
C -1.1792486 -0.4538706 2.0373772
C -1.0355679 1.7700997 1.2989351
C -2.4029705 1.9850299 1.4916835
C -3.1890964 0.9188300 1.9654244
C -2.5732740 -0.305667 2.2331667
C -0.4201235 -1.673136 2.3090137
C 0.9355425 -1.6886456 1.8509875
C 1.7276002 -2.8220221 2.1778069
C 1.2003632 -3.8950022 2.9016578
C -0.1504308 -3.8841555 3.3175383
C -0.9510923 -2.7789871 3.0201217
H -0.3899306 2.5751603 0.9165658
H -2.8381934 2.9706802 1.2663466
H -4.2734418 1.0429133 2.1195872
H -3.1670728 -1.1587135 2.5914871
H 2.779030 -2.8640172 1.8430276
H 1.8459733 -4.7541239 3.1503903
H -0.5662476 -4.7332208 3.8834527
H -1.9950363 -2.7600360 3.3732780
N -0.4304319 0.5901520 1.5618163
C 0.4252095 0.4646606 -1.9214119
C 1.0845783 1.6109801 -2.4406344
C 0.668475 2.1937363 -3.6394776
C -0.4316259 1.6717741 -4.3481923
C -1.1054294 0.5431403 -3.8415792
C -0.6837424 -0.0528002 -2.6485551
H 1.9388036 2.0406499 1.8981213
H 1.1940743 3.0839041 -4.0254955
C -0.8489076 2.2954447 -5.6585145
H -1.9705211 0.1313201 -4.3839526
H -2.180867 0.9313327 -2.2533843
C 0.8396665 -0.1949227 -0.7088548
C 1.0375226 -1.3347500 -0.1287520
H 1.2599484 -2.3733239 -0.3917808
F -0.7199966 3.6466930 -5.6358574
F -2.1388102 2.0147342 -5.9680578
F -0.0882877 1.8497925 -6.6939033

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number cm\(^{-1}\) | IR intensity km/mol | selection rules |
|---|------|---------|-----------------|-----------------|----------------|
| 1 | a | -221.56 | 0.00000 | YES | YES |
| 2 | | 0.00 | 0.00000 | - | - |
| 3 | | 0.00 | 0.00000 | - | - |
| 4 | | 0.00 | 0.00000 | - | - |
|   |   |   | 189   |   |
|---|---|---|-------|---|
| 5 | a |  50.00 |  0.00000 | - | - |
| 6 | a |  50.00 |  0.00000 | - | - |
| 7 | a |  50.00 |  0.00000 | - | - |
| 8 | a |   7.57 |   0.08787 | YES | YES |
| 9 | a |   12.70 |   0.02691 | YES | YES |
|10 | a |   17.57 |   0.40150 | YES | YES |
|11 | a |   39.40 |   0.11062 | YES | YES |
|12 | a |   53.16 |   0.26578 | YES | YES |
|13 | a |   64.57 |   0.09205 | YES | YES |
|14 | a |   68.37 |   0.13503 | YES | YES |
|15 | a |   84.86 |   0.30126 | YES | YES |
|16 | a |   88.58 |   0.21602 | YES | YES |
|17 | a |   90.97 |   0.86229 | YES | YES |
|18 | a |  101.75 |   0.61090 | YES | YES |
|19 | a |  107.00 |   0.11636 | YES | YES |
|20 | a |  111.52 |   0.04179 | YES | YES |
|21 | a |  123.67 |   0.39127 | YES | YES |
|22 | a |  166.48 |   2.85398 | YES | YES |
|23 | a |  169.78 |   0.80858 | YES | YES |
|24 | a |  189.44 |   0.55734 | YES | YES |
|25 | a |  197.50 |   1.45027 | YES | YES |
|26 | a |  205.67 |   1.38839 | YES | YES |
|27 | a |  234.18 |   0.76864 | YES | YES |
|28 | a |  258.19 |   0.93481 | YES | YES |
|29 | a |  278.23 |   0.21455 | YES | YES |
|30 | a |  294.42 |   2.80403 | YES | YES |
|31 | a |  333.91 |  12.63884 | YES | YES |
|32 | a |  358.35 |   1.03901 | YES | YES |
|33 | a |  383.65 |   2.02331 | YES | YES |
|34 | a |  400.39 |   5.40651 | YES | YES |
|35 | a |  402.37 |   1.56811 | YES | YES |
|36 | a |  411.18 |   1.44785 | YES | YES |
|37 | a |  426.61 |  12.14994 | YES | YES |
|38 | a |  435.36 |   0.54616 | YES | YES |
|39 | a |  455.25 |   4.11501 | YES | YES |
|40 | a |  464.66 |   8.39488 | YES | YES |
|41 | a |  466.98 |   0.81202 | YES | YES |
|42 | a |  476.39 |   0.76004 | YES | YES |
|43 | a |  492.10 |  1.01598 | YES | YES |
|44 | a |  497.58 |  11.50701 | YES | YES |
|45 | a |  502.37 |   4.21196 | YES | YES |
|46 | a |  521.29 |   1.91749 | YES | YES |
|47 | a |  542.49 |  12.24062 | YES | YES |
|48 | a |  545.04 |  10.18632 | YES | YES |
|49 | a |  553.10 |   1.46029 | YES | YES |
|50 | a |  564.73 |   0.25262 | YES | YES |
SCF Energy (au) BP86/SV(P) $-2614.309477147$
SCF Energy (au) PBE0/def2-TZVPP $-2613.929233249$
SCF Energy (au) PBE0/def2-TZVPP $-2613.9365857123$ (Toluene Correction)
Zero Point Energy (au) $0.2938482$
Chemical Potential (kJ mol$^{-1}$) $615.77$
Dispersion Correction (au) PBE0/def2-TZVPP $0.06657179$

xyz coordinates

Mn    1.0446202    2.2196695    0.5499048
C     1.1981552    2.6359065    2.3093251
C     2.7832881    1.8101785    0.4800956
C     1.3941553    3.8859223    -0.0312781
O     1.6281967    4.9485527    -0.4553341
O     3.9179773    1.5340174    0.444023
O     1.2902589    2.9124888    3.4368457
C     1.7905760    1.4788949    1.1355548
C     1.6847092    3.6702602    0.3070757
C     3.0724214    3.8273872    0.8344706
C     3.2011110    1.5661279    1.2096823
C     1.0016303    0.3123426    1.5382334
C     0.3728925    0.3073319    1.1399938
C     1.1861554    -0.7613311    1.5995115
C     0.6733319    -1.7655737    2.4267004
C     -0.6892004    -1.7600573    2.7968418
C     -1.5198851    -0.7277174    2.3494605
H     -1.0442952    4.4890153    -0.0557742
H     -0.5311239    7.8083199    0.0735908
H     -4.9451686    2.8235315    0.8929761
H     -3.7832541    0.6993749    1.5562845
H     -2.2456846    -0.8032007    1.2981667
H     -1.3391203    -2.5672179    2.7878006
H     -1.0941491    -2.5549752    3.4437029
H     -2.5744458    -0.7064679    2.6701195
N     -1.0519180    2.5341520    0.6732917
N     -0.5631348    2.2112433    -2.3631115
C     -0.6037548    1.7379934    -1.3765606
C     0.5771495    0.5524922    -0.8521550
C     0.7362246    -0.8300358    -1.3363065
C     1.0549481    -3.4210172    -2.4309260
C     1.0901820    -2.4157620    -2.7184140
C     1.8324125    -1.1303839    -2.1795329
C     -0.2001407    -1.8529545    -1.0541714
C     -0.0489507    -3.1298277    -1.6038352
C     -1.2296801    -4.8283375    -2.9552798
H     -2.8553113    -2.6375007    -3.3665245
H     2.5692766    -0.3425361    -2.4007842
H     -1.0604641    -1.6353141    -0.4029020
H     -0.7948139    -3.9112308    -1.3883314
F     1.5905075    -5.6834771    -1.9621783
F     2.1802621    -4.9093161    -3.9162865
F     0.0749786    -5.3095419    -3.4819251

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number (cm$^{-1}$) | IR intensity (km/mol) | selection rules |
|---|------|----------|-------------------------|----------------------|-----------------|
| 1 | a    |          | -255.12                 | 0.00000              | YES             |
| 2 |      |          | 0.00                    | 0.00000              | -               |
| 3 |      |          | 0.00                    | 0.00000              | -               |
| 4 |      |          | 0.00                    | 0.00000              | -               |
|   |     |               |     |     |      |      |
|---|-----|----------------|-----|-----|------|------|
|   |     | 0.00           |     | 0.00000 | -   | -   |
|   |     | 0.00           |     | 0.00000 | -   | -   |
|   |     | 0.00           |     | 0.00000 | -   | -   |
|   | a   | 19.38          |     | 0.35992 | YES | YES |
|   | a   | 27.80          |     | 0.03761 | YES | YES |
|   | a   | 36.47          |     | 0.52845 | YES | YES |
|   | a   | 39.58          |     | 0.21012 | YES | YES |
|   | a   | 53.23          |     | 0.14211 | YES | YES |
|   | a   | 64.72          |     | 0.08135 | YES | YES |
|   | a   | 68.31          |     | 0.41793 | YES | YES |
|   | a   | 84.55          |     | 0.02591 | YES | YES |
|   | a   | 89.92          |     | 0.66128 | YES | YES |
|   | a   | 98.38          |     | 0.68424 | YES | YES |
|   | a   | 99.94          |     | 0.07422 | YES | YES |
|   | a   | 106.78         |     | 0.31950 | YES | YES |
|   | a   | 114.25         |     | 0.24696 | YES | YES |
|   | a   | 134.60         |     | 0.04530 | YES | YES |
|   | a   | 147.90         |     | 0.70488 | YES | YES |
|   | a   | 158.95         |     | 0.91092 | YES | YES |
|   | a   | 174.99         |     | 0.16022 | YES | YES |
|   | a   | 205.88         |     | 0.13288 | YES | YES |
|   | a   | 222.42         |     | 2.44858 | YES | YES |
|   | a   | 227.63         |     | 0.35744 | YES | YES |
|   | a   | 249.15         |     | 0.21159 | YES | YES |
|   | a   | 278.70         |     | 1.18101 | YES | YES |
|   | a   | 283.25         |     | 0.15136 | YES | YES |
|   | a   | 349.26         |     | 9.91686 | YES | YES |
|   | a   | 359.42         |     | 6.76641 | YES | YES |
|   | a   | 383.55         |     | 2.45183 | YES | YES |
|   | a   | 395.33         |     | 2.70311 | YES | YES |
|   | a   | 398.54         |     | 1.47142 | YES | YES |
|   | a   | 416.19         |     | 6.80839 | YES | YES |
|   | a   | 430.08         |     | 0.93652 | YES | YES |
|   | a   | 447.93         |     | 4.21251 | YES | YES |
|   | a   | 457.31         |     | 0.25923 | YES | YES |
|   | a   | 464.37         |     | 2.95976 | YES | YES |
|   | a   | 475.72         |     | 0.71042 | YES | YES |
|   | a   | 487.97         |     | 2.61682 | YES | YES |
|   | a   | 494.87         |     | 3.04247 | YES | YES |
|   | a   | 509.69         |     | 1.79537 | YES | YES |
|   | a   | 521.65         |     | 1.12330 | YES | YES |
|   | a   | 523.98         |     | 8.59362 | YES | YES |
|   | a   | 536.63         |     | 14.48469 | YES | YES |
|   | a   | 550.84         |     | 2.04644 | YES | YES |
|   | a   | 557.50         |     | 1.58670 | YES | YES |
|   | a   | 570.14         |     | 0.27068 | YES | YES |
TS23bh
SCF Energy (au) BP86/SV(P) -2505.236367416
SCF Energy (au) PBE0/def2-TZVPP -2504.785704894
SCF Energy (au) PBE0/def2-TZVPP -2504.7950366914 (Toluene Correction)
Zero Point Energy (au) 0.3307489
Chemical Potential (kJ mol⁻¹) 706.50
Dispersion Correction (au) PBE0/def2-TZVPP -0.06699044

xyz coordinates
47

Mn  1.6754286 -0.0989474  1.7320687
C  2.0246866  0.1907221  3.4826619
C  3.3761028 -0.5732624  1.4381564
C  2.0663400  1.6058582  1.2761918
O  2.3505924  2.7059428  1.0062560
O  4.4836663 -0.8920963  1.2525671
O  2.2394096  0.3678434  4.6123541
C -1.1236676 -0.7355323  2.5456355
C -0.9827449  1.4824181  1.7886419
C -2.3512267  1.6956683  1.9750354
C -3.1364053  0.6318319  2.4558787
C -2.5185919 -0.5881900  2.8274500
C -0.9942939 -1.9519531  2.3738530
C  1.7871152 -3.0969841  2.7083437
C  1.2591085 -4.1680168  3.4348333
C -0.0931520 -4.1578398  3.8456843
C -0.8945836 -3.0551473  3.5412365
H -0.3378479  2.2853166  1.4005864
H -2.7881502  2.6779311  1.7388707
H -4.2216541  0.7544255  2.6044017
H -3.1116575 -1.4403217  3.0990710
H  2.8387260 -3.1386268  2.3775361
H  1.9051987 -5.0252121  3.6886868
H -0.5096903 -5.0056651  4.4129586
H -1.9400714 -3.0369371  3.8986727
N -0.3756995  0.3062179  2.0637330
C  0.4636371  0.1596775 -1.4108760
C  1.1217846  1.2999242 -1.9468962
C  0.6946638  1.8756950 -3.1472259
C -0.4168376  1.3493412 -3.8430565
C -1.0859068  0.2230198 -3.3128248
C -0.6556187 -0.3642270 -2.1220225
H  1.9853339  1.7276221 -1.4171679
H  1.2213671  2.7505785 -3.5564537
C -0.9245870  1.9319464 -5.1192142
H -1.9516267 -0.1796151 -3.8622928
H -1.1828555 -1.2410020 -1.7133119
C  0.8882290 -0.4932444 -0.2006888
C  1.0969078 -1.6260932  0.3897569
H  1.3282855 -2.6646696  0.1347985
O -0.1900944  3.0065661 -5.5221740
O -1.8845255  1.5108534 -5.7466551
C -0.6152721  3.6178162 -6.7452257
H -0.5710537  2.8924294 -7.5861685
H  0.0841179  4.4583675 -6.9218394
H -1.6584831  3.9917998 -6.6589589

$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm**(-1) km/mol IR RAMAN
1 a -220.95 0.00000 YES YES
|   |   |   |   |   |
|---|---|---|---|---|
| 2 | 0.00 | 0.00000 | - | - |
| 3 | 0.00 | 0.00000 | - | - |
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | 0.00 | 0.00000 | - | - |
| 8 | a | 7.19 | 0.62059 | YES | YES |
| 9 | a | 17.95 | 0.53375 | YES | YES |
| 10 | a | 33.13 | 0.60224 | YES | YES |
| 11 | a | 50.45 | 0.43904 | YES | YES |
| 12 | a | 62.46 | 0.22710 | YES | YES |
| 13 | a | 65.98 | 0.05742 | YES | YES |
| 14 | a | 71.16 | 0.53438 | YES | YES |
| 15 | a | 81.74 | 0.48049 | YES | YES |
| 16 | a | 88.35 | 0.37958 | YES | YES |
| 17 | a | 91.20 | 0.84586 | YES | YES |
| 18 | a | 100.95 | 0.52271 | YES | YES |
| 19 | a | 104.34 | 0.18076 | YES | YES |
| 20 | a | 110.48 | 0.04179 | YES | YES |
| 21 | a | 114.82 | 0.38083 | YES | YES |
| 22 | a | 122.64 | 0.13392 | YES | YES |
| 23 | a | 151.79 | 1.20487 | YES | YES |
| 24 | a | 162.80 | 2.63536 | YES | YES |
| 25 | a | 172.13 | 1.96656 | YES | YES |
| 26 | a | 186.96 | 2.89815 | YES | YES |
| 27 | a | 196.98 | 0.65384 | YES | YES |
| 28 | a | 234.08 | 0.43297 | YES | YES |
| 29 | a | 243.10 | 2.46732 | YES | YES |
| 30 | a | 258.63 | 1.81873 | YES | YES |
| 31 | a | 278.49 | 0.18283 | YES | YES |
| 32 | a | 310.30 | 17.10652 | YES | YES |
| 33 | a | 330.95 | 7.58735 | YES | YES |
| 34 | a | 357.39 | 4.72527 | YES | YES |
| 35 | a | 366.76 | 16.85249 | YES | YES |
| 36 | a | 406.16 | 0.17136 | YES | YES |
| 37 | a | 410.28 | 2.19811 | YES | YES |
| 38 | a | 419.15 | 3.05301 | YES | YES |
| 39 | a | 432.70 | 3.35204 | YES | YES |
| 40 | a | 444.49 | 1.07229 | YES | YES |
| 41 | a | 458.63 | 2.25641 | YES | YES |
| 42 | a | 463.19 | 6.28765 | YES | YES |
| 43 | a | 468.90 | 5.35694 | YES | YES |
| 44 | a | 481.86 | 0.52039 | YES | YES |
| 45 | a | 494.74 | 3.15862 | YES | YES |
| 46 | a | 502.91 | 11.21556 | YES | YES |
| 47 | a | 510.39 | 13.39519 | YES | YES |
| 48 | a | 531.24 | 6.55006 | YES | YES |
| 49 | a | 544.18 | 13.64828 | YES | YES |
| 50 | a | 549.57 | 6.58159 | YES | YES |
TS\textsubscript{23s}

SCF Energy (au) BP86/SV(P)  -2505.225492213
SCF Energy (au) PBE0/def2-TZVPP -2504.775890270
SCF Energy (au) PBE0/def2-TZVPP -2504.7853054603 (Toluene Correction)
Zero Point Energy (au) 0.3306400
Chemical Potential (kJ mol\textsuperscript{-1}) 709.19
Dispersion Correction (au) PBE0/def2-TZVPP -0.06918112

xyz coordinates

| Element | x (Å) | y (Å) | z (Å) |
|---------|-------|-------|-------|
| Mn      | 0.9887955 | 2.7402352 | 0.7706369 |
| C       | 1.0993447 | 3.1983377 | 2.5227002 |
| C       | 2.7327679 | 2.3462166 | 0.7441052 |
| C       | 1.3325783 | 4.3975058 | 0.1610897 |
| O       | 1.5635823 | 5.4539063 | -0.2801258 |
| O       | 3.8701017 | 2.0799175 | 0.7359770 |
| C       | -1.8493390 | 1.9787834 | 3.0698888 |
| O       | -1.7496036 | 4.1506747 | 0.4281616 |
| O       | -3.1406970 | 4.2900659 | 0.4562208 |
| O       | -3.9135692 | 3.2098363 | 0.9170475 |
| C       | -1.0562409 | 0.8339295 | 1.8991227 |
| O       | -0.6232379 | -1.198656 | 2.7438670 |

$vibrational spectrum$

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|-----------------|
| 1 | a    | -279.75  | 0.00000     | YES          | YES             |

S194
|   |     |          |          |     |     |
|---|-----|----------|----------|-----|-----|
| 2 | a   | 0.00     | 0.00000  | -   | -   |
| 3 | a   | 0.00     | 0.00000  | -   | -   |
| 4 | a   | 0.00     | 0.00000  | -   | -   |
| 5 | a   | 0.00     | 0.00000  | -   | -   |
| 6 | a   | 0.00     | 0.00000  | -   | -   |
| 7 | a   | 0.00     | 0.00000  | -   | -   |
| 8 | a   | 17.51    | 0.16059  | YES | YES |
| 9 | a   | 24.76    | 0.87042  | YES | YES |
| 10| a   | 32.68    | 0.08852  | YES | YES |
| 11| a   | 47.97    | 0.12715  | YES | YES |
| 12| a   | 64.95    | 0.28703  | YES | YES |
| 13| a   | 67.25    | 0.27949  | YES | YES |
| 14| a   | 70.35    | 0.90578  | YES | YES |
| 15| a   | 82.07    | 0.00642  | YES | YES |
| 16| a   | 87.39    | 0.43598  | YES | YES |
| 17| a   | 94.66    | 0.19779  | YES | YES |
| 18| a   | 100.79   | 0.72579  | YES | YES |
| 19| a   | 103.57   | 0.34623  | YES | YES |
| 20| a   | 112.09   | 1.05407  | YES | YES |
| 21| a   | 118.76   | 0.83993  | YES | YES |
| 22| a   | 127.62   | 0.31218  | YES | YES |
| 23| a   | 145.61   | 0.61791  | YES | YES |
| 24| a   | 153.40   | 2.18467  | YES | YES |
| 25| a   | 166.37   | 1.25911  | YES | YES |
| 26| a   | 184.68   | 2.11024  | YES | YES |
| 27| a   | 213.11   | 0.34696  | YES | YES |
| 28| a   | 220.16   | 0.27071  | YES | YES |
| 29| a   | 238.70   | 4.94535  | YES | YES |
| 30| a   | 250.11   | 1.12507  | YES | YES |
| 31| a   | 280.11   | 0.16457  | YES | YES |
| 32| a   | 311.94   | 19.32206 | YES | YES |
| 33| a   | 342.79   | 4.65277  | YES | YES |
| 34| a   | 352.63   | 5.38192  | YES | YES |
| 35| a   | 359.74   | 5.76677  | YES | YES |
| 36| a   | 406.74   | 0.90136  | YES | YES |
| 37| a   | 409.68   | 8.43837  | YES | YES |
| 38| a   | 417.12   | 3.65096  | YES | YES |
| 39| a   | 439.06   | 1.80633  | YES | YES |
| 40| a   | 456.81   | 4.34689  | YES | YES |
| 41| a   | 463.91   | 1.20800  | YES | YES |
| 42| a   | 472.63   | 7.62376  | YES | YES |
| 43| a   | 481.41   | 4.75192  | YES | YES |
| 44| a   | 490.61   | 0.25573  | YES | YES |
| 45| a   | 496.13   | 1.41333  | YES | YES |
| 46| a   | 506.21   | 4.74702  | YES | YES |
| 47| a   | 530.13   | 5.95655  | YES | YES |
| 48| a   | 533.50   | 3.73254  | YES | YES |
| 49| a   | 537.58   | 8.44805  | YES | YES |
| 50| a   | 551.81   | 5.46093  | YES | YES |
**TS23h1**

SCF Energy (au) BP86/SV(P) -2508.40094832

SCF Energy (au) PBE0/def2-TZVPP -2507.91553563

SCF Energy (au) PBE0/def2-TZVPP -2507.9234924354 (Toluene Correction)

Zero Point Energy (au) 0.3685873

Chemical Potential (kJ mol⁻¹) 807.17

Dispersion Correction (au) PBE0/def2-TZVPP 0.08050516

xyz coordinates

51

Mn 1.2284099 1.2096656 1.1382910
C 1.5620366 1.5138190 2.8913023
C 2.9273281 0.7258085 0.8612965
C 1.6434711 2.9064109 0.6896087
O 1.9471210 4.0056210 0.4325857
O 4.0370505 0.4075761 0.6800472
O 1.7693929 1.7061248 4.0206092
C -1.5930377 0.6161711 1.9181808
C -1.4230210 2.8073479 1.0951993
C -2.7945880 3.0321862 1.2429397
C -3.5965644 1.9873808 1.7374686
C -2.9914033 0.7740528 2.0703341
C -0.8419187 -0.5904372 2.2596235
C 0.5137302 -0.6407273 1.7985292
C 1.3020194 -1.7491283 2.2092476
C 0.7803488 4.0206092 0.8045580
C -1.9471210 -0.6407273 1.7985292
C -2.7945880 3.0321862 1.2429397
C -3.5965644 1.9873808 1.7374686
C -2.9914033 0.7740528 2.0703341
C -0.8419187 -0.5904372 2.2596235
C 0.5137302 -0.6407273 1.7985292
C 1.3020194 -1.7491283 2.2092476
C 0.7803488 4.0206092 0.8045580
C -1.9471210 -0.6407273 1.7985292
C -2.7945880 3.0321862 1.2429397
C -3.5965644 1.9873808 1.7374686
C -2.9914033 0.7740528 2.0703341
C -0.8419187 -0.5904372 2.2596235
C 0.5137302 -0.6407273 1.7985292
C 1.3020194 -1.7491283 2.2092476
C 0.7803488 4.0206092 0.8045580
C -1.9471210 -0.6407273 1.7985292
C -2.7945880 3.0321862 1.2429397
C -3.5965644 1.9873808 1.7374686
C -2.9914033 0.7740528 2.0703341
C -0.8419187 -0.5904372 2.2596235
C 0.5137302 -0.6407273 1.7985292
C 1.3020194 -1.7491283 2.2092476
C 0.7803488 4.0206092 0.8045580
C -1.9471210 -0.6407273 1.7985292
C -2.7945880 3.0321862 1.2429397
C -3.5965644 1.9873808 1.7374686
| #  | mode | symmetry | wave number (cm^{-1}) | IR intensity (km/mol) | selection rules |
|----|------|----------|-----------------------|-----------------------|-----------------|
| 1  | a    |          | -211.54               | 0.00000               | YES             |
| 2  | a    |          | 0.00                  | 0.00000               | -               |
| 3  | a    |          | 0.00                  | 0.00000               | -               |
| 4  | a    |          | 0.00                  | 0.00000               | -               |
| 5  | a    |          | 0.00                  | 0.00000               | -               |
| 6  | a    |          | 0.00                  | 0.00000               | -               |
| 7  | a    |          | 0.00                  | 0.00000               | -               |
| 8  | a    |          | 16.37                 | 0.10076               | YES             |
| 9  | a    |          | 21.57                 | 0.08172               | YES             |
| 10 | a    |          | 34.25                 | 0.18295               | YES             |
| 11 | a    |          | 36.01                 | 0.54213               | YES             |
| 12 | a    |          | 45.41                 | 0.04774               | YES             |
| 13 | a    |          | 59.27                 | 0.17249               | YES             |
| 14 | a    |          | 60.78                 | 0.21687               | YES             |
| 15 | a    |          | 72.34                 | 0.06198               | YES             |
| 16 | a    |          | 82.06                 | 0.05727               | YES             |
| 17 | a    |          | 90.47                 | 0.01476               | YES             |
| 18 | a    |          | 97.63                 | 0.96153               | YES             |
| 19 | a    |          | 100.50                | 0.54914               | YES             |
| 20 | a    |          | 109.58                | 0.14237               | YES             |
| 21 | a    |          | 119.03                | 0.26936               | YES             |
| 22 | a    |          | 134.60                | 0.28199               | YES             |
| 23 | a    |          | 163.90                | 1.12153               | YES             |
| 24 | a    |          | 169.91                | 0.74455               | YES             |
| 25 | a    |          | 182.93                | 0.83635               | YES             |
| 26 | a    |          | 195.42                | 2.51480               | YES             |
| 27 | a    |          | 222.37                | 2.35535               | YES             |
| 28 | a    |          | 228.13                | 0.18482               | YES             |
| 29 | a    |          | 246.98                | 1.73153               | YES             |
| 30 | a    |          | 254.70                | 0.90979               | YES             |
| 31 | a    |          | 282.61                | 0.22690               | YES             |
| 32 | a    |          | 357.35                | 1.85677               | YES             |
| 33 | a    |          | 376.57                | 1.37678               | YES             |
| 34 | a    |          | 386.15                | 5.82901               | YES             |
| 35 | a    |          | 402.20                | 0.10506               | YES             |
| 36 | a    |          | 403.17                | 0.31570               | YES             |
| 37 | a    |          | 416.22                | 4.47644               | YES             |
| 38 | a    |          | 433.54                | 0.99814               | YES             |
| 39 | a    |          | 438.89                | 1.17057               | YES             |
| 40 | a    |          | 458.10                | 0.65946               | YES             |
| 41 | a    |          | 471.77                | 1.49662               | YES             |
| 42 | a    |          | 475.05                | 1.42520               | YES             |
| 43 | a    |          | 491.89                | 0.85399               | YES             |
| 44 | a    |          | 497.24                | 0.46976               | YES             |
| 45 | a    |          | 503.12                | 0.85840               | YES             |
| 46 | a    |          | 522.33                | 51.85901              | YES             |
| 47 | a    |          | 537.37                | 6.88208               | YES             |
| 48 | a    |          | 545.03                | 6.98089               | YES             |
| 49 | a    |          | 552.23                | 0.60839               | YES             |
| 50 | a    |          | 558.89                | 6.15442               | YES             |
TS23bj

SCF Energy (au) BP86/SV(P) -2360.864038348
SCF Energy (au) PBE0/def2-TZVPP -2360.429227641
SCF Energy (au) PBE0/def2-TZVPP -2360.4352858128 (Toluene Correction)
Zero Point Energy (au) 0.4312018
Chemical Potential (kJ mol⁻¹) 963.71
Dispersion Correction (au) PBE0/def2-TZVPP -0.07320480

xyz coordinates

55

Mn    1.1107140  1.2303049  1.3664159
C     1.4536300  1.4391606  3.1321289
C     2.8216825  0.8326776  1.0473399
C     1.4253820  2.9528506  0.9656235
O     1.6383710  4.0679819  0.6816749
O     3.9410779  0.5625425  0.8435184
O     1.6673532  1.5794104  4.2692846
C     1.6730865  0.4395534  2.1100267
C     1.6057870  2.7156785  1.5460238
C     2.8823322  2.8642757  1.7337919
C     3.7346329  1.7350554  2.1086907
C     3.0747851  0.5186962  2.2928447
C     0.8665972  0.7623583  2.3160031
C     0.4756185  0.7158966  1.8125599
C     1.3177891  1.8216256  2.1160740
C     0.8546450  2.9182694  2.8506572
C     0.4826357  2.9653252  3.3041323
C     1.3333770  1.8882625  3.0373132
H     0.9843578  3.5731816  1.2442892
H     3.4533714  3.8434787  1.5829998
H     4.8252653  1.8056594  2.2523417
H     3.6384380  0.3837800  2.5721509
H     2.3676456  1.8105518  1.7788999
H     1.5448939  3.7457250  3.0870740
H     0.8465513  3.830140  3.8820871
H     2.363460  1.9043005  3.4300284
N     0.9591051  1.5423094  1.7231250
C     0.1966399  1.7365319  1.7972506
C     0.3998843  0.9469695  0.5521279
C     0.4971635  0.2772839  0.1349112
C     0.6203960  0.2772839  0.5923940
H     0.6203238  2.5382729  0.6982553
H     1.5056578  2.1689530  0.3929317
H     0.8285708  2.7767922  0.3683386
C     0.4533369  3.8450511  1.4918898
H     1.0594005  1.9814157  1.0763700
C     1.6815875  4.7616080  1.4184072
H     0.4416387  4.3915483  1.1106373
C     0.2312817  3.6059767  2.5592191
H     1.9058287  5.0516221  0.3672155
C     1.5273465  5.6969813  2.0005963
H     2.587613  4.2585816  1.8259528
C     1.5184950  2.1420550  2.4916082
H     0.4194166  1.1371300  2.5106304
C     0.3910740  2.6606134  1.5826174
H     2.1366295  2.7389659  1.7842564
C     1.2940266  2.9459554  3.7821047
H     2.1069365  1.2223677  2.7176136
C     2.6003986  3.3476417  4.4796392
H     0.7021094  3.8614864  3.5442694
H     0.6646045  2.3496998  4.4845199
### Vibrational Spectrum

| # | Mode | Symmetry | Wave Number | IR Intensity   | Selection Rules |
|---|------|----------|-------------|----------------|-----------------|
| 1 |      | a        | -219.60     | 0.00000        | YES  YES        |
| 2 |      | a        | 0.00        | 0.00000        | -    -          |
| 3 |      | a        | 0.00        | 0.00000        | -    -          |
| 4 |      | a        | 0.00        | 0.00000        | -    -          |
| 5 |      | a        | 0.00        | 0.00000        | -    -          |
| 6 |      | a        | 0.00        | 0.00000        | -    -          |
| 7 |      | a        | 0.00        | 0.00000        | -    -          |
| 8 |      | a        | 6.59        | 0.16626        | YES  YES        |
| 9 |      | a        | 21.63       | 0.11480        | YES  YES        |
| 10|      | a        | 21.79       | 0.04135        | YES  YES        |
| 11|      | a        | 21.87       | 0.04135        | YES  YES        |
| 12|      | a        | 21.97       | 0.04135        | YES  YES        |
| 13|      | a        | 21.97       | 0.04135        | YES  YES        |
| 14|      | a        | 21.97       | 0.04135        | YES  YES        |
| 15|      | a        | 21.97       | 0.04135        | YES  YES        |
| 16|      | a        | 21.97       | 0.04135        | YES  YES        |
| 17|      | a        | 21.97       | 0.04135        | YES  YES        |
| 18|      | a        | 21.97       | 0.04135        | YES  YES        |
| 19|      | a        | 21.97       | 0.04135        | YES  YES        |
| 20|      | a        | 21.97       | 0.04135        | YES  YES        |
| 21|      | a        | 21.97       | 0.04135        | YES  YES        |
| 22|      | a        | 21.97       | 0.04135        | YES  YES        |
| 23|      | a        | 21.97       | 0.04135        | YES  YES        |
| 24|      | a        | 21.97       | 0.04135        | YES  YES        |
| 25|      | a        | 21.97       | 0.04135        | YES  YES        |
| 26|      | a        | 21.97       | 0.04135        | YES  YES        |
| 27|      | a        | 21.97       | 0.04135        | YES  YES        |
| 28|      | a        | 21.97       | 0.04135        | YES  YES        |
| 29|      | a        | 21.97       | 0.04135        | YES  YES        |
| 30|      | a        | 21.97       | 0.04135        | YES  YES        |
| 31|      | a        | 21.97       | 0.04135        | YES  YES        |
| 32|      | a        | 21.97       | 0.04135        | YES  YES        |
| 33|      | a        | 21.97       | 0.04135        | YES  YES        |
| 34|      | a        | 21.97       | 0.04135        | YES  YES        |
| 35|      | a        | 21.97       | 0.04135        | YES  YES        |
| 36|      | a        | 21.97       | 0.04135        | YES  YES        |
| 37|      | a        | 21.97       | 0.04135        | YES  YES        |
| 38|      | a        | 21.97       | 0.04135        | YES  YES        |
| 39|      | a        | 21.97       | 0.04135        | YES  YES        |
| 40|      | a        | 21.97       | 0.04135        | YES  YES        |
| 41|      | a        | 21.97       | 0.04135        | YES  YES        |
| 42|      | a        | 21.97       | 0.04135        | YES  YES        |
| 43|      | a        | 21.97       | 0.04135        | YES  YES        |
| 44|      | a        | 21.97       | 0.04135        | YES  YES        |
| 45|      | a        | 21.97       | 0.04135        | YES  YES        |
| 46|      | a        | 21.97       | 0.04135        | YES  YES        |
| 47|      | a        | 21.97       | 0.04135        | YES  YES        |
| 48|      | a        | 21.97       | 0.04135        | YES  YES        |
| 49|      | a        | 21.97       | 0.04135        | YES  YES        |
| 50|      | a        | 21.97       | 0.04135        | YES  YES        |
### SCF Energy (au) BP86/SV(P)
-2678.188164496

### SCF Energy (au) PBE0/def2-TZVPP
-2677.701903263

### SCF Energy (au) PBE0/def2-TZVPP (Toluene Correction)
-2677.7129455643

### Zero Point Energy (au)
0.4155167

### Chemical Potential (kJ mol\(^{-1}\))
916.38

### Dispersion Correction (au) PBE0/def2-TZVPP
0.08439631

### xyz coordinates

| Mn    | 0.9098750 | 1.8356666 | -0.2916640 |
|-------|-----------|-----------|------------|
| C     | 1.2396347 | 1.7871900 | 1.4765609  |
| C     | 2.6475571 | 1.4826921 | -0.6359753 |
| C     | 1.2684348 | 3.6041827 | -0.4316902 |
| O     | 1.5234693 | 4.7442112 | -0.4771170 |
| O     | 3.7804513 | 1.3542633 | -0.8649219 |
| O     | 1.4479138 | 1.7134857 | 2.6212918  |
| C     | -1.8802210| 1.0356747 | 0.3493143  |
| C     | -1.7800896| 3.3400611 | -0.0736442 |
| C     | -3.1543107| 3.4950630 | 0.1368629  |
| C     | -3.9182654| 2.3601831 | 0.4620128  |
| C     | -3.2752138| 1.1242711 | 0.5635844  |
| C     | -1.0968017| -0.1954282| 0.4200711  |
| O     | 0.2443544 | -0.0788298| 0.0221512  |
| C     | 1.1020101 | -1.2669893| 0.0707704  |
| N     | 0.5215603 | -2.457193 | 0.6223414  |
| C     | -0.8134899| -2.5505430| 0.9935413  |
| C     | -1.6291399| -1.4425809| 0.8747245  |
| O     | 2.2686222 | -1.2951855| -0.3465440 |
| C     | -1.3307536| -3.8699686| 1.5038338  |
| N     | -1.1477021| 2.1506025 | 0.0307723  |
| C     | -0.2902579| 2.7328610 | -3.345501  |
| C     | 0.3587554 | 3.9618873 | -3.635746  |
| C     | -0.1252227| 4.8024539 | -4.6468580 |
| C     | -1.2719680| 4.4519655 | -5.3818446 |
| C     | -1.9313876| 3.2424671 | -5.0980075 |
| C     | -1.4509279| 2.3912803 | -4.0941614 |
| C     | 0.1940592 | 1.8083271 | -2.3515034 |
| C     | 0.4807960 | 0.6193957 | -1.9634753 |
| H     | -1.1527441| 4.2049584 | -0.3367287 |
| H     | -3.6108193| 4.4924433 | 0.0431678  |
| H     | -5.0045652| 2.4403470 | 0.6306485  |
| H     | -3.8477972| 0.2165580 | 0.8036044  |
| H     | -2.6803769| -1.5363013| 1.1820166  |
| H     | 1.2573669 | 4.2480346 | -3.0692580 |
| H     | 0.4019777 | 5.7466836 | -4.8629965 |
| H     | -1.6512502| 5.1200554 | -6.1726422 |
| H     | -2.8320578| 2.9567922 | -5.6672691 |
| H     | -1.9685037| 1.4439589 | -3.8730518 |
| H     | 0.8582417 | -0.3508818| -2.3010040 |
| H     | -2.3920439| -3.7659231| 1.8075188  |
| H     | -0.7512141| -4.2328524| 2.3812089  |
| H     | -1.2788372| -4.6654035| 0.7251127  |
| C     | 1.4364970 | -3.5980294| 0.7741268  |
| C     | 1.8947015 | -3.8576669| 2.2018580  |
| H     | 2.3122862 | -3.335121 | 0.1421400  |
| H     | 0.9677445 | -4.5078727| 0.3462925  |
| C     | 2.8641164 | -4.3778490| 4.8109069  |
| C     | 2.6104896 | -5.4404944| 3.9273811  |
| C     | 2.1261966 | -5.1802333| 2.6345091  |
| C     | 2.1530863 | -2.7975710| 3.0957061  |
| C     | 2.6320497 | -3.0567575| 4.3904190  |
| #  | mode | symmetry | wave number | IR intensity | selection rules |
|----|------|----------|-------------|--------------|----------------|
| 1  | a    | -158.39  | 0.00000     | YES          | YES            |
| 2  | a    | 0.00     | 0.00000     | -            | -              |
| 3  | a    | 0.00     | 0.00000     | -            | -              |
| 4  | a    | 0.00     | 0.00000     | -            | -              |
| 5  | a    | 0.00     | 0.00000     | -            | -              |
| 6  | a    | 0.00     | 0.00000     | -            | -              |
| 7  | a    | 0.00     | 0.00000     | -            | -              |
| 8  | a    | 16.31    | 0.16610     | YES          | YES            |
| 9  | a    | 19.21    | 0.14140     | YES          | YES            |
| 10 | a    | 20.70    | 0.05217     | YES          | YES            |
| 11 | a    | 24.15    | 0.13533     | YES          | YES            |
| 12 | a    | 28.69    | 0.60836     | YES          | YES            |
| 13 | a    | 43.50    | 0.11576     | YES          | YES            |
| 14 | a    | 55.93    | 2.17310     | YES          | YES            |
| 15 | a    | 70.63    | 0.18942     | YES          | YES            |
| 16 | a    | 75.08    | 0.18011     | YES          | YES            |
| 17 | a    | 83.27    | 0.01423     | YES          | YES            |
| 18 | a    | 85.27    | 0.56858     | YES          | YES            |
| 19 | a    | 97.48    | 0.55006     | YES          | YES            |
| 20 | a    | 103.95   | 0.30751     | YES          | YES            |
| 21 | a    | 111.46   | 0.39234     | YES          | YES            |
| 22 | a    | 115.39   | 0.63150     | YES          | YES            |
| 23 | a    | 126.26   | 0.45633     | YES          | YES            |
| 24 | a    | 145.84   | 0.24780     | YES          | YES            |
| 25 | a    | 153.38   | 0.50353     | YES          | YES            |
| 26 | a    | 162.83   | 0.10641     | YES          | YES            |
| 27 | a    | 192.28   | 0.83006     | YES          | YES            |
| 28 | a    | 192.55   | 0.52243     | YES          | YES            |
| 29 | a    | 204.96   | 1.16647     | YES          | YES            |
| 30 | a    | 213.33   | 0.26692     | YES          | YES            |
| 31 | a    | 245.14   | 0.49944     | YES          | YES            |
| 32 | a    | 252.28   | 0.39293     | YES          | YES            |
| 33 | a    | 255.49   | 0.28550     | YES          | YES            |
| 34 | a    | 260.15   | 1.10096     | YES          | YES            |
| 35 | a    | 305.23   | 0.85843     | YES          | YES            |
| 36 | a    | 326.12   | 2.04965     | YES          | YES            |
| 37 | a    | 350.42   | 7.12781     | YES          | YES            |
| 38 | a    | 368.62   | 4.52977     | YES          | YES            |
| 39 | a    | 383.52   | 3.78026     | YES          | YES            |
| 40 | a    | 400.95   | 0.02287     | YES          | YES            |
| 41 | a    | 401.52   | 0.22387     | YES          | YES            |
| 42 | a    | 411.81   | 10.99243    | YES          | YES            |
| 43 | a    | 430.02   | 7.43046     | YES          | YES            |
| 44 | a    | 440.22   | 13.87203    | YES          | YES            |
| 45 | a    | 450.45   | 13.59888    | YES          | YES            |
| 46 | a    | 460.14   | 1.30985     | YES          | YES            |
| 47 | a    | 464.12   | 4.29608     | YES          | YES            |
| 48 | a    | 468.65   | 9.67586     | YES          | YES            |
| 49 | a    | 478.93   | 0.85227     | YES          | YES            |
| 50 | a    | 492.04   | 2.00409     | YES          | YES            |
**TS23ca**

SCF Energy (au) BP86/SV(P)  
-2678.177478525

SCF Energy (au) PBE0/def2-TZVPP  
-2677.690686045

SCF Energy (au) PBE0/def2-TZVPP (Toluene Correction)  
-2677.7015428126

Zero Point Energy (au)  
0.4152541

Chemical Potential (kJ mol\(^{-1}\))  
916.57

Dispersion Correction (au) PBE0/def2-TZVPP  
0.08703529

xyz coordinates

Mn 0.7138071 2.8980516 -0.5336869
C 1.1068390 2.9124074 1.2304921
C 2.4330774 2.5191573 -0.9176994
C 1.0673393 4.6427539 -0.8047677
O 1.2919132 5.7699489 -1.0160662
O 3.5587450 2.3776686 -1.1815661
O 1.3553517 2.9018747 2.3702301
C -2.1057198 2.1386502 0.1223057
C -1.9501941 4.4577347 -0.1693790
C -3.3216873 4.6340174 0.0451723
C -4.1161799 3.4991076 0.2881568
C -3.5023884 2.2449093 0.1766645
C -0.0125015 0.9761958 -0.2680189
C 0.8685198 -0.1849968 -0.0775572
N 0.2665812 -1.3659019 0.4587460
C -1.0716427 -1.4466455 0.8181379
C -1.8769306 -0.308541 0.6869901
O 2.0773055 -0.1866064 -0.3435158
C -1.6044607 -2.7531520 1.3442330
N -1.3467834 3.2502233 -0.1343219
H -0.1032397 3.4828033 -3.3241380
C 0.0146097 2.8232305 -2.4592061
C 0.0568635 1.5599712 -2.1817017
H -1.2997601 5.3214130 -0.376251
H -3.7533767 5.6464581 0.0168647
H -5.2027305 3.5943436 0.4475574
H -4.0977751 1.3370573 0.4986173
H -2.9203268 -0.4004872 1.0261529
C 0.1335619 0.2634315 -2.8797375
H -2.6641268 -2.6326257 1.6477354
H -1.0283502 -3.1150192 2.2242253
H -1.5641031 -3.5554622 0.5720072
C 1.1742491 -2.5126875 0.6429649
C 1.6278683 -2.7425968 2.0771552
H 2.0556937 -2.2718138 0.0110307
H 0.6944240 -3.4261753 0.2371900
C 2.5715018 -3.2122539 4.7051519
C 2.2125776 -4.2920695 3.8813847
C 1.7410718 -4.0560628 2.5787635
C 1.9956023 -1.6648834 2.9105629
C 2.4601761 -1.8991837 4.2149380
H 2.9379800 -3.3932633 5.7292854
H 2.2948495 -5.3264140 4.2551135
H 1.4581802 -4.9098036 1.9380594
H 1.9264470 -0.6309753 2.5351710
H 2.7442227 -1.0452621 4.8521320
C 0.2436835 -2.1439634 -4.3543183
C 1.4121581 -1.3909553 -4.1411569
C 1.3624037 -0.1939805 -3.4101481
C -1.0348033 -0.5068422 -3.0829668
C -0.9801775 -1.6970952 -3.8257625
| #  | mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules | IR | Raman |
|---|------|----------|---------------------|---------------------|-----------------|----|-------|
| 1 | a    | -281.77  | 0.00000             | YES                 | 0.11677         | YES| YES   |
| 2 | a    | 0.00     | 0.00000             | -                   | 0.48793         | YES| YES   |
| 3 | a    | 23.35    | 0.50714             | YES                 | 0.50714         | YES| YES   |
| 4 | a    | 27.88    | 0.38305             | YES                 | 0.38305         | YES| YES   |
| 5 | a    | 35.47    | 0.34503             | YES                 | 0.34503         | YES| YES   |
| 6 | a    | 41.64    | 0.12674             | YES                 | 0.12674         | YES| YES   |
| 7 | a    | 45.75    | 0.06490             | YES                 | 0.06490         | YES| YES   |
| 8 | a    | 64.64    | 1.23398             | YES                 | 1.23398         | YES| YES   |
| 9 | a    | 79.99    | 0.08681             | YES                 | 0.08681         | YES| YES   |
| 10| a    | 81.42    | 0.30846             | YES                 | 0.30846         | YES| YES   |
| 11| a    | 86.23    | 0.18885             | YES                 | 0.18885         | YES| YES   |
| 12| a    | 86.86    | 2.02877             | YES                 | 2.02877         | YES| YES   |
| 13| a    | 100.20   | 0.10912             | YES                 | 0.10912         | YES| YES   |
| 14| a    | 112.65   | 1.15652             | YES                 | 1.15652         | YES| YES   |
| 15| a    | 117.48   | 0.75015             | YES                 | 0.75015         | YES| YES   |
| 16| a    | 127.85   | 0.27572             | YES                 | 0.27572         | YES| YES   |
| 17| a    | 145.38   | 0.60008             | YES                 | 0.60008         | YES| YES   |
| 18| a    | 159.80   | 0.21392             | YES                 | 0.21392         | YES| YES   |
| 19| a    | 176.84   | 5.07115             | YES                 | 5.07115         | YES| YES   |
| 20| a    | 185.84   | 0.24957             | YES                 | 0.24957         | YES| YES   |
| 21| a    | 191.89   | 0.82374             | YES                 | 0.82374         | YES| YES   |
| 22| a    | 198.90   | 2.00031             | YES                 | 2.00031         | YES| YES   |
| 23| a    | 206.45   | 2.92257             | YES                 | 2.92257         | YES| YES   |
| 24| a    | 229.40   | 0.29347             | YES                 | 0.29347         | YES| YES   |
| 25| a    | 239.23   | 0.17811             | YES                 | 0.17811         | YES| YES   |
| 26| a    | 250.82   | 0.28528             | YES                 | 0.28528         | YES| YES   |
| 27| a    | 260.98   | 0.06373             | YES                 | 0.06373         | YES| YES   |
| 28| a    | 293.01   | 0.12201             | YES                 | 0.12201         | YES| YES   |
| 29| a    | 319.69   | 4.39261             | YES                 | 4.39261         | YES| YES   |
| 30| a    | 337.75   | 4.13786             | YES                 | 4.13786         | YES| YES   |
| 31| a    | 364.47   | 3.52406             | YES                 | 3.52406         | YES| YES   |
| 32| a    | 387.66   | 2.19276             | YES                 | 2.19276         | YES| YES   |
| 33| a    | 400.14   | 0.42898             | YES                 | 0.42898         | YES| YES   |
| 34| a    | 401.41   | 0.15064             | YES                 | 0.15064         | YES| YES   |
| 35| a    | 426.70   | 1.66304             | YES                 | 1.66304         | YES| YES   |
| 36| a    | 441.21   | 13.80089            | YES                 | 13.80089        | YES| YES   |
| 37| a    | 447.88   | 0.16682             | YES                 | 0.16682         | YES| YES   |
| 38| a    | 456.14   | 2.72252             | YES                 | 2.72252         | YES| YES   |
| 39| a    | 463.93   | 2.63819             | YES                 | 2.63819         | YES| YES   |
| 40| a    | 466.75   | 2.08337             | YES                 | 2.08337         | YES| YES   |
| 41| a    | 478.66   | 1.74876             | YES                 | 1.74876         | YES| YES   |
| 42| a    | 489.42   | 2.32141             | YES                 | 2.32141         | YES| YES   |
| 43| a    | 498.68   | 7.04635             | YES                 | 7.04635         | YES| YES   |
SCF Energy (au) BP86/SV(P) -2408.995112972
SCF Energy (au) PBE0/def2-TZVPP -2408.528811114
SCF Energy (au) PBE0/def2-TZVPP -2408.5368518917 (Toluene Correction)
Zero Point Energy (au) 0.3176652
Chemical Potential (kJ mol\(^{-1}\)) 684.72
Dispersion Correction (au) PBE0/def2-TZVPP -0.06668154

xyz coordinates
45

Mn  1.7275223  0.7999167  0.3898309
C   2.0895483  1.0816028  2.1407390
C   3.4216148  0.2952688  0.0980376
C   2.1216996  2.5065434 -0.0548414
O   2.3942681  3.6123101 -0.3122392
O   4.5224521 -0.0452347 -0.0826326
O   2.3138259  1.2506852  3.2695325
C   1.0696555 -0.1494737  1.1735573
C   0.9452402  2.3772016  0.4726763
C   2.3206936  2.5655412  0.6310084
C   3.0971991  1.4675657  1.0421106
C   2.4752166  0.2452548  1.3058193
N   -0.3278659 -0.9901403  1.4304791
C   1.0302861  1.0331570  0.9837798
C   1.5669268 -2.2391538  1.4195374
C   0.5609475 -2.9614117  2.1463357
C   -0.6310173 -2.1594269  2.1567726
H   -0.3007874  3.1946902  0.1159326
H   -2.7694426  3.5462976  0.4137220
H   -4.1910040  1.5577266  1.1436460
H   -3.0675080 -0.6361346  1.5774146
H   -2.5910470 -2.5809008  1.2200111
C   -1.7803764 -2.5716864  2.8541962
N   -0.3242258  1.2063843  0.7356993
C   0.6087933  1.1297135 -2.7764697
C   1.3596298  2.2162507 -3.2967806
C   0.9857201 -2.8322139 -4.4990762
C   -0.1538459  2.4000883 -5.2007365
C   -0.9146119  1.3319305 -5.6916026
C   -0.5397590  0.7002888 -3.4987574
H   2.2522018  2.5678695 -2.7584966
H   1.5912388  3.6665749 -4.8906988
H   -0.4499531  2.8952950 -6.1401784
H   -1.8107552  0.9834489 -5.2321667
H   -1.1363767 -0.1372632 -3.1019966
C   0.9754901  0.4321249 -1.5662732
C   1.1101977 -0.7218231 -1.0021441
H   1.2974738 -1.7667095 -1.2600597
C   -1.7454693 -3.8123328  3.5148773
H   -2.6863943 -1.9549698  2.9228964
H   -2.6384791 -4.1486237  4.0663696
C   -0.5891616 -4.6246356  3.4900499
H   -0.5951833 -5.5931240  4.0167712
C   0.5654396 -4.2057824  2.8175284
H   1.4741595 -4.8294912  2.8158191

$vibrational spectrum$
# mode  symmetry wave number IR intensity selection rules
  1    a         -237.37    0.00000   YES   YES
  2                        0.00    0.00000   -     -
  3                        0.00    0.00000   -     -
|   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
|4  |0.00|0.00000| - | - |
|5  |0.00|0.00000| - | - |
|6  |0.00|0.00000| - | - |
|7  |0.00|0.00000| - | - |
|8  | a |16.90|0.00794|YES|YES |
|9  | a |27.26|0.08611|YES|YES |
|10 | a |33.16|0.11095|YES|YES |
|11 | a |54.27|0.16625|YES|YES |
|12 | a |68.89|0.30671|YES|YES |
|13 | a |73.22|0.49740|YES|YES |
|14 | a |76.42|0.13529|YES|YES |
|15 | a |84.67|0.22794|YES|YES |
|16 | a |93.42|0.06507|YES|YES |
|17 | a |100.15|0.60557|YES|YES |
|18 | a |107.55|0.04497|YES|YES |
|19 | a |128.61|0.17288|YES|YES |
|20 | a |137.13|0.25235|YES|YES |
|21 | a |158.03|4.13126|YES|YES |
|22 | a |169.02|0.72987|YES|YES |
|23 | a |200.40|1.72411|YES|YES |
|24 | a |211.16|2.18243|YES|YES |
|25 | a |236.27|3.70321|YES|YES |
|26 | a |239.25|2.39867|YES|YES |
|27 | a |250.95|1.06395|YES|YES |
|28 | a |300.23|1.10439|YES|YES |
|29 | a |336.42|8.93386|YES|YES |
|30 | a |362.82|4.04049|YES|YES |
|31 | a |364.60|3.32119|YES|YES |
|32 | a |400.79|6.52216|YES|YES |
|33 | a |402.21|0.08097|YES|YES |
|34 | a |425.77|8.35193|YES|YES |
|35 | a |433.33|1.36559|YES|YES |
|36 | a |451.84|7.72534|YES|YES |
|37 | a |467.18|1.43404|YES|YES |
|38 | a |482.53|1.07415|YES|YES |
|39 | a |489.01|7.91623|YES|YES |
|40 | a |497.36|1.87821|YES|YES |
|41 | a |502.11|2.52264|YES|YES |
|42 | a |513.86|2.19350|YES|YES |
|43 | a |528.63|4.72170|YES|YES |
|44 | a |536.72|19.06779|YES|YES |
|45 | a |546.95|16.32610|YES|YES |
|46 | a |566.74|0.55150|YES|YES |
|47 | a |573.19|9.51230|YES|YES |
|48 | a |590.52|8.76627|YES|YES |
|49 | a |605.37|8.55967|YES|YES |
|50 | a |611.88|3.41869|YES|YES |
TS23da'

SCF Energy (au) BP86/SV(P) -2408.986641492
SCF Energy (au) PBE0/def2-TZVPP -2408.520986012
SCF Energy (au) PBE0/def2-TZVPP -2408.5290620226 (Toluene Correction)
Zero Point Energy (au) 0.3174132
Chemical Potential (kJ mol⁻¹) 684.77
Dispersion Correction (au) PBE0/def2-TZVPP -0.06880878

xyz coordinates
45

Mn    1.3929405    2.1179321    0.0346053
C     1.5920354    2.4758324    1.8024534
C     3.1193805    1.6611721 -0.0761235
C     1.7583553    3.8001150 -0.4949705
O     1.9946440    4.8771940 -0.879786
O     4.2431992    1.3514463 -0.1390355
O     1.7222591    2.7126864  2.9351880
C     1.4348519    1.3721376  0.6037112
C     1.3380177    3.5979133 -0.0999468
C     2.7269111    3.7407853 -0.0340012
C     3.4928823    2.6191133  0.3312722
C     2.8484693    1.4195798  0.6425246
N     0.6766299    0.2559087  0.9168210
C     0.7030024    0.2367931  0.5363423
C     1.2498842    0.9340909  1.0457297
C     0.2394481    1.6424615  0.5363423
C     0.9732203    0.8764538  1.7014801
H     0.6975913    4.4361886 -0.4145309
H     3.1929470    4.7058657 -0.2834772
H     4.5933515    2.6730763  0.3596596
H     3.4263285    0.5176568  0.8777316
H     2.2870153    1.2597861  0.8958340
C     2.1347038    1.2771427  2.3859537
N     0.6966783    2.4499950  0.2097932
C     0.8708690    2.2675579  2.8666379
C     0.9239950    1.7187705  1.9211631
C     0.8921691    0.5014069  1.4887468
C     1.0615201    0.8629432  2.0061543
H     2.0883262    2.4734346  3.1229722
H     3.0576234    0.6815185  2.3865140
H     2.9892199    2.8001588  3.6674636
C     0.9111694    3.2539717  3.1835882
H     0.9094097    4.1884285  3.7685879
C     0.2537007    2.8445431  2.5232639
H     1.1781725    3.4410599  2.5878421
C     1.3873297    3.4133154  3.1850301
H     2.3456125    3.1695796  3.4036839
C     2.1833224    1.1849638  2.8239487
C     1.079126    1.8843728  1.7845339
C     0.2664994    3.1444326  2.3776991
H     1.5134272    4.4086686  3.6423504
H     3.2295294    2.6135106  4.0305493
H     2.9334823    0.3513558  2.9890131
H     0.7698230    1.6806500  1.1517711
H     0.4915512    3.9263131  2.2055020

$vibrational spectrum

# mode symmetry wave number IR intensity selection rules
#                          cm⁻¹   km/mol     IR     RAMAN
1   a   -287.02  0.00000  YES     YES
2   b   0.00   0.00000  -       -
|   |     |     |     |
|---|-----|-----|-----|
| 3 | 0.00 | 0.0000 | -   |
| 4 | 0.00 | 0.0000 | -   |
| 5 | 0.00 | 0.0000 | -   |
| 6 | 0.00 | 0.0000 | -   |
| 7 | 0.00 | 0.0000 | -   |
| 8 | a   | 20.67 | 0.60655 | YES | YES |
| 9 | a   | 28.74 | 0.41890 | YES | YES |
|10 | a   | 42.36 | 0.06185 | YES | YES |
|11 | a   | 48.42 | 0.04076 | YES | YES |
|12 | a   | 62.97 | 0.44129 | YES | YES |
|13 | a   | 71.63 | 0.08685 | YES | YES |
|14 | a   | 77.65 | 0.26895 | YES | YES |
|15 | a   | 86.77 | 0.22815 | YES | YES |
|16 | a   | 89.66 | 0.18222 | YES | YES |
|17 | a   | 96.58 | 0.02826 | YES | YES |
|18 | a   | 102.25| 0.40104 | YES | YES |
|19 | a   | 131.02| 0.25623 | YES | YES |
|20 | a   | 132.36| 0.74006 | YES | YES |
|21 | a   | 161.35| 2.79207 | YES | YES |
|22 | a   | 176.38| 7.58770 | YES | YES |
|23 | a   | 197.25| 1.11695 | YES | YES |
|24 | a   | 205.64| 1.84132 | YES | YES |
|25 | a   | 228.37| 3.45277 | YES | YES |
|26 | a   | 233.19| 0.79052 | YES | YES |
|27 | a   | 255.52| 1.79123 | YES | YES |
|28 | a   | 300.11| 0.94208 | YES | YES |
|29 | a   | 326.31| 4.03321 | YES | YES |
|30 | a   | 363.15| 4.81019 | YES | YES |
|31 | a   | 367.03| 1.79414 | YES | YES |
|32 | a   | 402.97| 0.07985 | YES | YES |
|33 | a   | 416.28| 5.42703 | YES | YES |
|34 | a   | 433.86| 0.86468 | YES | YES |
|35 | a   | 456.32| 1.84925 | YES | YES |
|36 | a   | 458.93| 1.96833 | YES | YES |
|37 | a   | 474.37| 5.79367 | YES | YES |
|38 | a   | 484.31| 0.73568 | YES | YES |
|39 | a   | 493.32| 9.72999 | YES | YES |
|40 | a   | 497.86| 19.72214| YES | YES |
|41 | a   | 504.56| 1.35928 | YES | YES |
|42 | a   | 516.71| 2.70257 | YES | YES |
|43 | a   | 530.08| 20.04411| YES | YES |
|44 | a   | 538.14| 5.12531 | YES | YES |
|45 | a   | 554.22| 11.05044| YES | YES |
|46 | a   | 555.69| 18.32082| YES | YES |
|47 | a   | 567.67| 1.46299 | YES | YES |
|48 | a   | 591.43| 10.61040| YES | YES |
|49 | a   | 611.96| 3.40366 | YES | YES |
|50 | a   | 613.21| 0.62181 | YES | YES |
TS23aa

SCF Energy (au) BP86/SV(P) -2583.753044495
SCF Energy (au) PBE0/def2-TZVPP -2583.299586047
SCF Energy (au) PBE0/def2-TZVPP -2583.3092723309 (Toluene Correction)
Zero Point Energy (au) 0.3857030
Chemical Potential (kJ mol⁻¹) 843.61
Dispersion Correction (au) PBE0/def2-TZVPP -0.07220089

xyz coordinates

Mn 2.3833058 0.8483205 0.3108484
C 2.6727450 1.1691657 2.0615271
C 4.1166155 0.4487440 0.0725329
C 2.6466621 2.5783517 -0.1538424
O 2.8190904 3.7029692 -0.4141811
O 5.2432486 0.1718222 -0.0696683
O 2.8494658 1.3606284 3.1967976
C -0.4004547 0.1554101 0.9220468
C -1.8785234 0.2888813 0.9662264
C 0.3311949 -1.0383896 1.3080514
C 1.7274833 -1.0184595 0.9764134
C 2.5353600 -2.1001426 1.415396
C 1.9793464 -2.3120991 2.1320991
C 0.5878700 -2.1397654 2.4353188
C -0.2173080 -2.1328742 2.0301947
H 3.6098354 -2.0926353 1.1731258
O 2.6855051 -4.2349131 2.6000951
H 0.1863604 -4.0397473 3.0079205
H -1.2853858 -2.1288642 2.3014784
N 0.3690596 1.1381350 0.5004391
C 1.2656167 0.9684925 -2.9026942
C 1.7993636 2.1870718 -3.3979245
C 1.3830038 2.7006197 -4.6345102
C 0.4137082 2.0276644 -5.395675
C -0.1341568 0.8245695 -4.9168780
C 0.2844428 0.2986441 -3.6880383
H 2.5531545 2.7282996 -2.8080934
H 1.8191197 3.6441258 -5.0027592
H 0.0829049 2.4402888 -6.3669099
H -0.8972491 0.2883857 -5.5058238
H -0.1471660 -0.6420084 -3.3100178
C 1.6874677 0.3688457 -1.6591208
C 1.9467988 -0.7307784 -1.0314793
H 2.2581332 -1.7603291 -1.2274445
H -4.7037107 0.6189425 0.9711380
C -4.1194987 -0.5712115 0.4755624
C -2.7330312 -0.7332381 0.4793554
C -2.4747491 1.4726042 1.4537188
C -3.8675218 1.6450218 1.4648803
O -6.0608174 0.6777296 0.9309396
H -4.7856424 -1.3557750 0.0837907
H -2.2967469 -1.6576109 0.0685523
H -1.8356938 2.2731621 1.8627868
H -4.2889202 2.5770713 1.8687505
H -0.1328790 1.9651192 0.1475545
C 4.0842964 -4.2897159 2.3632922
C -6.7122521 1.8464633 1.4041348
H 4.6123053 -3.4217927 2.8227643
H 4.3166356 -4.3214205 1.2730434
H 4.4385375 -5.2266522 2.8382625
H -6.5048590 2.0246182 2.4856943
H -7.7977912 1.6687913 1.2676145
| # | mode | symmetry | wave number cm\(^{-1}\) | IR intensity km/mol | selection rules |
|---|-----|---------|-------------------------|---------------------|-----------------|
| 1 | a   | -208.55 | 0.00000 | YES | YES |
| 2 | a   | 0.00 | 0.00000 | - | - |
| 3 | a   | 0.00 | 0.00000 | - | - |
| 4 | a   | 0.00 | 0.00000 | - | - |
| 5 | a   | 0.00 | 0.00000 | - | - |
| 6 | a   | 0.00 | 0.00000 | - | - |
| 7 | a   | 0.00 | 0.00000 | - | - |
| 8 | a   | 15.47 | 0.07161 | YES | YES |
| 9 | a   | 16.51 | 0.10232 | YES | YES |
| 10 | a | 33.01 | 0.47225 | YES | YES |
| 11 | a | 38.56 | 0.38207 | YES | YES |
| 12 | a | 43.92 | 0.70894 | YES | YES |
| 13 | a | 46.39 | 0.32732 | YES | YES |
| 14 | a | 61.18 | 0.20756 | YES | YES |
| 15 | a | 73.20 | 0.46680 | YES | YES |
| 16 | a | 75.48 | 0.18658 | YES | YES |
| 17 | a | 86.94 | 0.06247 | YES | YES |
| 18 | a | 89.04 | 0.29431 | YES | YES |
| 19 | a | 97.18 | 0.31965 | YES | YES |
| 20 | a | 105.22 | 2.00191 | YES | YES |
| 21 | a | 113.00 | 0.98813 | YES | YES |
| 22 | a | 125.65 | 0.79241 | YES | YES |
| 23 | a | 134.73 | 1.05068 | YES | YES |
| 24 | a | 151.30 | 1.78706 | YES | YES |
| 25 | a | 160.31 | 1.44935 | YES | YES |
| 26 | a | 179.53 | 0.32215 | YES | YES |
| 27 | a | 188.52 | 0.23415 | YES | YES |
| 28 | a | 197.77 | 0.33095 | YES | YES |
| 29 | a | 213.48 | 0.36455 | YES | YES |
| 30 | a | 233.72 | 0.26149 | YES | YES |
| 31 | a | 241.14 | 0.49848 | YES | YES |
| 32 | a | 260.07 | 0.76530 | YES | YES |
| 33 | a | 265.83 | 2.10419 | YES | YES |
| 34 | a | 297.40 | 3.78161 | YES | YES |
| 35 | a | 321.18 | 0.63206 | YES | YES |
| 36 | a | 338.79 | 4.50691 | YES | YES |
| 37 | a | 342.71 | 7.05066 | YES | YES |
| 38 | a | 367.37 | 3.38791 | YES | YES |
| 39 | a | 401.37 | 1.93286 | YES | YES |
| 40 | a | 402.87 | 0.12617 | YES | YES |
| 41 | a | 416.51 | 0.58616 | YES | YES |
| 42 | a | 418.70 | 2.95551 | YES | YES |
| 43 | a | 435.27 | 1.24917 | YES | YES |
| 44 | a | 449.98 | 3.46461 | YES | YES |
| 45 | a | 454.81 | 2.85799 | YES | YES |
| 46 | a | 468.62 | 10.92685 | YES | YES |
| 47 | a | 482.98 | 0.52244 | YES | YES |
| 48 | a | 493.07 | 3.92736 | YES | YES |
| 49 | a | 499.16 | 7.85117 | YES | YES |
| 50 | a | 501.98 | 5.34270 | YES | YES |
SCF Energy (au) BP86/SV(P)  -2583.738258985
SCF Energy (au) PBE0/def2-TZVPP  -2583.285628368
SCF Energy (au) PBE0/def2-TZVPP  -2583.2957410864 (Toluene Correction)
Zero Point Energy (au)  0.3849902
Chemical Potential (kJ mol\(^{-1}\))  841.35
Dispersion Correction (au) PBE0/def2-TZVPP  -0.07451576

xyz coordinates

Mn 2.1746510 1.9645105 -0.4690860
C 2.6450634 2.4250908 1.2145880
C 3.8781896 1.5626495 -0.8563270
C 2.3534054 3.6185339 -1.1566146
O 2.4489731 4.6785438 -1.6355252
O 4.9897225 1.2963138 -1.1038729
O 2.9325961 2.7213873 2.3051651
C -0.5284013 1.3313376 0.5157799
C 0.2253290 0.1323297 0.8434505
C 1.5604853 0.0882302 0.2933244
C 2.4022337 -0.9653430 0.7115988
C 1.9613766 -1.9532893 1.6126250
C 0.6165517 -1.9494312 2.0721544
C -0.2359884 -1.9152057 1.6749787
H 2.8839293 -2.8864229 1.9698074
H 0.2372654 -2.7409785 2.7340992
H -1.2772839 -0.9105281 2.0351930
N 0.1895135 2.2659540 -0.0653128
H 1.0940955 1.7766872 -3.2253331
C 1.3346492 1.3755574 -2.2357727
C 1.5101649 0.2213884 -1.6611739
C 1.7568852 -1.1496442 -2.1513247
C 2.1801818 -3.7175437 -3.2623512
C 3.0246732 -2.6504279 -3.6120825
C 2.8127054 -1.3738298 -3.0662641
C 0.9208420 -2.2337256 -1.7958153
C 1.1257378 -3.5032770 -2.3559522
H 2.3440281 -4.7186166 -3.6948865
H 3.8567578 -2.8102908 -4.3178720
H 3.4747769 -0.5355053 -3.3349262
H 0.0965800 -2.0672438 -1.0839022
H 0.4559344 -4.3353256 -2.0814602
H -0.3288160 3.1216373 -0.3112567
C -1.9823949 1.5233350 0.7739732
C -4.7489168 1.9946365 1.2280657
C -3.8909273 1.6593259 2.3018371
C -2.5326718 1.4245519 2.0765794
C -2.8455695 1.8705045 -0.2867300
C -4.2146754 2.1003417 -0.0747566
O -6.0547404 2.1985750 1.5494690
H -4.3200517 1.5997385 3.3143149
H -1.8771432 1.1958545 2.9321193
H -2.4418454 1.9427006 -1.3104591
H -4.8538629 2.3556583 -0.9324763
C -6.9667337 2.5488890 0.5205927
H -7.0386567 1.7516628 -0.2567495
H -6.6867477 3.5119097 0.0316236
H -7.9533948 2.6655222 1.0119679
C 2.5211775 -3.9033562 2.8892150
H 1.7176168 -4.5622496 2.4824823
H 2.1870458 -3.4786642 3.8650232
| # | mode | symmetry | wave number (cm**(-1)) | IR intensity (km/mol) | IR | RAMAN |
|---|------|----------|------------------------|----------------------|----|--------|
| 1 | a    |          | 296.98                 | 0.00000              | YES | YES    |
| 2 | a    |          | 0.00                   | 0.00000              | -   | -      |
| 3 | a    |          | 0.00                   | 0.00000              | -   | -      |
| 4 | a    |          | 0.00                   | 0.00000              | -   | -      |
| 5 | a    |          | 0.00                   | 0.00000              | -   | -      |
| 6 | a    |          | 0.00                   | 0.00000              | -   | -      |
| 7 | a    |          | 0.00                   | 0.00000              | -   | -      |
| 8 | a    |          | 18.22                  | 0.22944              | YES | YES    |
| 9 | a    |          | 24.31                  | 0.09629              | YES | YES    |
| 10| a    |          | 29.57                  | 0.35562              | YES | YES    |
| 11| a    |          | 32.77                  | 0.12955              | YES | YES    |
| 12| a    |          | 43.30                  | 0.28450              | YES | YES    |
| 13| a    |          | 48.40                  | 1.17254              | YES | YES    |
| 14| a    |          | 52.25                  | 0.33172              | YES | YES    |
| 15| a    |          | 65.12                  | 0.13582              | YES | YES    |
| 16| a    |          | 78.99                  | 0.14413              | YES | YES    |
| 17| a    |          | 85.48                  | 0.13030              | YES | YES    |
| 18| a    |          | 86.69                  | 0.50394              | YES | YES    |
| 19| a    |          | 94.09                  | 0.75043              | YES | YES    |
| 20| a    |          | 99.10                  | 2.62791              | YES | YES    |
| 21| a    |          | 100.03                 | 0.58182              | YES | YES    |
| 22| a    |          | 125.70                 | 0.20917              | YES | YES    |
| 23| a    |          | 143.38                 | 0.32313              | YES | YES    |
| 24| a    |          | 145.97                 | 0.79017              | YES | YES    |
| 25| a    |          | 152.13                 | 1.76887              | YES | YES    |
| 26| a    |          | 177.98                 | 0.13994              | YES | YES    |
| 27| a    |          | 193.14                 | 1.65087              | YES | YES    |
| 28| a    |          | 203.26                 | 3.59753              | YES | YES    |
| 29| a    |          | 208.08                 | 0.83531              | YES | YES    |
| 30| a    |          | 231.47                 | 1.19931              | YES | YES    |
| 31| a    |          | 239.87                 | 1.29797              | YES | YES    |
| 32| a    |          | 244.45                 | 2.03842              | YES | YES    |
| 33| a    |          | 253.73                 | 1.06308              | YES | YES    |
| 34| a    |          | 288.48                 | 1.17820              | YES | YES    |
| 35| a    |          | 306.57                 | 4.12109              | YES | YES    |
| 36| a    |          | 314.39                 | 1.27095              | YES | YES    |
| 37| a    |          | 332.66                 | 0.94044              | YES | YES    |
| 38| a    |          | 355.46                 | 0.48843              | YES | YES    |
| 39| a    |          | 402.18                 | 0.02761              | YES | YES    |
| 40| a    |          | 411.11                 | 4.82695              | YES | YES    |
| 41| a    |          | 412.86                 | 3.42446              | YES | YES    |
| 42| a    |          | 423.23                 | 0.47428              | YES | YES    |
| 43| a    |          | 452.15                 | 0.15110              | YES | YES    |
| 44| a    |          | 459.15                 | 2.51377              | YES | YES    |
| 45| a    |          | 466.24                 | 2.50035              | YES | YES    |
| 46| a    |          | 479.31                 | 5.60076              | YES | YES    |
| 47| a    |          | 491.13                 | 4.47747              | YES | YES    |
| 48| a    |          | 495.62                 | 4.84184              | YES | YES    |
| 49| a    |          | 499.16                 | 4.12463              | YES | YES    |
| 50| a    |          | 512.83                 | 3.08282              | YES | YES    |
**TS23wJ**

SCF Energy (au) BP86/SV(P)  -2814.645959297
SCF Energy (au) PBE0/def2-TZVPP  -2814.155882277
SCF Energy (au) PBE0/def2-TZVPP (Toluene Correction)  -2814.1661111849
Zero Point Energy (au)  0.4648176
Chemical Potential (kJ mol⁻¹)  1034.42
Dispersion Correction (au) PBE0/def2-TZVPP  -0.09273178

xyz coordinates

63

Mn  1.9306911  1.4020002  0.6830458
C  2.1838181  1.7351582  2.4392325
C  3.6641337  0.9860875  0.4910235
C  2.2510348  3.1212471  0.2232937
O  2.4712664  4.2408521  -0.0256646
O  4.7959451  0.7116684  0.3802884
O  2.3372093  1.9384693  3.5758549
C  -0.8818569  0.7680615  1.2417821
C  -2.3576784  0.9247761  1.2413331
C  -0.1766581  -0.4235535  1.6783525
C  1.2250130  -0.4418934  1.3598469
C  2.0102907  -1.5083179  2.6499970
C  0.0410310  -1.4663571  2.4562785
H  3.0839960  -1.5361476  1.6273815
O  2.1235925  -3.5612119  3.1902086
H  -0.3769380  -3.3106800  3.5600084
H  -1.8189575  -1.4320486  2.7145749
N  -0.0842866  1.7267082  0.8160727
C  0.8260154  1.4855016  -2.5115280
C  1.2304284  2.7687591  -2.9640986
C  0.8216903  3.2503419  -4.2164899
C  -0.0126781  2.4769118  -5.0424273
C  -0.4330863  1.2069388  -4.6039751
C  -0.0216378  0.7153266  -3.3591703
H  1.8769689  3.3893508  -2.3273141
H  1.1563737  4.2473776  -4.5482167
H  -0.3388016  2.8627253  -6.0224091
H  -1.0902393  0.5914373  -5.2412450
H  -0.3540159  -0.2781091  -3.0184706
C  1.2445243  0.9213366  -1.2469878
C  1.4821055  -0.2274950  -0.6770971
C  1.9529371  -1.5431340  -1.1375304
C  -5.1764461  1.2964760  1.1526703
C  -4.5985342  0.0748947  0.7319111
C  -3.2157782  -0.1069035  0.7812849
C  -2.9480030  2.1390221  1.6509444
C  -4.3374039  2.3326881  1.6198692
O  -6.5306659  1.3738259  1.0713401
H  -5.2665135  -0.7177467  0.3601128
H  -2.7833855  -1.0560987  0.4266622
H  -2.3076940  2.9487000  2.0447980
H  -4.7543672  3.2893905  1.9665970
H  -0.5606966  2.5486784  0.4189116
C  3.5214601  -3.6573375  2.9519756
C  -7.1755115  2.5767779  1.4668446
H  4.0669060  -2.7732336  3.3570887
H  3.7460199  -3.7599460  1.8653516
H  3.8590608  -4.5694592  3.4840392
H  -6.9955334  2.8036794  2.5436660
H  -8.2595994  2.4068834  1.3080940
| #  | mode | symmetry | wave number (cm^{-1}) | IR intensity (km/mol) | IR | Raman |
|----|------|----------|-----------------------|-----------------------|----|-------|
| 1  | a    | a        | -194.57               | 0.0000                | YES | YES   |
| 2  | a    | a        | 0.00                  | 0.0000                | -   | -     |
| 3  | a    | a        | 0.00                  | 0.0000                | -   | -     |
| 4  | a    | a        | 0.00                  | 0.0000                | -   | -     |
| 5  | a    | a        | 0.00                  | 0.0000                | -   | -     |
| 6  | a    | a        | 0.00                  | 0.0000                | -   | -     |
| 7  | a    | a        | 0.00                  | 0.0000                | -   | -     |
| 8  | a    | a        | 16.41                 | 0.09106               | YES | YES   |
| 9  | a    | a        | 18.69                 | 0.13939               | YES | YES   |
| 10 | a    | a        | 24.84                 | 0.06883               | YES | YES   |
| 11 | a    | a        | 32.84                 | 0.18714               | YES | YES   |
| 12 | a    | a        | 36.53                 | 0.67747               | YES | YES   |
| 13 | a    | a        | 43.45                 | 0.75136               | YES | YES   |
| 14 | a    | a        | 45.03                 | 0.09858               | YES | YES   |
| 15 | a    | a        | 49.04                 | 0.02101               | YES | YES   |
| 16 | a    | a        | 57.92                 | 0.23317               | YES | YES   |
| 17 | a    | a        | 63.05                 | 0.29982               | YES | YES   |
| 18 | a    | a        | 74.95                 | 0.57612               | YES | YES   |
| 19 | a    | a        | 76.87                 | 0.04162               | YES | YES   |
| 20 | a    | a        | 86.54                 | 0.07244               | YES | YES   |
| 21 | a    | a        | 92.38                 | 0.33303               | YES | YES   |
| 22 | a    | a        | 98.55                 | 0.34466               | YES | YES   |
| 23 | a    | a        | 106.72                | 2.23100               | YES | YES   |
| 24 | a    | a        | 114.66                | 0.40203               | YES | YES   |
| 25 | a    | a        | 124.04                | 0.64485               | YES | YES   |
| 26 | a    | a        | 137.05                | 1.94375               | YES | YES   |
| 27 | a    | a        | 150.70                | 1.72182               | YES | YES   |
| 28 | a    | a        | 160.05                | 1.53666               | YES | YES   |
| 29 | a    | a        | 168.98                | 0.45894               | YES | YES   |
| 30 | a    | a        | 186.71                | 1.45702               | YES | YES   |
| 31 | a    | a        | 189.01                | 0.60705               | YES | YES   |
| 32 | a    | a        | 198.14                | 2.37796               | YES | YES   |
| 33 | a    | a        | 222.80                | 0.28299               | YES | YES   |
| 34 | a    | a        | 230.16                | 0.23786               | YES | YES   |
| 35 | a    | a        | 237.45                | 1.45215               | YES | YES   |
| 36 | a    | a        | 249.75                | 1.01148               | YES | YES   |
| 37 | a    | a        | 253.15                | 0.14093               | YES | YES   |
| 38 | a    | a        | 261.15                | 2.60947               | YES | YES   |
| 39 | a    | a        | 294.73                | 4.15721               | YES | YES   |
| 40 | a    | a        | 323.23                | 3.05680               | YES | YES   |
| 41 | a    | a        | 339.69                | 0.67976               | YES | YES   |
| 42 | a    | a        | 357.65                | 4.33796               | YES | YES   |
| 43 | a    | a        | 374.48                | 0.60465               | YES | YES   |
| 44 | a    | a        | 398.95                | 3.36470               | YES | YES   |
| 45 | a    | a        | 402.20                | 0.12622               | YES | YES   |
| 46 | a    | a        | 405.90                | 2.63261               | YES | YES   |
| 47 | a    | a        | 416.83                | 0.45536               | YES | YES   |
| 48 | a    | a        | 419.15                | 2.87869               | YES | YES   |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 49 | a | 435.25 | 1.41876 | YES | YES |
| 50 | a | 450.38 | 0.19487 | YES | YES |
### SCF Energy (au) BP86/SV(P)

-2391.953906106

### SCF Energy (au) PBE0/def2-TZVPP

-2391.506807198

### SCF Energy (au) PBE0/def2-TZVPP (Toluene Correction)

-2391.514569127

### Zero Point Energy (au)

0.3208594

### Chemical Potential (kJ mol\(^{-1}\))

692.48

### Dispersion Correction (au) PBE0/def2-TZVPP

0.06636323

### xyz coordinates

45

| Element | X            | Y            | Z            |
|---------|--------------|--------------|--------------|
| Mn      | 1.6823049    | -0.1540813   | 0.7119304    |
| C       | 2.0823667    | 0.0299876    | 2.4662496    |
| C       | 3.3142989    | -0.7703630   | 0.3633362    |
| C       | 2.2916770    | 1.5080239    | 0.3104084    |
| O       | 2.8051040    | -1.1888982   | 0.0645810    |
| O       | 4.3832846    | -1.1888982   | 0.0645810    |
| O       | 0.3252325    | -0.6715825   | 1.5897830    |
| C       | -1.1529180   | -0.6715825   | 1.5897830    |
| C       | -0.9430170   | 1.5831402    | 0.9670982    |
| C       | -2.3147607   | 1.8220671    | 1.1899400    |
| C       | -3.1142375   | 0.7522986    | 1.6162800    |
| C       | -2.5383478   | -0.5024504   | 1.816618     |
| C       | -0.4436773   | -1.9368414   | 1.7767137    |
| C       | 0.8891064    | -2.0045914   | 1.2620044    |
| C       | 1.6189977    | -3.2041245   | 1.4916431    |
| C       | 1.0557362    | -4.2830285   | 2.1764479    |
| C       | -0.2732070   | -4.2137822   | 2.6538585    |
| C       | -1.0127998   | -3.0473244   | 2.4508552    |
| O       | -0.0854716   | 2.5354261    | 0.5597101    |
| H       | -2.7477230   | 2.8191459    | 1.0333578    |
| H       | -4.1919682   | 0.9070197    | 1.7894065    |
| H       | -3.1526392   | -1.3556750   | 2.1355549    |
| C       | 2.6507360    | -3.2910846   | 1.1112435    |
| H       | 1.6561477    | -5.1924837   | 2.3484406    |
| H       | -0.7180477   | -5.0658746   | 3.1926222    |
| H       | -2.0376043   | -2.9848091   | 2.8513895    |
| N       | -0.3729834   | 0.3672597    | 1.1560503    |
| C       | 0.3526155    | 0.3818633    | -2.3524857   |
| C       | 0.9943495    | 1.5649540    | -2.8046371   |
| C       | 0.5520736    | 2.2219353    | -3.9617036   |
| C       | -0.5528760   | 1.7362858    | -4.6840251   |
| C       | -1.2105295   | 0.5744263    | -4.2394100   |
| C       | -0.7656216   | -0.0968195   | -3.0932606   |
| H       | 1.8555215    | 1.9605836    | -2.2470897   |
| H       | 1.0769613    | 3.1301816    | -4.3027952   |
| H       | -0.9020385   | 2.2615575    | -5.5884173   |
| H       | -2.0800711   | 0.1837491    | -4.7945666   |
| H       | -1.2829623   | -1.0061058   | -2.7462792   |
| C       | 0.7881228    | -0.3593225   | -1.1930104   |
| C       | 0.9329506    | -1.5439861   | -0.6899098   |
| H       | 1.0768716    | -2.5764308   | -1.0226138   |
| C       | -0.5505492   | 3.8496392    | 0.2821474    |
| H       | -1.3018194   | 3.8476272    | -0.5401194   |
| H       | 0.3453502    | 4.4159264    | -0.0394656   |
| H       | -0.9839389   | 4.3282658    | 1.1902184    |

### $\nu$ Vibrational spectrum

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|-----------------|
| 1 | a    | -228.81  | 0.00000     | YES          | YES             |
| 2 | 0.00 | 0.00000  | -           | -            | -               |
| 3 | 0.00 | 0.00000  | -           | -            | -               |
| a  | b       | c         | d         | e    | f    |
|----|---------|-----------|-----------|------|------|
| b1 | 0.00    | 0.00000   | -         | -    | -    |
| b2 | 0.00    | 0.00000   | -         | -    | -    |
| b3 | 0.00    | 0.00000   | -         | -    | -    |
| b4 | 0.00    | 0.00000   | -         | -    | -    |
| b5 | 19.11   | 0.00795   | YES       | YES  |
| b6 | 25.55   | 0.42080   | YES       | YES  |
| b7 | 36.80   | 0.24743   | YES       | YES  |
| b8 | 50.02   | 0.01194   | YES       | YES  |
| b9 | 62.78   | 0.35860   | YES       | YES  |
| b10| 74.19   | 1.54238   | YES       | YES  |
| b11| 88.21   | 0.46670   | YES       | YES  |
| b12| 90.75   | 0.18401   | YES       | YES  |
| b13| 99.41   | 1.03121   | YES       | YES  |
| b14| 106.93  | 0.10587   | YES       | YES  |
| b15| 115.06  | 0.57837   | YES       | YES  |
| b16| 124.51  | 0.24267   | YES       | YES  |
| b17| 130.62  | 0.61017   | YES       | YES  |
| b18| 142.11  | 0.86214   | YES       | YES  |
| b19| 157.29  | 0.55479   | YES       | YES  |
| b20| 184.92  | 0.19479   | YES       | YES  |
| b21| 196.86  | 1.19340   | YES       | YES  |
| b22| 215.56  | 1.28885   | YES       | YES  |
| b23| 219.99  | 0.16940   | YES       | YES  |
| b24| 237.14  | 1.67363   | YES       | YES  |
| b25| 259.45  | 0.14314   | YES       | YES  |
| b26| 289.72  | 0.20098   | YES       | YES  |
| b27| 304.37  | 0.88957   | YES       | YES  |
| b28| 332.98  | 0.97419   | YES       | YES  |
| b29| 351.21  | 9.54902   | YES       | YES  |
| b30| 385.30  | 2.59182   | YES       | YES  |
| b31| 403.53  | 0.11870   | YES       | YES  |
| b32| 406.94  | 0.93506   | YES       | YES  |
| b33| 428.32  | 0.72794   | YES       | YES  |
| b34| 447.17  | 1.62589   | YES       | YES  |
| b35| 452.76  | 2.13332   | YES       | YES  |
| b36| 465.85  | 10.10407  | YES       | YES  |
| b37| 478.61  | 2.11244   | YES       | YES  |
| b38| 492.64  | 1.85906   | YES       | YES  |
| b39| 495.93  | 11.69786  | YES       | YES  |
| b40| 510.21  | 5.47025   | YES       | YES  |
| b41| 522.54  | 0.68273   | YES       | YES  |
| b42| 538.58  | 11.69373  | YES       | YES  |
| b43| 549.24  | 15.95716  | YES       | YES  |
| b44| 551.00  | 3.74202   | YES       | YES  |
| b45| 581.07  | 5.63391   | YES       | YES  |
| b46| 584.20  | 14.70772  | YES       | YES  |
| b47| 609.52  | 14.07838  | YES       | YES  |
SCF Energy (au) BP86/SV(P) -2391.943845351
SCF Energy (au) PBE0/def2-TZVPP -2391.497946159
SCF Energy (au) PBE0/def2-TZVPP -2391.5061895680 (Toluene Correction)
Zero Point Energy (au) 0.3205041
Chemical Potential (kJ mol⁻¹) 691.29
Dispersion Correction (au) PBE0/def2-TZVPP 0.06768189

xyz coordinates
45

Mn  1.3110392  1.2919826  0.4372025
C   1.4509833  1.6980167  2.1987554
C   3.0228283  0.8213585  0.3786671
C   1.7953893  2.9380234 -0.1248740
O   2.2046709  3.9514035 -0.5338050
O   4.1482855  0.5024836  0.3461756
O   1.5310264  1.9758415  3.3279080
C  -1.5523798  0.5457394  1.0418146
C  -1.4986120  2.7521652  0.2485363
C  -2.9024106  2.8677863  0.3315387
C  -3.6342364  1.7570910  0.7744980
C  -2.9629776  0.5862788  1.1280883
C  -0.7457941 -0.6191727  1.4129148
C   0.6175561 -0.6239367  0.9817123
C   1.4303899 -1.7145122  1.3919974
C   0.9321047 -2.7317726  2.2105416
C  -0.4190106 -2.7209434  2.6219262
C  -1.2508336 -1.6730210  2.2171497
O  -0.7002393  3.7487217 -0.1755946
H  -3.4111534  3.8006983  0.0535798
H  -4.7332901  1.8131157  0.8378185
H  -3.5200531 -0.3020652  1.4585336
H   2.4804194 -1.7603028  1.0605214
H   1.6004942 -3.5474605  2.5338769
H  -0.8132982 -3.5238275  3.2654803
H  -2.2957236 -1.6486816  2.5674539
N  -0.8365671  1.6221262  0.5948643
H   0.7824923  1.3877611 -2.4572689
C   0.8270174  0.8827240 -1.4868665
C   0.7844700 -0.3219684 -1.0065775
C   0.9209701 -1.6842854 -1.5522209
C   1.1695360 -4.2139431 -2.8018412
C   2.1030016 -3.1991099 -3.0733444
C   1.9792576 -1.9436023 -2.4576369
C  -0.0051991 -2.7178798 -1.2778888
C   0.1145770 -3.9666638 -1.9047448
H   1.2648857 -5.1996778 -3.2869415
H   2.9370347 -3.3850051 -3.7704585
H   2.7109546 -1.1462934 -2.6638590
H  -0.8306913 -2.5304744 -0.5734895
H  -0.6238435  4.7568831 -1.6894224
C  -1.2549939  4.9970395 -0.5660557
H   1.9479366  4.8831263 -1.4315429
H  -0.3905350  5.6213350 -0.0662557
H  -1.7896031  5.4880350  0.2793667

$vibrational spectrum
#  mode     symmetry     wave number   IR intensity    selection rules
#                         cm**(-1)        km/mol         IR     RAMAN
 1   a       -281.82        0.00000       YES     YES
 2   0.00        0.00000       -       -
 3   0.00        0.00000       -       -
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | 0.00 | 0.00000 | - | - |
| 8 | a | 21.96 | 0.54731 | YES | YES |
| 9 | a | 27.17 | 0.31688 | YES | YES |
| 10 | a | 39.40 | 0.07178 | YES | YES |
| 11 | a | 45.13 | 0.01735 | YES | YES |
| 12 | a | 59.30 | 0.80359 | YES | YES |
| 13 | a | 73.87 | 1.42854 | YES | YES |
| 14 | a | 81.25 | 0.11047 | YES | YES |
| 15 | a | 89.84 | 0.12936 | YES | YES |
| 16 | a | 91.63 | 0.10392 | YES | YES |
| 17 | a | 109.10 | 0.05579 | YES | YES |
| 18 | a | 111.04 | 1.52700 | YES | YES |
| 19 | a | 129.12 | 0.58316 | YES | YES |
| 20 | a | 130.00 | 0.22055 | YES | YES |
| 21 | a | 142.74 | 0.77459 | YES | YES |
| 22 | a | 160.87 | 1.01154 | YES | YES |
| 23 | a | 184.29 | 0.59976 | YES | YES |
| 24 | a | 185.71 | 2.74327 | YES | YES |
| 25 | a | 209.39 | 0.21746 | YES | YES |
| 26 | a | 219.24 | 3.52486 | YES | YES |
| 27 | a | 226.92 | 2.15658 | YES | YES |
| 28 | a | 261.16 | 0.23288 | YES | YES |
| 29 | a | 284.51 | 0.53013 | YES | YES |
| 30 | a | 300.92 | 1.42087 | YES | YES |
| 31 | a | 315.13 | 2.22167 | YES | YES |
| 32 | a | 333.70 | 0.64837 | YES | YES |
| 33 | a | 402.41 | 0.38858 | YES | YES |
| 34 | a | 403.00 | 0.12920 | YES | YES |
| 35 | a | 410.69 | 4.78803 | YES | YES |
| 36 | a | 443.69 | 3.35847 | YES | YES |
| 37 | a | 457.29 | 0.26555 | YES | YES |
| 38 | a | 467.58 | 0.25933 | YES | YES |
| 39 | a | 475.36 | 3.06914 | YES | YES |
| 40 | a | 479.63 | 3.18434 | YES | YES |
| 41 | a | 502.35 | 7.87649 | YES | YES |
| 42 | a | 509.01 | 11.22374 | YES | YES |
| 43 | a | 510.08 | 10.04585 | YES | YES |
| 44 | a | 526.74 | 6.49210 | YES | YES |
| 45 | a | 541.34 | 9.55862 | YES | YES |
| 46 | a | 548.14 | 6.24154 | YES | YES |
| 47 | a | 558.45 | 15.13916 | YES | YES |
| 48 | a | 564.90 | 6.13221 | YES | YES |
| 49 | a | 581.38 | 3.49303 | YES | YES |
| 50 | a | 606.71 | 40.94505 | YES | YES |
TS_{23ga}

SCF Energy (au) B3LYP/6-311G(d,p) -2508.390483009
SCF Energy (au) B3LYP/6-311G++(d,p) -2507.907823752
SCF Energy (au) B3LYP/6-311G++(d,p) -2507.9156889379 (Toluene Correction)
Zero Point Energy (au) 0.3677427
Chemical Potential (kJ mol^{-1}) 805.67
Dispersion Correction (au) B3LYP/def2-TZVPP -0.08080308

dxyz coordinates

Mn    1.5248441  -0.5845365  0.6397492
C     1.9479276  -0.1680022  2.3451840
C     3.1531787  -1.2378222  0.3611675
C     2.1434209   0.9801826  -0.0458451
O     2.6918521   1.9009823  -0.5073779
O     4.2221277  -1.6797369   0.1922384
O     4.2221277  -1.6797369   0.1922384
O     4.2221277  -1.6797369   0.1922384
C     2.0340646   0.0904312  3.4519353
C     -1.3262784  -1.0784282  1.4637251
C     -1.1652883  -1.1729122  0.7906054
C     -2.5693532  -1.2931026  0.7780946
C     -3.3670493   0.1875560  1.1054350
C     -2.7381636  -1.0002992  1.4764198
C     -0.5901441  -2.2833859  1.8490622
C     0.7694752  -2.3633513  1.4202424
C     1.5213038  -3.4987701  1.8290059
C     0.9525439  -4.5042281  2.6153884
C     -0.4005685  -4.4235477  3.0150732
C     -1.1636811  -3.3192696  2.6284128
C     -0.3684453   2.4183943  0.5898400
H     -3.0168061   2.2711242  0.5453896
H     -4.4666993   0.2630063  1.0922184
H     -3.3295190  -1.8843629  1.7555811
H     2.5741119  -3.5971104  1.5150369
H     1.5690844  -5.3632896  2.9303901
H     -0.8469301  -5.2157813  3.6375045
H     -2.2094528  -3.2406564  2.9683437
N     -0.5553920  -0.0151934  1.0669763
C     0.1552864  -0.4653066 -2.4658343
C     0.8115630   0.6114667  -3.1182067
C     0.3520392   1.0840650  -4.3563685
C     -0.7830842   0.5178294  -4.9641111
C     -1.4555771  -0.5377193  -4.3206713
C     -0.9942453  -1.0266136  -3.0914358
H     1.6965534   1.0694607  -2.6547579
H     0.8886911   1.904129  -4.8516946
H     -1.1442849   0.8987999  -5.9335844
H     -2.3490344  -0.9888064  -4.7841610
H     -1.5217427  -1.8530576  -2.5889030
C     0.6129898  -1.0354979  -1.2186079
C     0.7942461  -2.1456615  -0.5795400
H     0.9486033  -3.2104797  -0.7768708
C     0.9675526   4.8921174  0.3197217
C     1.0864307   4.1530671  1.5096814
C     0.4248956   2.9235896  1.6455242
C     -0.4989074  3.1762558  -0.5944436
C     0.1746010   4.4006849  -0.7311774
H     1.4944440   5.8545831  0.2121793
H     1.7004501   4.5366872  2.3410568
H     0.5127752   2.3515817  2.5829314
H     -1.1148258   2.7881814  -1.4221905
H     0.0810448   4.9738029  -1.6683325
| # | mode | symmetry | wave number  | IR intensity | selection rules |
|---|------|----------|--------------|--------------|----------------|
| 1 | a    |          | -220.39      | 0.00000      | YES YES        |
| 2 |      |          | 0.00         | 0.00000      | - -            |
| 3 |      |          | 0.00         | 0.00000      | - -            |
| 4 |      |          | 0.00         | 0.00000      | - -            |
| 5 |      |          | 0.00         | 0.00000      | - -            |
| 6 |      |          | 0.00         | 0.00000      | - -            |
| 7 |      |          | 0.00         | 0.00000      | - -            |
| 8 | a    |          | 7.18         | 0.04481      | YES YES        |
| 9 | a    |          | 25.98        | 0.14963      | YES YES        |
| 10| a    |          | 28.35        | 0.07413      | YES YES        |
| 11| a    |          | 46.66        | 0.05710      | YES YES        |
| 12| a    |          | 59.46        | 0.24527      | YES YES        |
| 13| a    |          | 68.02        | 0.05833      | YES YES        |
| 14| a    |          | 74.15        | 0.04441      | YES YES        |
| 15| a    |          | 75.96        | 0.56208      | YES YES        |
| 16| a    |          | 89.54        | 0.52008      | YES YES        |
| 17| a    |          | 93.41        | 0.21133      | YES YES        |
| 18| a    |          | 104.63       | 0.29995      | YES YES        |
| 19| a    |          | 112.39       | 0.18400      | YES YES        |
| 20| a    |          | 119.55       | 0.10028      | YES YES        |
| 21| a    |          | 126.31       | 0.36676      | YES YES        |
| 22| a    |          | 133.97       | 0.32997      | YES YES        |
| 23| a    |          | 156.06       | 0.27131      | YES YES        |
| 24| a    |          | 162.45       | 0.56834      | YES YES        |
| 25| a    |          | 186.04       | 0.40033      | YES YES        |
| 26| a    |          | 205.73       | 0.28924      | YES YES        |
| 27| a    |          | 217.74       | 0.64486      | YES YES        |
| 28| a    |          | 233.91       | 0.23953      | YES YES        |
| 29| a    |          | 243.74       | 1.42955      | YES YES        |
| 30| a    |          | 292.38       | 0.46312      | YES YES        |
| 31| a    |          | 311.96       | 0.57499      | YES YES        |
| 32| a    |          | 334.06       | 0.79096      | YES YES        |
| 33| a    |          | 352.03       | 9.28848      | YES YES        |
| 34| a    |          | 368.04       | 0.39060      | YES YES        |
| 35| a    |          | 390.04       | 4.82528      | YES YES        |
| 36| a    |          | 401.29       | 0.38297      | YES YES        |
| 37| a    |          | 402.85       | 0.11789      | YES YES        |
| 38| a    |          | 423.04       | 1.79015      | YES YES        |
| 39| a    |          | 442.50       | 0.64033      | YES YES        |
| 40| a    |          | 449.25       | 2.87375      | YES YES        |
| 41| a    |          | 464.05       | 9.91506      | YES YES        |
| 42| a    |          | 470.92       | 3.87025      | YES YES        |
| 43| a    |          | 485.37       | 1.17087      | YES YES        |
| 44| a    |          | 496.16       | 4.18584      | YES YES        |
| 45| a    |          | 496.70       | 7.06281      | YES YES        |
| 46| a    |          | 509.12       | 5.45970      | YES YES        |
| 47| a    |          | 522.80       | 0.52314      | YES YES        |
| 48| a    |          | 544.46       | 10.99192     | YES YES        |
| 49| a    |          | 548.38       | 10.35088     | YES YES        |
| 50| a    |          | 553.61       | 7.49606      | YES YES        |
**TS23ga**

| SCF Energy (au) BP86/SV(P) | -2508.381424342 |
|---------------------------|------------------|
| SCF Energy (au) PBE0/def2-TZVPP | -2507.899292682 |
| SCF Energy (au) PBE0/def2-TZVPP (Toluene Correction) | -2507.9076218786 |
| Zero Point Energy (au) | 0.3672553 |
| Chemical Potential (kJ mol⁻¹) | 806.64 |
| Dispersion Correction (au) PBE0/def2-TZVPP | -0.08140660 |

**xyz coordinates**

| 51 |
|---------------------------|
| Mn | 1.2410302 | 0.5333857 | 0.2961025 |
| C | 1.5263352 | 1.0929493 | 1.9927023 |
| C | 2.9071938 | -0.0668038 | 0.1951247 |
| C | 1.8221134 | 2.0394922 | -0.5207088 |
| O | 2.306189 | 2.9125814 | -1.1210368 |
| O | 4.0048967 | 0.4683008 | 0.1367038 |
| O | 1.6945615 | 1.4668466 | 3.0848500 |
| C | -1.6575623 | -0.0149824 | 0.9417047 |
| C | -1.5364748 | 2.1990646 | 0.1567478 |
| C | -2.4119747 | 2.2625908 | 0.0498340 |
| C | -3.7195572 | 1.0499970 | 0.3851796 |
| C | -3.0711123 | 0.0031825 | 0.8574349 |
| C | -0.9090923 | 1.1670358 | 1.4404657 |
| O | 0.4594018 | -1.2690511 | 0.1439718 |
| C | 1.2150706 | -2.3528122 | 1.5680757 |
| O | 0.6652456 | -3.266542 | 2.4657516 |
| C | -0.7007262 | -3.1607172 | 2.8435114 |
| C | -1.4788625 | -2.1225976 | 2.3227578 |
| C | -0.7715030 | 3.4558025 | -0.0874276 |
| H | -3.4081654 | 3.2081733 | -0.2644633 |
| H | -4.8162981 | 1.1754567 | 0.2970408 |
| C | -3.6447395 | -0.8918064 | 1.1399669 |
| H | 2.2676031 | -2.4767398 | 1.2651584 |
| H | 1.2811689 | -4.0761009 | 2.8790807 |
| C | -1.1410555 | -3.8821409 | 3.5506334 |
| H | -2.5291042 | -2.0190188 | 2.6420475 |
| N | -0.9031486 | 1.0552181 | 0.5435537 |
| H | 0.4499847 | 0.4216045 | -2.5439982 |
| C | 0.5607354 | -0.0039046 | -1.5418071 |
| C | 0.5742943 | -1.1626540 | -0.9586258 |
| C | 0.7256616 | -2.5658496 | -1.3849620 |
| C | 1.0037271 | -5.1939512 | -2.3999772 |
| C | 1.9159538 | -4.1931897 | -2.7769453 |
| C | 1.7767054 | -2.884252 | -2.2778509 |
| C | -0.1787191 | 3.5841268 | -1.0032094 |
| C | -0.0447128 | -4.8831180 | -1.5151326 |
| H | 1.1107196 | -6.2183806 | -2.7938696 |
| H | 2.7439438 | -4.4283081 | -3.4657565 |
| H | 2.4910807 | -2.1013343 | -2.5668104 |
| H | -0.9984457 | -3.3465788 | -0.3078007 |
| H | -0.7656718 | -5.6628181 | -1.2180546 |
| C | 0.5151899 | 5.9401442 | -0.4778100 |
| C | 0.6249282 | 5.2747137 | 0.7554304 |
| C | -0.0111497 | 4.0399951 | 0.9510863 |
| C | -0.8937585 | 4.1414036 | -1.3158616 |
| C | -0.2447296 | 5.3703487 | -1.5131783 |
| H | 1.0235453 | 6.9062034 | -0.6319847 |
| H | 1.2129245 | 5.7201377 | 1.5746824 |
| H | 0.0709041 | 3.5264374 | 1.9220227 |
| H | -1.4872165 | 3.6941213 | -2.1308931 |
| H | -0.3312525 | 5.8854934 | -2.4841767 |
| #  | mode | symmetry | wave number  | IR intensity | selection rules |
|----|------|----------|--------------|--------------|-----------------|
| 1  |      | a        | -284.04      | 0.00000      | YES YES         |
| 2  |      |          | 0.00         | 0.00000      | -               |
| 3  |      |          | 0.00         | 0.00000      | -               |
| 4  |      |          | 0.00         | 0.00000      | -               |
| 5  |      |          | 0.00         | 0.00000      | -               |
| 6  |      |          | 0.00         | 0.00000      | -               |
| 7  |      |          | 0.00         | 0.00000      | -               |
| 8  |      | a        | 21.83        | 0.24742      | YES YES         |
| 9  |      | a        | 26.53        | 0.04054      | YES YES         |
| 10 |      | a        | 27.55        | 0.22997      | YES YES         |
| 11 |      | a        | 55.52        | 0.15441      | YES YES         |
| 12 |      | a        | 58.54        | 0.19895      | YES YES         |
| 13 |      | a        | 61.78        | 0.23479      | YES YES         |
| 14 |      | a        | 71.79        | 0.06660      | YES YES         |
| 15 |      | a        | 76.28        | 0.41529      | YES YES         |
| 16 |  a   | a        | 83.91        | 0.31739      | YES YES         |
| 17 |      | a        | 95.67        | 0.03798      | YES YES         |
| 18 |      | a        | 99.00        | 0.00329      | YES YES         |
| 19 |      | a        | 107.45       | 0.22463      | YES YES         |
| 20 |      | a        | 121.83       | 0.36120      | YES YES         |
| 21 |      | a        | 126.36       | 0.65725      | YES YES         |
| 22 |      | a        | 137.69       | 0.31483      | YES YES         |
| 23 |      | a        | 150.00       | 0.32541      | YES YES         |
| 24 |      | a        | 162.20       | 1.30034      | YES YES         |
| 25 |      | a        | 188.41       | 2.47324      | YES YES         |
| 26 |      | a        | 206.75       | 0.28675      | YES YES         |
| 27 |      | a        | 213.47       | 0.30054      | YES YES         |
| 28 |      | a        | 219.86       | 2.90087      | YES YES         |
| 29 |      | a        | 243.29       | 2.20485      | YES YES         |
| 30 |      | a        | 286.50       | 0.19870      | YES YES         |
| 31 |      | a        | 310.92       | 0.22004      | YES YES         |
| 32 |      | a        | 315.82       | 3.21257      | YES YES         |
| 33 |      | a        | 336.36       | 0.22768      | YES YES         |
| 34 |      | a        | 363.76       | 0.87637      | YES YES         |
| 35 |      | a        | 400.50       | 0.19138      | YES YES         |
| 36 |      | a        | 403.33       | 0.02312      | YES YES         |
| 37 |      | a        | 410.28       | 4.24302      | YES YES         |
| 38 |      | a        | 428.24       | 3.94233      | YES YES         |
| 39 |      | a        | 452.97       | 0.04614      | YES YES         |
| 40 |      | a        | 463.34       | 1.26011      | YES YES         |
| 41 |      | a        | 471.28       | 2.93625      | YES YES         |
| 42 |      | a        | 476.39       | 2.12371      | YES YES         |
| 43 |      | a        | 491.14       | 1.06595      | YES YES         |
| 44 |      | a        | 499.32       | 3.23268      | YES YES         |
| 45 |      | a        | 509.11       | 20.73100     | YES YES         |
| 46 |      | a        | 511.47       | 2.04412      | YES YES         |
| 47 |      | a        | 527.22       | 1.86051      | YES YES         |
| 48 |      | a        | 542.20       | 12.79466     | YES YES         |
| 49 |      | a        | 553.78       | 5.71313      | YES YES         |
| 50 |      | a        | 559.95       | 14.88453     | YES YES         |
TS23a

SCF Energy (au) BP86/SV(P) \(-2354.86230783\)
SCF Energy (au) PBE0/def2-TZVPP \(-2354.40635475\)
SCF Energy (au) PBE0/def2-TZVPP (Toluene Correction) \(-2354.4142715193\)

Zero Point Energy (au) 0.3226651
Chemical Potential (kJ mol\(^{-1}\)) 696.08
Dispersion Correction (au) PBE0/def2-TZVPP -0.06451629

xyz coordinates

| Symbol | X (au) | Y (au) | Z (au) |
|--------|--------|--------|--------|
| Mn     | 2.2084975 | 0.5250623 | 0.5478324 |
| C      | 2.6176997 | 0.7441853 | 2.2909833 |
| C      | 3.9129016 | 0.0878398 | 0.1836519 |
| C      | 2.5072647 | 2.2676112 | 0.1533830 |
| O      | 2.7042883 | 3.3973215 | -0.0618477 |
| O      | 5.0195021 | -0.2048262 | -0.0461420 |
| H      | 3.3550933 | -2.5382253 | 1.1887155 |
| H      | 2.3632348 | -4.4427922 | 2.4280768 |
| N      | -0.0603429 | -4.4147024 | 3.1066682 |
| C      | -1.4689279 | -2.4092071 | 2.5857970 |
| N      | 0.2270115 | 0.8730877 | 0.8742984 |
| C      | 0.9202487 | 0.8497547 | -2.5944228 |
| C      | 1.4599919 | 2.0800371 | -3.0524654 |
| O      | 0.9950442 | 2.6676223 | -4.2376942 |
| O      | -0.0284697 | 2.0583820 | -4.9852224 |
| C      | -0.5822600 | 0.8443132 | -4.5379431 |
| C      | -0.1163384 | 0.2449687 | -3.3610110 |
| H      | 2.2572383 | 2.5714496 | -2.4764361 |
| H      | 1.4363998 | 3.6186356 | -4.5793264 |
| H      | -0.3965910 | 2.5289268 | -5.9117454 |
| H      | -1.3869890 | 0.3575339 | -5.1140262 |
| H      | -0.5514575 | -0.7048071 | -3.0108143 |
| C      | 1.3904782 | 0.1728235 | -1.4093728 |
| C      | 1.6563040 | -0.9615126 | -0.8514462 |
| H      | 1.9301743 | -1.9875303 | -1.118527 |
| C      | -4.8044947 | 0.5537602 | 1.6782051 |
| C      | -4.3265595 | -0.6013673 | 1.0345916 |
| C      | -2.9461264 | -0.8304895 | 0.9262954 |
| C      | -2.5138801 | 1.2629604 | 2.0949284 |
| H      | -3.8947102 | 1.4844429 | 2.2095130 |
| H      | -5.8894386 | 0.7282725 | 1.7672252 |
| H      | -5.0359508 | -1.3295173 | 0.6079751 |
| H      | -2.5756396 | -1.7276806 | 0.4049310 |
| H      | -1.8032385 | 1.9844021 | 2.5317119 |
| H      | -4.2629510 | 2.3874861 | 2.7235636 |
| H      | -0.2585430 | 1.7449751 | 0.6173225 |

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number |
|---|------|----------|-------------|
| 1 | a    | -211.06  | 0.00000     |
| 2 |      | 0.00     | 0.00000     |
| 3 |      | 0.00     | 0.00000     |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 4 | 0.00 | 0.00000 | - | - |
| 5 | 0.00 | 0.00000 | - | - |
| 6 | 0.00 | 0.00000 | - | - |
| 7 | 0.00 | 0.00000 | - | - |
| 8 | a | 18.67 | 0.09950 | YES | YES |
| 9 | a | 21.60 | 0.02891 | YES | YES |
| 10 | a | 38.38 | 0.00779 | YES | YES |
| 11 | a | 48.05 | 0.09372 | YES | YES |
| 12 | a | 51.86 | 0.11616 | YES | YES |
| 13 | a | 69.55 | 0.22643 | YES | YES |
| 14 | a | 73.33 | 0.08989 | YES | YES |
| 15 | a | 80.49 | 0.12999 | YES | YES |
| 16 | a | 88.89 | 0.07702 | YES | YES |
| 17 | a | 94.68 | 0.23259 | YES | YES |
| 18 | a | 103.22 | 0.02377 | YES | YES |
| 19 | a | 110.35 | 0.25271 | YES | YES |
| 20 | a | 134.35 | 0.18439 | YES | YES |
| 21 | a | 143.04 | 0.44549 | YES | YES |
| 22 | a | 176.35 | 0.76100 | YES | YES |
| 23 | a | 195.95 | 0.47683 | YES | YES |
| 24 | a | 204.67 | 0.63859 | YES | YES |
| 25 | a | 212.39 | 0.45590 | YES | YES |
| 26 | a | 238.72 | 0.78590 | YES | YES |
| 27 | a | 269.37 | 1.77691 | YES | YES |
| 28 | a | 304.64 | 0.65671 | YES | YES |
| 29 | a | 340.16 | 8.47923 | YES | YES |
| 30 | a | 358.93 | 0.43972 | YES | YES |
| 31 | a | 395.36 | 1.89545 | YES | YES |
| 32 | a | 402.38 | 0.02315 | YES | YES |
| 33 | a | 404.64 | 0.38999 | YES | YES |
| 34 | a | 420.53 | 1.91042 | YES | YES |
| 35 | a | 436.65 | 0.58360 | YES | YES |
| 36 | a | 447.96 | 4.00709 | YES | YES |
| 37 | a | 461.40 | 20.24491 | YES | YES |
| 38 | a | 465.05 | 2.25747 | YES | YES |
| 39 | a | 485.47 | 0.85113 | YES | YES |
| 40 | a | 492.96 | 2.86485 | YES | YES |
| 41 | a | 497.08 | 3.33844 | YES | YES |
| 42 | a | 504.77 | 8.24943 | YES | YES |
| 43 | a | 521.80 | 0.45494 | YES | YES |
| 44 | a | 540.22 | 19.26793 | YES | YES |
| 45 | a | 544.86 | 15.56428 | YES | YES |
| 46 | a | 564.68 | 28.71926 | YES | YES |
| 47 | a | 590.89 | 1.48234 | YES | YES |
| 48 | a | 609.57 | 1.75365 | YES | YES |
| 49 | a | 611.76 | 5.86176 | YES | YES |
| 50 | a | 618.68 | 13.41133 | YES | YES |
TS231a

SCF Energy (au) BP86/SV(P)  -2183.11397934
SCF Energy (au) PBE0/def2-TZVPP  -2182.694332982
SCF Energy (au) PBE0/def2-TZVPP  -2182.7012637601 (Toluene Correction)
Zero Point Energy (au)  0.2578498
Chemical Potential (kJ mol\(^{-1}\))  537.65
Dispersion Correction (au) PBE0/def2-TZVPP  -0.05000930

xyz coordinates
37

Mn  1.3012750  0.6735212  0.8636467
C  1.6923990  0.9350102  2.6106761
C  3.0056460  0.2982574  0.5195438
C  1.5195873  2.4381721  0.4701240
O  1.6680679  3.5695831  0.2467560
O  4.1188443  0.0253376  0.2925176
O  1.9402074  1.0881191  3.7374012
C  -1.4133247  0.0725285  1.6759428
C  -2.893810  0.2622864  1.9251222
C  -0.7102733  1.1720529  1.9402837
C  0.484269  -1.933217  1.4760537
C  1.410669  -2.349571  1.7900079
C  0.8606475  -3.417294  2.4976908
C  -0.4970065  -3.399882  2.9059424
C  -1.2792418  -2.281359  2.6211696
H  2.4683728  -2.408447  1.4609439
H  1.4988509  -4.290543  2.7409042
H  -0.9242473  -4.257620  3.4497033
H  -2.3326827  -2.247159  2.9453367
O  -0.7429383  1.032698  1.2089872
C  0.1325468  0.9718078  -2.2911245
C  0.7714301  2.134574  -2.7930459
C  0.3824316  2.689619  -4.0202216
C  -0.6628773  2.115240  -4.7650935
C  -1.3143103  0.968571  -4.2745778
C  -0.9219310  0.399731  -3.0562753
H  1.5860925  2.598505  -2.2181170
H  0.8988533  3.588285  -4.3963692
H  -0.9726876  2.569145  -5.7242020
H  -2.1370795  0.510746  -4.8488992
H  -1.4327901  -0.497935  -2.6718159
C  0.5245875  0.331029  -1.0565555
C  0.7064571  -0.818313  -0.4815302
H  0.9010254  -1.857359  -0.7651214
H  -3.1924575  1.277144  1.5999085
H  -3.1200868  0.1456830  3.0077219
H  -3.4886102  -0.4975339  1.3765547

# mode symmetry wave number IR intensity selection rules
#              cm**(-1) km/mol    IR     RAMAN
1   a   -228.38  0.00000  YES    YES
2   0.00  0.00000  -    -
3   0.00  0.00000  -    -
4   0.00  0.00000  -    -
5   0.00  0.00000  -    -
6   0.00  0.00000  -    -
7   0.00  0.00000  -    -
8   a   18.98  0.12008  YES    YES
9   a   28.24  0.16870  YES    YES
10  a   56.30  0.07960  YES    YES
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 11 | a | 57.56 | 0.36639 | YES | YES |
| 12 | a | 73.76 | 0.43554 | YES | YES |
| 13 | a | 77.76 | 0.29842 | YES | YES |
| 14 | a | 90.84 | 0.23664 | YES | YES |
| 15 | a | 98.00 | 0.44156 | YES | YES |
| 16 | a | 103.22 | 0.33827 | YES | YES |
| 17 | a | 109.70 | 0.29581 | YES | YES |
| 18 | a | 123.22 | 0.04442 | YES | YES |
| 19 | a | 139.00 | 0.13164 | YES | YES |
| 20 | a | 160.46 | 0.60555 | YES | YES |
| 21 | a | 183.73 | 0.72674 | YES | YES |
| 22 | a | 202.28 | 0.19418 | YES | YES |
| 23 | a | 217.24 | 1.59049 | YES | YES |
| 24 | a | 246.57 | 1.24502 | YES | YES |
| 25 | a | 268.54 | 0.12494 | YES | YES |
| 26 | a | 284.53 | 0.22753 | YES | YES |
| 27 | a | 344.37 | 6.19449 | YES | YES |
| 28 | a | 378.18 | 1.40902 | YES | YES |
| 29 | a | 401.89 | 0.07019 | YES | YES |
| 30 | a | 410.53 | 2.74233 | YES | YES |
| 31 | a | 412.51 | 0.38710 | YES | YES |
| 32 | a | 437.47 | 1.28361 | YES | YES |
| 33 | a | 451.81 | 0.33644 | YES | YES |
| 34 | a | 461.91 | 10.89574 | YES | YES |
| 35 | a | 474.64 | 1.21843 | YES | YES |
| 36 | a | 489.37 | 4.15812 | YES | YES |
| 37 | a | 499.02 | 12.59916 | YES | YES |
| 38 | a | 507.71 | 2.91113 | YES | YES |
| 39 | a | 523.72 | 0.68396 | YES | YES |
| 40 | a | 536.45 | 21.31995 | YES | YES |
| 41 | a | 544.19 | 10.51342 | YES | YES |
| 42 | a | 587.29 | 45.28376 | YES | YES |
| 43 | a | 601.55 | 8.05846 | YES | YES |
| 44 | a | 605.21 | 3.61664 | YES | YES |
| 45 | a | 610.37 | 16.40323 | YES | YES |
| 46 | a | 618.62 | 32.05822 | YES | YES |
| 47 | a | 629.66 | 5.92647 | YES | YES |
| 48 | a | 650.99 | 6.48357 | YES | YES |
| 49 | a | 662.64 | 77.38872 | YES | YES |
| 50 | a | 683.14 | 75.60527 | YES | YES |
SCF Energy (au) BP86/SV(P) -2183.10398116
SCF Energy (au) PBE0/def2-TZVPP -2182.684894240
SCF Energy (au) PBE0/def2-TZVPP -2182.6918100274 (Toluene Correction)
Zero Point Energy (au) 0.2574986
Chemical Potential (kJ mol$^{-1}$) 536.55
Dispersion Correction (au) PBE0/def2-TZVPP -0.05277314

xyz coordinates
37

Mn  0.8656508  2.1918527  0.3154680
C   1.1790350  2.5549686  2.0654266
C   2.5879855  1.8447707  0.0639702
C   1.0592617  3.9108963 -0.2271348
O   1.1764375  5.0000906 -0.6170753
O   3.7169389  1.5924075 -0.1107837
O   1.3780395  2.7885345  3.1888876
C   0.8851770  1.5606129  1.0314934
C   -3.3749241  1.7211766  1.2143033
C   -1.1676374  0.3385116  1.3637880
C   0.1928795  0.2976471  0.8966920
C   0.9769784 -0.8171162  1.3068905
O   1.1764375 -1.8082698  2.1384112
O   0.9031338 -1.7728671  2.5530957
O   1.3780395 -2.5215978  3.1888876
C   2.0212614 -0.8984200  0.9639711
C   1.0995558 -2.6375996  2.4677812
C   -1.3097820 -2.5737732  3.1913226
C   -2.7632831 -0.6596729  2.4818752
O   -1.2156307  2.5215978  0.5717577
C   0.0508076  2.2612256 -2.5157530
C   0.2007315  1.7823629 -1.5430835
C   0.2860686  0.5846236 -1.0359000
C   0.5162019 -0.7600306 -1.6056033
H   -3.6912993  2.7092654  0.8251728
H   -3.6424525  1.6592183  2.2930281
H   -3.6440442  0.9161822  0.6885007
C   0.9322564 -3.2571365  2.8686490
C   1.8416603 -2.2050001 -3.0704459
C   1.6339749 -0.9629319  2.4495997
C   -0.3846345 -1.8296872 -1.3973801
C   -0.1825077 -3.0636265 -2.0324442
H   1.0923530 -4.2302003 -3.3619071
H   2.7212031 -2.3489816 -3.7198076
H   2.3454830 -0.1362331 -2.6045609
H   -1.2567891 -1.6828597 -0.7402380
H   -0.9026940 -3.8833917 -1.8738868

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number cm$^{-1}$ | IR intensity km/mol | selection rules |
|---|------|----------|-----------------------|---------------------|-----------------|
| 1 | a    | -289.58  | 0.00000               | YES                 | YES             |
| 2 |      | 0.00     | 0.00000               | -                   | -               |
| 3 |      | 0.00     | 0.00000               | -                   | -               |
| 4 |      | 0.00     | 0.00000               | -                   | -               |
| 5 |      | 0.00     | 0.00000               | -                   | -               |
| 6 |      | 0.00     | 0.00000               | -                   | -               |
| 7 |      | 0.00     | 0.00000               | -                   | -               |
| 8 | a    | 19.52    | 0.07940               | YES                 | YES             |
| 9 | a    | 29.50    | 0.44592               | YES                 | YES             |
| 10| a    | 47.00    | 0.00881               | YES                 | YES             |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 11 | a | 66.99 | 0.70250 | YES | YES |
| 12 | a | 69.94 | 0.36195 | YES | YES |
| 13 | a | 75.16 | 0.35748 | YES | YES |
| 14 | a | 87.37 | 0.16474 | YES | YES |
| 15 | a | 92.36 | 0.09761 | YES | YES |
| 16 | a | 100.95 | 0.18382 | YES | YES |
| 17 | a | 105.08 | 0.60387 | YES | YES |
| 18 | a | 125.50 | 0.05780 | YES | YES |
| 19 | a | 145.83 | 0.68043 | YES | YES |
| 20 | a | 161.43 | 0.37167 | YES | YES |
| 21 | a | 189.20 | 2.75605 | YES | YES |
| 22 | a | 201.91 | 1.88209 | YES | YES |
| 23 | a | 214.20 | 1.99503 | YES | YES |
| 24 | a | 233.76 | 2.14063 | YES | YES |
| 25 | a | 247.68 | 0.55556 | YES | YES |
| 26 | a | 280.54 | 0.32179 | YES | YES |
| 27 | a | 305.53 | 1.16879 | YES | YES |
| 28 | a | 391.57 | 2.59632 | YES | YES |
| 29 | a | 400.96 | 0.00811 | YES | YES |
| 30 | a | 409.44 | 2.07552 | YES | YES |
| 31 | a | 418.83 | 5.94734 | YES | YES |
| 32 | a | 445.08 | 0.94194 | YES | YES |
| 33 | a | 466.52 | 0.52551 | YES | YES |
| 34 | a | 474.78 | 0.62650 | YES | YES |
| 35 | a | 486.70 | 3.71712 | YES | YES |
| 36 | a | 497.96 | 17.15639 | YES | YES |
| 37 | a | 510.90 | 0.65377 | YES | YES |
| 38 | a | 514.70 | 9.50928 | YES | YES |
| 39 | a | 523.80 | 7.85160 | YES | YES |
| 40 | a | 535.03 | 12.63137 | YES | YES |
| 41 | a | 562.79 | 13.26407 | YES | YES |
| 42 | a | 569.97 | 6.56249 | YES | YES |
| 43 | a | 599.46 | 22.92425 | YES | YES |
| 44 | a | 604.08 | 9.15845 | YES | YES |
| 45 | a | 610.41 | 63.96900 | YES | YES |
| 46 | a | 613.73 | 5.51951 | YES | YES |
| 47 | a | 628.85 | 10.60410 | YES | YES |
| 48 | a | 656.49 | 38.14813 | YES | YES |
| 49 | a | 681.82 | 76.06539 | YES | YES |
| 50 | a | 689.44 | 19.04587 | YES | YES |
TS23s

SCF Energy (au) BP86/SV(P) = -2452.07412234
SCF Energy (au) PBE0/def2-TZVPP = -2451.611763009
SCF Energy (au) PBE0/def2-TZVPP = -2451.6198030278 (Toluene Correction)
Zero Point Energy (au) = 0.3426121
Chemical Potential (kJ mol$^{-1}$) = 738.90
Dispersion Correction (au) PBE0/def2-TZVPP = -0.06697983

xyz coordinates

Mn  1.5654786  0.9681938  0.4627900
C  1.9182416  1.2711050  2.2078398
C  3.2854914  0.6398468  0.1205255
C  1.7410987  2.7390327  0.0539965
O  1.8481311  3.8736680 -0.1726503
O  4.4094621  0.4308376 -0.1165767
O  2.1443005  1.4632721  3.3334955
C -1.1354830  0.3230288  1.1767272
C -2.5924500  0.4860401  1.4246771
C -0.4263610  0.8978221  1.4068286
C  0.9262225 -0.8932344  1.0551879
C  1.7359861 -2.1102219  1.3285877
O -0.4687028  1.3262799  0.7545599
O  0.4294030  1.343794 -2.7203335
C  1.0947815  2.4917352 -3.2222126
O  0.6939823  3.074199 -4.4328112
C -0.3837235  2.536352 -5.1609371
C -1.0597128  1.4079526 -4.6693880
C -0.6607253  0.8148338 -3.4650582
H  1.9398299  2.9201504 -2.6636380
H  1.2293198  3.9607478 -4.8111972
H -0.6992564  3.0056133 -6.1089827
H -1.9080140  0.9816840 -5.2305998
H -1.1914557  0.0692529 -3.0769267
C  0.8343937  0.6607428 -1.5140208
C  1.0386082 -0.4801990 -0.9434658
H  1.2698459 -1.5240326 -1.1830719
C  3.2211616 -4.4623286  1.9036248
C  1.9746975 -4.5548126  1.2605153
C  1.2370539 -3.3932483  0.9855944
C  3.0006889 -2.0360127  1.9592241
C  3.7266886 -3.1994438  2.2567531
H  3.8001881 -5.3739688  2.1256541
H  1.5719437 -5.5398198  0.9715006
H  0.2581377 -3.4736495  0.4834480
H  3.4100301 -1.0544150  2.2403214
H  4.7072422 -3.1159529  2.7634979
H -5.3471196  0.8537170  1.9156071
C -4.8631252 -0.4103499  1.5360898
C -3.4918806 -0.5979408  1.3053365
C -3.0919689  1.7596975  1.7845470
C -4.4577647  1.9373832  2.0431648
H -6.4229519  0.9971777  2.1104698
H -5.5601838 -1.2565457  1.4170325
H -3.1189453 -1.5882096  0.9971250
H -2.3856525  2.5997060  1.8729524
H -4.8346486  2.9278332  2.3479318
H -0.9072833 -1.7670527  1.8862643
| #  | mode | symmetry | wave number | IR intensity | selection rules |
|----|------|----------|-------------|--------------|----------------|
| 1  |      | a        | -180.13     | 0.00000      | YES YES        |
| 2  |      |          | 0.00        | 0.00000      | - -            |
| 3  |      |          | 0.00        | 0.00000      | - -            |
| 4  |      |          | 0.00        | 0.00000      | - -            |
| 5  |      |          | 0.00        | 0.00000      | - -            |
| 6  |      |          | 0.00        | 0.00000      | - -            |
| 7  |      |          | 0.00        | 0.00000      | - -            |
| 8  |      | a        | 16.16       | 0.08999      | YES YES        |
| 9  |      | a        | 20.23       | 0.17454      | YES YES        |
| 10 |      | a        | 34.71       | 0.06401      | YES YES        |
| 11 |      | a        | 37.61       | 0.19479      | YES YES        |
| 12 |      | a        | 43.85       | 0.24760      | YES YES        |
| 13 |      | a        | 51.29       | 0.13596      | YES YES        |
| 14 |      | a        | 54.50       | 0.27276      | YES YES        |
| 15 |      | a        | 63.64       | 0.23335      | YES YES        |
| 16 |      | a        | 74.41       | 0.09767      | YES YES        |
| 17 |      | a        | 93.89       | 0.26720      | YES YES        |
| 18 |      | a        | 99.92       | 0.26287      | YES YES        |
| 19 |      | a        | 102.96      | 0.22256      | YES YES        |
| 20 |      | a        | 105.64      | 0.21123      | YES YES        |
| 21 |      | a        | 116.39      | 0.20491      | YES YES        |
| 22 |      | a        | 143.20      | 0.60293      | YES YES        |
| 23 |      | a        | 149.93      | 0.16503      | YES YES        |
| 24 |      | a        | 190.48      | 1.23144      | YES YES        |
| 25 |      | a        | 205.11      | 1.14525      | YES YES        |
| 26 |      | a        | 214.53      | 0.46048      | YES YES        |
| 27 |      | a        | 220.33      | 0.23064      | YES YES        |
| 28 |      | a        | 237.52      | 0.32706      | YES YES        |
| 29 |      | a        | 247.55      | 0.52677      | YES YES        |
| 30 |      | a        | 282.57      | 2.82391      | YES YES        |
| 31 |      | a        | 341.14      | 1.83436      | YES YES        |
| 32 |      | a        | 353.75      | 3.35426      | YES YES        |
| 33 |      | a        | 366.36      | 8.42762      | YES YES        |
| 34 |      | a        | 401.05      | 0.75597      | YES YES        |
| 35 |      | a        | 401.37      | 0.17593      | YES YES        |
| 36 |      | a        | 404.09      | 1.14187      | YES YES        |
| 37 |      | a        | 421.75      | 0.55163      | YES YES        |
| 38 |      | a        | 438.05      | 4.88263      | YES YES        |
| 39 |      | a        | 445.64      | 5.18937      | YES YES        |
| 40 |      | a        | 467.10      | 3.82912      | YES YES        |
| 41 |      | a        | 469.55      | 9.05303      | YES YES        |
| 42 |      | a        | 492.57      | 4.87405      | YES YES        |
| 43 |      | a        | 495.94      | 4.92155      | YES YES        |
| 44 |      | a        | 498.59      | 9.00082      | YES YES        |
| 45 |      | a        | 516.90      | 5.21897      | YES YES        |
| 46 |      | a        | 522.34      | 2.90990      | YES YES        |
| 47 |      | a        | 539.29      | 7.89970      | YES YES        |
| 48 |      | a        | 550.81      | 20.25726     | YES YES        |
| 49 |      | a        | 556.18      | 47.74073     | YES YES        |
| 50 |      | a        | 584.71      | 36.46291     | YES YES        |
**TS3sia**

SCF Energy (au) BP86/SV(P) \(-2183.131539912\)

SCF Energy (au) PBE0/def2-TZVPP \(-2182.721878063\)

SCF Energy (au) PBE0/def2-TZVPP \(-2182.729117777\) (Toluene Correction)

Zero Point Energy (au) \(0.2598847\)

Chemical Potential (kJ mol\(^{-1}\)) \(548.92\)

Dispersion Correction (au) PBE0/def2-TZVPP \(-0.05353197\)

**xyz coordinates**

37

C 1.3367351 -0.3768756 2.2988397
C -0.8696697 0.8718326 2.5792574
C 0.2856535 0.5555105 -0.1853000
C -0.8282425 -1.6478829 2.9806592
C 1.2519233 -1.5778408 -0.5630382
C 2.2661993 -2.5523916 -0.6927707
C 0.7030816 -4.2683414 0.1152815
C -0.3271217 -3.3227472 0.2125609
C -0.0654066 -1.9849484 -0.1596621
C -1.1360361 -0.9068470 0.338982
C -1.5758540 -0.6336499 1.7822888

Mn -0.3279993 -0.5396906 1.6508554
O -2.0534784 -0.8175555 0.5732889
O 2.4163054 -0.2735892 2.7286415
O -1.2253325 1.7938260 3.1976814
O -1.3383776 -0.141305 -0.7477564
O -1.1596605 -2.3668982 3.8350984
C 1.9817374 -3.8823686 -0.3520192
H 2.1689385 0.3057951 -1.3249510
C -0.0172476 1.9784906 -0.3980815
C -0.6588662 4.7126596 -0.8344551
C -1.6449917 3.8175246 -0.3849215
C -1.3271176 2.4705144 -0.1582523
C 0.9650262 2.8969337 -0.8540831
C 0.6494950 4.2465958 -1.0614716
H -0.9056341 5.7744510 -0.9996448
H -2.6712222 4.1733747 -0.1962435
H -2.1011877 1.7750955 0.2048468
H 1.9976462 2.5529194 -1.0266605
H 1.4329602 4.9443609 -1.4014742
H -1.3413772 -3.6078647 0.5360664
H 0.5161972 -5.3184823 0.3920617
H 2.7777451 -4.6417863 -0.4299211
H 3.2777694 -2.2619577 -1.0205504
H -0.7404145 -0.7323922 -2.5036776
H -2.0291270 0.3746046 -1.8699356
H -2.3597839 -1.3883484 -2.0190815

$\text{vibrational spectrum}$

| #  | mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules |
|----|------|----------|----------------------|---------------------|-----------------|
| 1  | a    | -178.15  | 0.00000              | YES                | YES             |
| 2  | 0.00 | 0.00000  | -                    | -                   | -               |
| 3  | 0.00 | 0.00000  | -                    | -                   | -               |
| 4  | 0.00 | 0.00000  | -                    | -                   | -               |
| 5  | 0.00 | 0.00000  | -                    | -                   | -               |
| 6  | 0.00 | 0.00000  | -                    | -                   | -               |
| 7  | 0.00 | 0.00000  | -                    | -                   | -               |
| 8  | a    | 38.07    | 0.17468              | YES                | YES             |
| 9  | a    | 42.16    | 0.34856              | YES                | YES             |
| 10 | a    | 57.65    | 0.64808              | YES                | YES             |
| 11 | a    | 69.07    | 0.05984              | YES                | YES             |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
|   |   |   |   |   |   |   |
| 12 | a | 79.69 | 1.20659 | YES | YES |
| 13 | a | 85.09 | 0.07459 | YES | YES |
| 14 | a | 91.20 | 0.11329 | YES | YES |
| 15 | a | 101.05 | 0.11238 | YES | YES |
| 16 | a | 108.83 | 0.07859 | YES | YES |
| 17 | a | 109.28 | 0.33871 | YES | YES |
| 18 | a | 129.11 | 1.29873 | YES | YES |
| 19 | a | 172.76 | 1.55207 | YES | YES |
| 20 | a | 197.82 | 1.60561 | YES | YES |
| 21 | a | 218.20 | 1.84289 | YES | YES |
| 22 | a | 229.25 | 1.86660 | YES | YES |
| 23 | a | 250.83 | 0.90614 | YES | YES |
| 24 | a | 261.45 | 5.14381 | YES | YES |
| 25 | a | 277.68 | 0.84444 | YES | YES |
| 26 | a | 299.35 | 0.12607 | YES | YES |
| 27 | a | 346.64 | 4.71924 | YES | YES |
| 28 | a | 365.64 | 21.12433 | YES | YES |
| 29 | a | 405.32 | 0.81981 | YES | YES |
| 30 | a | 442.72 | 2.88639 | YES | YES |
| 31 | a | 448.97 | 1.12164 | YES | YES |
| 32 | a | 463.59 | 3.13786 | YES | YES |
| 33 | a | 472.79 | 2.09847 | YES | YES |
| 34 | a | 486.71 | 13.64170 | YES | YES |
| 35 | a | 489.97 | 4.34087 | YES | YES |
| 36 | a | 498.19 | 5.76372 | YES | YES |
| 37 | a | 518.61 | 14.10605 | YES | YES |
| 38 | a | 526.22 | 1.99394 | YES | YES |
| 39 | a | 532.54 | 1.56273 | YES | YES |
| 40 | a | 538.83 | 2.68195 | YES | YES |
| 41 | a | 545.65 | 5.39873 | YES | YES |
| 42 | a | 578.06 | 50.23447 | YES | YES |
| 43 | a | 605.11 | 1.59629 | YES | YES |
| 44 | a | 612.32 | 2.01782 | YES | YES |
| 45 | a | 625.64 | 19.88850 | YES | YES |
| 46 | a | 631.86 | 24.17884 | YES | YES |
| 47 | a | 640.70 | 6.88353 | YES | YES |
| 48 | a | 687.72 | 43.96053 | YES | YES |
| 49 | a | 697.76 | 24.66806 | YES | YES |
| 50 | a | 707.48 | 1.42323 | YES | YES |
TS_{383a}

SCF Energy (au) BP86/SV(P) -2452.085970536
SCF Energy (au) PBE0/def2-TZVPP -2451.630064256
SCF Energy (au) PBE0/def2-TZVPP -2451.6393433949 (Toluene Correction)
Zero Point Energy (au) 0.3438944
Chemical Potential (kJ mol^{-1}) 742.05
Dispersion Correction (au) PBE0/def2-TZVPP -0.07029183

xyz coordinates
48

C     1.4459651  -0.1758419  2.8322908
C     -0.8719835  0.8033845  3.3521899
C      0.0125768  0.8884238  0.4443620
C      -0.5083544 -1.7779318  3.3370157
C      1.0132788 -1.2451803  0.1905398
C      2.1795258 -2.1580859  0.1205537
C      -0.3067399 -1.6681079  0.429187
C      -1.4034456  0.6318798  0.2980345
C      -2.0187606 -0.3064184 -1.0455662
Mn     -0.2219443 -0.4141605  2.2012076
O      -2.1573556 -0.5843903  1.3513091
O      2.5026577 -0.0181497  3.3015286
O      -1.3089156  1.5830339  4.0958950
C      1.0950577  0.1951911 -0.0519171
O      -0.7006179 -2.6852305  4.0434619
H      1.9811696  0.6399284 -0.5426852
C      -0.2991287  2.3090379  0.2745308
C      -0.9605832  5.0546709 -0.0279566
C      -1.8643864  4.1740186  0.5920341
C      -1.5362569  2.8195546  0.7454660
C      0.5953798  3.2118691 -0.3598140
C      0.2720649  4.5675809 -0.5018172
H      -1.2138114  6.1218979 -0.1407718
H      -2.8323003  4.5476008  0.9648278
H      -2.2417561  2.1306412  1.2353915
H      1.5655869  2.8492619 -0.7365969
H      0.9880235  5.2532203 -0.9851804
C      4.3876931 -3.9295352 -0.0631820
C      4.4216323 -2.6878733 -0.7187161
C      3.3334881 -1.8068533 -0.6202468
C      2.1615645 -3.4136922  0.7770749
C      3.2539196 -4.2864338  0.6895042
H      5.2462816 -4.6173137 -0.1331958
H      5.3049295 -2.3975818 -1.3107729
H      3.3789063 -0.8420686 -1.1485920
H      1.2920379 -3.6977317  1.3904486
H      3.2228163 -5.2524159  1.2194816
C      -3.3354897  0.2099527 -3.4882376
C      -2.0171691 -0.2836324 -3.4855670
C      -1.3643536 -0.5440095 -2.2721703
C      -3.3403718  0.1856946 -1.0537263
C      -3.9954496  0.4391063 -2.2694879
H      -3.8483526  0.4108975 -4.4436166
H      -1.4963679 -0.4734897 -4.4387979
H      -0.3342230 -0.9371152 -2.2802273
H      -3.8489404  0.3411595 -0.0895448
H      -5.0318163  0.8173070 -2.2638959
H      -0.5956271 -2.7183371  0.5856160
| #  | mode | symmetry | wave number (cm\(^{-1}\)) | IR intensity (km/mol) | selection rules |
|----|------|----------|-----------------------------|-----------------------|-----------------|
| 1  | a    |          | -257.50                     | 0.00000               | YES            |
| 2  | a    |          | 0.00                        | 0.00000               | -              |
| 3  | a    |          | 0.00                        | 0.00000               | -              |
| 4  | a    |          | 0.00                        | 0.00000               | -              |
| 5  | a    |          | 0.00                        | 0.00000               | -              |
| 6  | a    |          | 0.00                        | 0.00000               | -              |
| 7  | a    |          | 0.00                        | 0.00000               | -              |
| 8  | a    |          | 16.16                       | 0.35618               | YES            |
| 9  | a    |          | 19.51                       | 0.10998               | YES            |
| 10 | a    |          | 30.74                       | 0.85372               | YES            |
| 11 | a    |          | 37.52                       | 0.01350               | YES            |
| 12 | a    |          | 40.58                       | 0.13918               | YES            |
| 13 | a    |          | 47.33                       | 0.01430               | YES            |
| 14 | a    |          | 51.11                       | 0.28303               | YES            |
| 15 | a    |          | 59.59                       | 0.80674               | YES            |
| 16 | a    |          | 74.06                       | 0.79660               | YES            |
| 17 | a    |          | 84.46                       | 0.71821               | YES            |
| 18 | a    |          | 89.28                       | 0.09853               | YES            |
| 19 | a    |          | 100.80                      | 0.74385               | YES            |
| 20 | a    |          | 110.29                      | 1.42942               | YES            |
| 21 | a    |          | 124.54                      | 0.19616               | YES            |
| 22 | a    |          | 133.27                      | 0.44369               | YES            |
| 23 | a    |          | 157.79                      | 2.33843               | YES            |
| 24 | a    |          | 187.55                      | 0.58258               | YES            |
| 25 | a    |          | 203.50                      | 1.02218               | YES            |
| 26 | a    |          | 218.94                      | 3.89951               | YES            |
| 27 | a    |          | 235.58                      | 1.10036               | YES            |
| 28 | a    |          | 242.37                      | 0.84239               | YES            |
| 29 | a    |          | 249.53                      | 0.58950               | YES            |
| 30 | a    |          | 290.62                      | 8.45380               | YES            |
| 31 | a    |          | 355.98                      | 18.12758              | YES            |
| 32 | a    |          | 373.78                      | 1.88651               | YES            |
| 33 | a    |          | 396.89                      | 1.42140               | YES            |
| 34 | a    |          | 400.74                      | 0.64740               | YES            |
| 35 | a    |          | 402.24                      | 0.55560               | YES            |
| 36 | a    |          | 416.32                      | 11.16342              | YES            |
| 37 | a    |          | 438.96                      | 1.67739               | YES            |
| 38 | a    |          | 456.34                      | 7.67132               | YES            |
| 39 | a    |          | 462.49                      | 3.16918               | YES            |
| 40 | a    |          | 473.97                      | 8.00078               | YES            |
| 41 | a    |          | 478.28                      | 0.19856               | YES            |
| 42 | a    |          | 480.96                      | 1.70836               | YES            |
| 43 | a    |          | 494.62                      | 8.40481               | YES            |
| 44 | a    |          | 507.88                      | 11.33733              | YES            |
| 45 | a    |          | 517.95                      | 4.88110               | YES            |
| 46 | a    |          | 528.96                      | 16.19087              | YES            |
| 47 | a    |          | 541.68                      | 2.52103               | YES            |
| 48 | a    |          | 576.51                      | 14.87999              | YES            |
| 49 | a    |          | 588.03                      | 27.43969              | YES            |
| 50 | a    |          | 607.72                      | 15.80706              | YES            |
TS391a

SCF Energy (au) BP86/SV(P) -2183.125430263
SCF Energy (au) PBE0/def2-TZVPP -2182.704202665
SCF Energy (au) PBE0/def2-TZVPP -2182.7106225495 (Toluene Correction)
Zero Point Energy (au) 0.2592413
Chemical Potential (kJ mol\(^{-1}\)) 544.22
Dispersion Correction (au) PBE0/def2-TZVPP -0.04988049

xyz coordinates

37
C  1.6215828   0.0130222   2.8637253
C -0.5552919   1.2926508   2.8384885
C  0.3174606   0.8443706   0.1505579
C -0.5744828  -1.3750881   3.0075668
C  0.7261198  -1.6256458   0.3393932
C  1.7321269  -2.6532331   0.5664832
C  0.2907708  -4.3516046  -0.4519661
C -0.7080140  -3.4292694  -0.6772707
C -0.5704676  -2.0679884  -0.2341211
C -1.5464973  -1.0762966  -0.3232095
C -2.7473448  -1.0344039  -1.2212595
Mn  0.1193950  -0.0917515   1.9197951
O  -1.3230132   0.0275928   0.4074424
O   2.6326727   0.0755906   3.4481464
O  -0.9747757   2.1891404   3.4576197
C   1.731735   -0.2558642   0.0899197
O  -1.0479384  -2.1858525   3.6955779
C   1.5161086  -3.9529029   0.1995257
H   2.2538640  -0.0815612  -0.0572638
C   0.3137643   2.1154790   0.0544509
H  -1.6541747  -3.7437835  -1.1471547
O   0.1515968  -5.4016114  -0.7567116
H   2.2932074  -4.7181989   0.3894030
H   2.684546   -2.3521242   1.0258805
H  -2.8894473  -1.9851829  -1.7739075
H  -2.6294363  -0.2159190  -1.9692374
H  -3.6716583  -0.8108671  -0.6431154
C   0.3086756   4.5642397  -1.9674185
C   0.8512904   3.4089457  -2.5600222
C   0.8486286   2.1954004  -1.8602233
C  -0.2351322   3.2887501   0.0356064
C  -0.2339798   4.4938769  -0.6702443
H   0.3059966   5.5188076  -2.5194580
H   1.2749335   3.4550747  -3.5766716
H   1.2615609   1.2851469  -2.3259539
H  -0.6594449   3.2401770   1.0493161
H  -0.6602843   5.4023044  -0.2047327

$\text{vibrational spectrum}$

| # | mode | symmetry | wave number cm**(-1) | IR intensity km/mol | selection rules |
|---|------|----------|----------------------|---------------------|-----------------|
| 1 | a    | a        | -313.32              | 0.00000             | YES             |
| 2 |      |          | 0.00                 | 0.00000             | -               |
| 3 |      |          | 0.00                 | 0.00000             | -               |
| 4 |      |          | 0.00                 | 0.00000             | -               |
| 5 |      |          | 0.00                 | 0.00000             | -               |
| 6 |      |          | 0.00                 | 0.00000             | -               |
| 7 |      |          | 0.00                 | 0.00000             | -               |
| 8 | a    | a        | 31.63                | 0.03949             | YES             |
| 9 | a    |          | 40.30                | 0.01775             | YES             |
| 10| a    |          | 53.45                | 0.53751             | YES             |
| 11| a    |          | 60.98                | 0.12144             | YES             |
| 12| a    |          | 69.36                | 0.04757             | YES             |
|   | a   |     |     |      |      |    |    |
|---|-----|-----|-----|------|------|----|----|
| 13|     | 80.92 | 0.16401 | YES  | YES  |
| 14|     | 88.84 | 0.18539 | YES  | YES  |
| 15|     | 91.39 | 0.29083 | YES  | YES  |
| 16|     | 98.17 | 0.47781 | YES  | YES  |
| 17|     | 104.25 | 0.53446 | YES  | YES  |
| 18|     | 122.27 | 0.27990 | YES  | YES  |
| 19|     | 147.04 | 0.95015 | YES  | YES  |
| 20|     | 154.86 | 1.55796 | YES  | YES  |
| 21|     | 192.89 | 0.67278 | YES  | YES  |
| 22|     | 223.70 | 0.31201 | YES  | YES  |
| 23|     | 235.13 | 0.54397 | YES  | YES  |
| 24|     | 257.58 | 0.44732 | YES  | YES  |
| 25|     | 279.00 | 0.69986 | YES  | YES  |
| 26|     | 318.53 | 1.92914 | YES  | YES  |
| 27|     | 387.67 | 4.46802 | YES  | YES  |
| 28|     | 403.37 | 0.08995 | YES  | YES  |
| 29|     | 417.51 | 2.41069 | YES  | YES  |
| 30|     | 432.74 | 1.95993 | YES  | YES  |
| 31|     | 441.60 | 2.11914 | YES  | YES  |
| 32|     | 461.74 | 0.87129 | YES  | YES  |
| 33|     | 477.70 | 3.83105 | YES  | YES  |
| 34|     | 478.89 | 0.99679 | YES  | YES  |
| 35|     | 482.93 | 1.29028 | YES  | YES  |
| 36|     | 501.38 | 0.56334 | YES  | YES  |
| 37|     | 510.65 | 3.16652 | YES  | YES  |
| 38|     | 520.78 | 7.08188 | YES  | YES  |
| 39|     | 535.43 | 14.46453 | YES  | YES  |
| 40|     | 542.00 | 5.87021 | YES  | YES  |
| 41|     | 566.54 | 4.99136 | YES  | YES  |
| 42|     | 581.36 | 9.04895 | YES  | YES  |
| 43|     | 603.70 | 18.18185 | YES  | YES  |
| 44|     | 614.09 | 33.72873 | YES  | YES  |
| 45|     | 631.46 | 6.20273 | YES  | YES  |
| 46|     | 642.41 | 31.94297 | YES  | YES  |
| 47|     | 657.03 | 5.78668 | YES  | YES  |
| 48|     | 685.30 | 47.75021 | YES  | YES  |
| 49|     | 688.80 | 33.16830 | YES  | YES  |
| 50|     | 701.59 | 14.32620 | YES  | YES  |
TS39a

SCF Energy (au) BP86/SV(P)  -2452.101612798
SCF Energy (au) PBE0/def2-TZVPP -2451.637427819
SCF Energy (au) PBE0/def2-TZVPP -2451.6455080397 (Toluene Correction)
Zero Point Energy (au) 0.3446137
Chemical Potential (kJ mol\(^{-1}\)) 746.48
Dispersion Correction (au) PBE0/def2-TZVPP -0.06671155

xyz coordinates

48

C   1.6911518   0.6228639   2.9599087
C  -0.5381033   1.8319302   2.8699088
C   0.5156193   1.3664366   0.2758119
C  -0.4804033  -0.7971369   3.1531878
C   0.8488824  -1.1533185   0.4898860
C   1.9238833  -2.1593889   0.7807363
C  -0.4299699  -1.6306059  -0.0101577
C  -1.4614591  -0.7019179   0.1204781
C  -2.6568288  -0.7785329  -0.9969108
Mn   0.1931996   0.4441162   2.0089345
O  -1.3093976   0.4176004   0.5715432
O   2.6893899   0.7487136   3.5529774
O  -1.0018127   2.7373071   3.4424823
C   1.2831257   0.2088211   0.1935954
O  -0.9329596  -0.9329596  -1.5831127
C   2.3746248   0.3488222   0.0759198
C   0.5527362   2.6114123  -0.4457787
C  -4.9714533  -0.8042816  -2.6347098
C  -4.0882095  -1.8996863  -2.6367533
C  -2.9367838  -1.8859868  -1.8347872
C  -3.5595053   0.3131106  -0.9985137
C  -4.6981174   0.3043616  -1.8148038
H  -5.8716749  -0.8147227  -3.2716781
H  -4.2965941  -2.7715272  -3.2790539
H  -2.2505973  -2.7475411  -1.8679982
H  -3.3418301  -1.7061813  -0.3448872
H  -5.3818132   1.1696513  -1.8054271
H  -0.4897308  -2.6480544  -0.4272459
C   0.6920922   5.0397000  -1.8938761
C   0.9948020   3.8226459  -2.5346432
C   0.9269590   2.6209065  -1.8209363
C   0.2278337   3.8473862   0.1774812
C   0.3075455   5.0470284  -0.5391237
H   0.7528175   5.9872565  -2.4544869
H   1.2854998   3.8151227  -3.5979841
H   1.1568459   1.6635327  -2.3166701
H  -0.0799994   3.8505724   1.2334426
H   0.0669994   5.9995647  -0.0392820
C   3.9630695  -4.0219373   1.4494328
C   4.2023586  -3.0250814   0.4899196
C   3.1928921  -2.1067782   0.1579381
C   1.6877952  -3.1905233   1.7206998
C   2.6976743  -4.1047987   2.0573633
H   4.7601895  -4.7329263   1.7225311
H   5.1837171  -2.9583326  -0.0085284
H   3.3961008  -1.3491768  -0.6167166
H   0.7101998  -3.2455799   2.2256543
H   2.4992385  -4.8785330   2.8172817
| #  | mode | symmetry | wave number cm**(-1) | IR intensity km/mol | IR | RAMAN |
|----|------|----------|---------------------|---------------------|----|-------|
| 1  | a    |          | -101.84             | 0.00000             | YES| YES   |
| 2  | 0.00 |          | 0.00000             | -                   | -  | -     |
| 3  | 0.00 |          | 0.00000             | -                   | -  | -     |
| 4  | 0.00 |          | 0.00000             | -                   | -  | -     |
| 5  | 0.00 |          | 0.00000             | -                   | -  | -     |
| 6  | 0.00 |          | 0.00000             | -                   | -  | -     |
| 7  | 0.00 |          | 0.00000             | -                   | -  | -     |
| 8  | a    |          | 19.82               | 0.04668             | YES| YES   |
| 9  | a    |          | 31.80               | 0.37669             | YES| YES   |
| 10 | a    |          | 40.20               | 0.20557             | YES| YES   |
| 11 | a    |          | 43.70               | 0.03615             | YES| YES   |
| 12 | a    |          | 47.80               | 0.24022             | YES| YES   |
| 13 | a    |          | 53.12               | 0.20842             | YES| YES   |
| 14 | a    |          | 58.20               | 0.16989             | YES| YES   |
| 15 | a    |          | 76.82               | 0.14507             | YES| YES   |
| 16 | a    |          | 88.16               | 0.32927             | YES| YES   |
| 17 | a    |          | 92.55               | 0.19181             | YES| YES   |
| 18 | a    |          | 101.18              | 0.19223             | YES| YES   |
| 19 | a    |          | 115.84              | 0.51378             | YES| YES   |
| 20 | a    |          | 134.32              | 0.28560             | YES| YES   |
| 21 | a    |          | 142.23              | 0.83050             | YES| YES   |
| 22 | a    |          | 169.68              | 0.93431             | YES| YES   |
| 23 | a    |          | 186.56              | 0.09386             | YES| YES   |
| 24 | a    |          | 206.28              | 1.66894             | YES| YES   |
| 25 | a    |          | 229.73              | 0.47084             | YES| YES   |
| 26 | a    |          | 237.12              | 0.49147             | YES| YES   |
| 27 | a    |          | 250.38              | 1.77895             | YES| YES   |
| 28 | a    |          | 261.02              | 3.38600             | YES| YES   |
| 29 | a    |          | 304.35              | 1.70317             | YES| YES   |
| 30 | a    |          | 353.95              | 5.54405             | YES| YES   |
| 31 | a    |          | 390.73              | 6.44978             | YES| YES   |
| 32 | a    |          | 400.70              | 0.74591             | YES| YES   |
| 33 | a    |          | 402.44              | 0.39983             | YES| YES   |
| 34 | a    |          | 403.13              | 0.39119             | YES| YES   |
| 35 | a    |          | 432.59              | 2.42700             | YES| YES   |
| 36 | a    |          | 445.95              | 6.51090             | YES| YES   |
| 37 | a    |          | 453.39              | 3.00818             | YES| YES   |
| 38 | a    |          | 469.58              | 1.35279             | YES| YES   |
| 39 | a    |          | 480.02              | 0.97809             | YES| YES   |
| 40 | a    |          | 484.42              | 0.28655             | YES| YES   |
| 41 | a    |          | 491.23              | 0.85186             | YES| YES   |
| 42 | a    |          | 510.47              | 5.91320             | YES| YES   |
| 43 | a    |          | 521.15              | 4.56488             | YES| YES   |
| 44 | a    |          | 532.73              | 7.72744             | YES| YES   |
| 45 | a    |          | 544.33              | 11.44481            | YES| YES   |
| 46 | a    |          | 556.94              | 15.98299            | YES| YES   |
| 47 | a    |          | 572.11              | 11.88796            | YES| YES   |
| 48 | a    |          | 592.99              | 11.20011            | YES| YES   |
| 49 | a    |          | 610.97              | 1.19647             | YES| YES   |