C$_2$H$_5$NO Isomers: from

Acetamide to 1,2-Oxazetidine

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#1 1-amino-ethanol

Charge = 0 Multiplicity = 1 Stoichiometry C$_2$H$_5$NO

| Center Number | Atomic Number | Atomic Type | X (Å) | Y (Å) | Z (Å) |
|---------------|---------------|-------------|-------|-------|-------|
| 1             | 6             | 0           | -0.098496 | -0.000636 | 0.003809 |
| 2             | 6             | 0           | -1.401390 | -0.278992 | 0.007973 |
| 3             | 7             | 0           | 0.949461  | -0.926260 | -0.081140 |
| 4             | 8             | 0           | 0.347858  | 1.290565  | 0.047666 |
| 5             | 1             | 0           | -1.748741 | -1.296192 | 0.097672 |
| 6             | 1             | 0           | -2.125624 | 0.514648  | -0.075791 |
| 7             | 1             | 0           | 1.626073  | -0.829060 | 0.666100 |
| 8             | 1             | 0           | 0.630137  | -1.881171 | -0.147386 |
| 9             | 1             | 0           | 1.188381  | 1.328843  | -0.424640 |

A, B, C / GHz 10.4676840 9.8787368 5.1622496

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|-----------|--------------|
| 1         | vib      | 322.49         | 0.00             | A         | 22.8881      |
| 2         | vib      | 450.45         | 0.00             | A         | 106.8977     |
| 3         | vib      | 457.13         | 0.00             | A         | 21.1293      |
| 4         | vib      | 502.88         | 0.00             | A         | 26.1824      |
| 5         | vib      | 584.42         | 0.00             | A         | 72.0742      |
| 6         | vib      | 681.22         | 0.00             | A         | 42.1468      |
| 7         | vib      | 782.81         | 0.00             | A         | 77.5178      |
| 8         | vib      | 799.90         | 0.00             | A         | 146.1423     |
| 9         | vib      | 920.80         | 0.00             | A         | 27.7564      |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 10 | vib | 981.63 | 0.00 | A | 23.0046 |
| 11 | vib | 1150.46 | 0.00 | A | 18.4855 |
| 12 | vib | 1242.28 | 0.00 | A | 61.3117 |
| 13 | vib | 1366.82 | 0.00 | A | 183.2122 |
| 14 | vib | 1440.02 | 0.00 | A | 3.1579 |
| 15 | vib | 1635.49 | 0.00 | A | 45.7097 |
| 16 | vib | 1747.15 | 0.00 | A | 215.9462 |
| 17 | vib | 3173.27 | 0.00 | A | 1.1042 |
| 18 | vib | 3263.93 | 0.00 | A | 5.3890 |
| 19 | vib | 3505.60 | 0.00 | A | 3.6441 |
| 20 | vib | 3616.78 | 0.00 | A | 10.1448 |
| 21 | vib | 3774.52 | 0.00 | A | 37.7459 |
| 22 | rot | 0.3491644 | - | - | - |
| 23 | rot | 0.3295192 | - | - | - |
| 24 | rot | 0.1721941 | - | - | - |

------------------------ ZPE and THERMAL CONTRIBUTIONS ------------------------

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| Eelectronic | [kJ/mol] | = -549416.559 |
| Ezpe | [kJ/mol] | = +193.796 |
| Eelectronic+Ezpe | [kJ/mol] | = -549222.763 |

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| Eelectronic | [hartrees] | = -209.261687 |
| Ezpe | [hartrees] | = +0.073813 |
| Eelectronic+Ezpe | [hartrees] | = -209.187874 |

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| Thermal Correction to Energy | [kJ/mol] | = +205.776 |
| Thermal Correction to Enthalpy | [kJ/mol] | = +208.255 |
| Thermal Correction to Gibbs | [kJ/mol] | = +124.457 |

#10 Figure 17a

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO
| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|-----------------|----------|--------------|
| 1         | vib      | 378.64         | 0.00            | A        | 6.5531       |
| 2         | vib      | 423.17         | 0.00            | A        | 94.2689      |
| 3         | vib      | 492.02         | 0.00            | A        | 6.6798       |
| 4         | vib      | 560.06         | 0.00            | A        | 1.6772       |
| 5         | vib      | 748.84         | 0.00            | A        | 7.4922       |
| 6         | vib      | 820.14         | 0.00            | A        | 67.3257      |
| 7         | vib      | 848.48         | 0.00            | A        | 36.8659      |
| 8         | vib      | 914.22         | 0.00            | A        | 1.1653       |
| 9         | vib      | 943.49         | 0.00            | A        | 199.7825     |
| 10        | vib      | 1076.30        | 0.00            | A        | 115.0154     |
| 11        | vib      | 1111.89        | 0.00            | A        | 9.8776       |
| 12        | vib      | 1228.42        | 0.00            | A        | 3.0498       |
| 13        | vib      | 1252.57        | 0.00            | A        | 112.2166     |
| 14        | vib      | 1328.46        | 0.00            | A        | 37.0050      |
| 15        | vib      | 1441.39        | 0.00            | A        | 32.2993      |
| 16        | vib      | 1603.14        | 0.00            | A        | 23.2838      |
| 17        | vib      | 2997.52        | 0.00            | A        | 97.6250      |
| 18        | vib      | 3075.12        | 0.00            | A        | 51.5406      |
| 19        | vib      | 3471.11        | 0.00            | A        | 8.4229       |
| 20        | vib      | 3606.36        | 0.00            | A        | 41.3069      |
| 21        | vib      | 3774.71        | 0.00            | A        | 10.2099      |
| 22        | rot      | 0.5831022      | -               |          |              |
| 23        | rot      | 0.2381264      | -               |          |              |
| 24        | rot      | 0.1999046      | -               |          |              |

**ZPE and THERMAL CONTRIBUTIONS**

- Electronic [kJ/mol] = -549117.166
- Zpe [kJ/mol] = +191.977
- Electronic+Zpe [kJ/mol] = -548925.189

- Electronic [hartrees] = -209.147654
- Zpe [hartrees] = +0.073120
- Electronic+Zpe [hartrees] = -209.074534

Thermal Correction to Energy [kJ/mol] = +203.248
Thermal Correction to Enthalpy [kJ/mol] = +205.726
Thermal Correction to Gibbs [kJ/mol] = +123.441

#100 methyl formimidate

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

--------------- OPTIMIZED GEOMETRY -------------------

| Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X    | Y    | Z    |
|--------|---------------|--------------|-------------------------|------|------|------|
| 1      | 6             | 0            | -0.783408               | 0.48306 | 0.000000 |
| 2      | 6             | 0            | 1.380787                | -0.443150 | -0.000000 |
| 3      | 7             | 0            | -1.292877               | -0.666913 | 0.000000 |
| 4      | 8             | 0            | 0.537020                | 0.716794 | -0.000000 |
| 5      | 1             | 0            | 2.398289                | -0.063728 | -0.000000 |
| 6      | 1             | 0            | 1.196007                | -1.050848 | -0.884813 |
| 7      | 1             | 0            | 1.196008                | -1.050847 | 0.884814 |
| 8      | 1             | 0            | -2.306149               | -0.612143 | -0.000000 |
| 9      | 1             | 0            | -1.314455               | 1.440671 | -0.000000 |

A, B, C / GHz 19.6545885 6.6674288 5.1383084

--------------- FREQUENCIES AND ROTATIONAL CONSTANTS -------------------

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|-----------|--------------|
| 1         | vib      | 169.43         | 0.00             | A         | 0.0111       |
| 2         | vib      | 306.17         | 0.00             | A         | 49.1396      |
| 3         | vib      | 315.73         | 0.00             | A         | 15.0746      |
| 4         | vib      | 724.56         | 0.00             | A         | 5.6492       |
| 5         | vib      | 831.80         | 0.00             | A         | 38.9329      |
| 6         | vib      | 926.19         | 0.00             | A         | 53.7011      |
| 7         | vib      | 1042.82        | 0.00             | A         | 1.1242       |
| 8         | vib      | 1077.36        | 0.00             | A         | 144.9285     |
| 9         | vib      | 1176.08        | 0.00             | A         | 1.1308       |
| 10        | vib      | 1216.71        | 0.00             | A         | 26.3922      |
| 11        | vib      | 1303.77        | 0.00             | A         | 125.1285     |
| 12        | vib      | 1400.36        | 0.00             | A         | 24.2800      |
| 13        | vib      | 1469.04        | 0.00             | A         | 8.8960       |
| 14        | vib      | 1480.68        | 0.00             | A         | 9.0281       |
| 15        | vib      | 1500.94        | 0.00             | A         | 11.2284      |
| 16        | vib      | 1704.85        | 0.00             | A         | 228.2464     |
| 17        | vib      | 3044.23        | 0.00             | A         | 31.4146      |
|   |   |       |     |   |   |
|---|---|-------|-----|---|---|
| 18| vib| 3085.39 | 0.00 | A | 38.4930 |
| 19| vib| 3110.48 | 0.00 | A | 22.5721 |
| 20| vib| 3145.82 | 0.00 | A | 18.1015 |
| 21| vib| 3521.64 | 0.00 | A | 5.1660 |
| 22| rot| 0.6556065 | - | - | - |
| 23| rot| 0.2224015 | - | - | - |
| 24| rot| 0.1713955 | - | - | - |

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### ZPE and THERMAL CONTRIBUTIONS

- Electronic [kJ/mol] = -549412.653
- Zpe [kJ/mol] = +194.718
- Electronic+Zpe [kJ/mol] = -549217.935

- Electronic [hartrees] = -209.260199
- Zpe [hartrees] = +0.074164
- Electronic+Zpe [hartrees] = -209.186035

- Thermal Correction to Energy [kJ/mol] = +206.811
- Thermal Correction to Enthalpy [kJ/mol] = +209.292
- Thermal Correction to Gibbs [kJ/mol] = +124.598

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### #11 Figure 17c

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

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#### OPTIMIZED GEOMETRY

| Center Number | Atomic Number | Atomic Type | X       | Y       | Z       |
|---------------|---------------|-------------|---------|---------|---------|
| 1             | 6             | 0           | 0.801331| 0.830041| -0.313137|
| 2             | 6             | 0           | 1.000255| -0.646338| -0.148602|
| 3             | 7             | 0           | -0.158352| 0.041907| 0.439166 |
| 4             | 8             | 0           | -1.474224| -0.122497| -0.110812|
| 5             | 1             | 0           | 1.382107 | 1.455512| 0.360233 |
| 6             | 1             | 0           | 0.747167 | -1.304756| -0.971837|
| 7             | 1             | 0           | 1.646128 | -1.106870| 0.600322 |
| 8             | 1             | 0           | -0.268817| 0.034405| 1.447329 |
| 9             | 1             | 0           | -1.413842| 0.506111| -0.853284|

A, B, C / GHz 18.4378574 7.1491507 6.2362163
| INDEX NO. | DOF TYPE | CM\(^{-1}\)(UNSCALED) | CM\(^{-1}\)(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|-----------------------|--------------------------|----------|--------------|
| 1         | vib      | 378.66                | 0.00                     | A        | 17.3513      |
| 2         | vib      | 419.13                | 0.00                     | A        | 34.8569      |
| 3         | vib      | 468.08                | 0.00                     | A        | 73.5050      |
| 4         | vib      | 711.44                | 0.00                     | A        | 104.2360     |
| 5         | vib      | 739.61                | 0.00                     | A        | 27.2633      |
| 6         | vib      | 842.48                | 0.00                     | A        | 12.9437      |
| 7         | vib      | 901.65                | 0.00                     | A        | 17.5883      |
| 8         | vib      | 909.69                | 0.00                     | A        | 26.9837      |
| 9         | vib      | 1087.72               | 0.00                     | A        | 40.6640      |
| 10        | vib      | 1102.81               | 0.00                     | A        | 7.2579       |
| 11        | vib      | 1137.60               | 0.00                     | A        | 6.9932       |
| 12        | vib      | 1212.08               | 0.00                     | A        | 12.7329      |
| 13        | vib      | 1234.41               | 0.00                     | A        | 0.9451       |
| 14        | vib      | 1370.52               | 0.00                     | A        | 39.1199      |
| 15        | vib      | 1469.00               | 0.00                     | A        | 39.1816      |
| 16        | vib      | 1514.67               | 0.00                     | A        | 2.0352       |
| 17        | vib      | 3032.87               | 0.00                     | A        | 80.0570      |
| 18        | vib      | 3100.81               | 0.00                     | A        | 25.4395      |
| 19        | vib      | 3138.21               | 0.00                     | A        | 17.3608      |
| 20        | vib      | 3485.79               | 0.00                     | A        | 11.5232      |
| 21        | vib      | 3620.32               | 0.00                     | A        | 43.6435      |
| 22        | rot      | 0.6150207             | -                        |          |              |
| 23        | rot      | 0.2384700             | -                        |          |              |
| 24        | rot      | 0.2080178             | -                        |          |              |

| Eelectronic [kJ/mol] | = -548987.878 |
| Ezpe [kJ/mol]        | = +190.669   |
| Eelectronic+Ezpe [kJ/mol] | = -548797.209 |

| Eelectronic [hartrees] | = -209.098411 |
| Ezpe [hartrees]        | = +0.072622 |
| Eelectronic+Ezpe [hartrees] | = -209.025789 |

| Thermal Correction to Energy [kJ/mol] | = +201.707 |
| Thermal Correction to Enthalpy [kJ/mol] | = +204.185 |
| Thermal Correction to Gibbs [kJ/mol] | = +122.327 |
#111 Figure 17r

Charge = 0 Multiplicity = 1  Stoichiometry  C2H5NO

---------------------------------------- OPTIMIZED GEOMETRY ----------------------------------------

| Center Number | Atomic Number | Atomic Type | Coordinates (Å) |
|---------------|---------------|-------------|-----------------|
|               | 6             | 0           | 0.601314 -0.382304 0.278004 |
|               | 6             | 0           | 1.726511 0.089878 -0.223849 |
|               | 7             | 0           | -0.642826 0.389628 0.286519 |
|               | 8             | 0           | -1.620678 -0.254546 -0.406442 |
|               | 1             | 0           | 0.440586 -1.384422 0.643201 |
|               | 1             | 0           | 2.611791 -0.526646 -0.274764 |
|               | 1             | 0           | 1.800690 1.096315 -0.616459 |
|               | 1             | 0           | -0.437393 1.324279 -0.099624 |
|               | 1             | 0           | -0.917413 0.553995 1.268624 |

A, B, C / GHz  27.7340126  4.7366673  4.5999598

---------------------------------------- FREQUENCIES AND ROTATIONAL CONSTANTS ----------------------------------------

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY A) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|-------------------|-----------|--------------|
| 1         | vib      | 135.37         | 0.00              | A         | 22.0712      |
| 2         | vib      | 348.31         | 0.00              | A         | 45.9921      |
| 3         | vib      | 443.83         | 0.00              | A         | 4.4302       |
| 4         | vib      | 665.26         | 0.00              | A         | 10.0557      |
| 5         | vib      | 903.35         | 0.00              | A         | 5.6812       |
| 6         | vib      | 935.50         | 0.00              | A         | 3.5221       |
| 7         | vib      | 944.54         | 0.00              | A         | 102.6400     |
| 8         | vib      | 983.41         | 0.00              | A         | 6.5381       |
| 9         | vib      | 1001.32        | 0.00              | A         | 6.2500       |
| 10        | vib      | 1163.60        | 0.00              | A         | 6.6664       |
| 11        | vib      | 1273.86        | 0.00              | A         | 4.1904       |
| 12        | vib      | 1310.11        | 0.00              | A         | 0.9378       |
| 13        | vib      | 1390.97        | 0.00              | A         | 17.4523      |
| 14        | vib      | 1444.52        | 0.00              | A         | 6.9676       |
| 15        | vib      | 1645.55        | 0.00              | A         | 16.9625      |
| 16        | vib      | 1710.33        | 0.00              | A         | 31.7243      |
| 17        | vib      | 3143.01        | 0.00              | A         | 2.1298       |
| 18        | vib      | 3191.09        | 0.00              | A         | 34.8990      |
| 19        | vib      | 3212.40        | 0.00              | A         | 11.0872      |
| 20        | vib      | 3224.20        | 0.00              | A         | 4.1093       |
| 21        | vib      | 3239.79        | 0.00              | A         | 2.7204       |
| 22        | rot      | 0.9251071      | -                 | -         | -            |
| 23        | rot      | 0.1579982      | -                 | -         | -            |
| 24        | rot      | 0.1534381      | -                 | -         | -            |
#118 Z,E ethanimidic acid

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

OPTIMIZED GEOMETRY

| Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X     | Y     | Z     |
|--------|---------------|-------------|--------------------------|-------|-------|-------|
| 1      | 6             | 0           | -0.117617                | -0.104509 | 0   | 0.000000 |
| 2      | 6             | 0           | 1.380143                 | -0.194380 | -0.000000 |
| 3      | 7             | 0           | -0.858549                | -1.123639 | 0   | 0.000000 |
| 4      | 8             | 0           | 0.634042                 | 1.166854  | 0   | 0.000000 |
| 5      | 1             | 0           | 1.683680                 | -1.236135 | 0   | 0.000000 |
| 6      | 1             | 0           | 1.794625                 | 0.298522  | 0.882712 |
| 7      | 1             | 0           | 1.794625                 | 0.298522  | -0.882712 |
| 8      | 1             | 0           | -1.841894                | -0.854209 | 0.000000 |
| 9      | 1             | 0           | 0.075982                 | 1.817274  | 0.000002 |

A, B, C / GHz 10.6804968 9.3604650 5.1481232

FREQUENCIES AND ROTATIONAL CONSTANTS

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|-----------------|----------|--------------|
| 1         | vib      | 166.71         | 0.00            | A        | 0.1372       |
| 2         | vib      | 374.64         | 0.00            | A        | 107.5016     |
| 3         | vib      | 427.26         | 0.00            | A        | 3.0209       |
| vib | 542.31 | 0.00 | A  | 26.5921 |
|-----|--------|------|----|---------|
| vib | 543.86 | 0.00 | A  | 11.6583 |
| vib | 853.72 | 0.00 | A  | 40.7383 |
| vib | 915.98 | 0.00 | A  | 64.4434 |
| vib | 1007.12| 0.00 | A  | 5.6625  |
| vib | 1077.52| 0.00 | A  | 0.7500  |
| vib | 1116.43| 0.00 | A  | 44.2791 |
| vib | 1229.20| 0.00 | A  | 50.6291 |
| vib | 1354.95| 0.00 | A  | 265.1785|
| vib | 1415.44| 0.00 | A  | 70.3546 |
| vib | 1478.43| 0.00 | A  | 1.9424  |
| vib | 1488.56| 0.00 | A  | 7.8695  |
| vib | 1771.98| 0.00 | A  | 165.4072|
| vib | 3026.09| 0.00 | A  | 13.1582 |
| vib | 3074.06| 0.00 | A  | 13.5538 |
| vib | 3152.93| 0.00 | A  | 3.8625  |
| vib | 3462.95| 0.00 | A  | 2.7823  |
| vib | 3805.86| 0.00 | A  | 40.2240 |
| rot | 0.3562630 | - |   |        |
| rot | 0.3122315 | - |   |        |
| rot | 0.1717229 | - |   |        |

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### ZPE and THERMAL CONTRIBUTIONS

**Electronic** [kJ/mol] = -549458.685

**Ezpe** [kJ/mol] = +193.113

**Electronic+Ezpe** [kJ/mol] = -549265.572

**Electronic** [hartrees] = -209.277732

**Ezpe** [hartrees] = +0.073553

**Electronic+Ezpe** [hartrees] = -209.204179

**Thermal Correction to Energy** [kJ/mol] = +205.451

**Thermal Correction to Enthalpy** [kJ/mol] = +207.929

**Thermal Correction to Gibbs** [kJ/mol] = +122.808

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### #119 tZt oxime-acetaldehyde

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

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---------------------- OPTIMIZED GEOMETRY ---------------------------

| Center | Atomic | Atomic | Coordinates (Angstroms) |
| Number | Number | Type | X       | Y       | Z       |
|--------|--------|------|---------|---------|---------|
| 1      | 6      | 0    | -0.521186 | 0.704092 | -0.000001 |
| 2      | 6      | 0    | -1.418567 | -0.492619 | -0.000000 |
| 3      | 7      | 0    | 0.749582  | 0.696472  | -0.000000 |
| 4      | 8      | 0    | 1.255814  | -0.618245 | 0.000001  |
| 5      | 1      | 0    | -0.945857 | 1.701687  | -0.000001 |
| 6      | 1      | 0    | -1.225398 | -1.15946  | -0.874961 |
| 7      | 1      | 0    | -2.464883 | -0.195695 | -0.000007 |
| 8      | 1      | 0    | -1.225408 | -1.15937  | 0.874969  |
| 9      | 1      | 0    | 2.206481  | -0.472290 | 0.000001  |

A, B, C / GHz  17.4449931  6.5814875  4.9222861

| INDEX NO. | DOF | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|-----|----------------|------------------|-----------|--------------|
| 1         | vib | 53.15          | 0.00             | A         | 0.0104       |
| 2         | vib | 284.06         | 0.00             | A         | 1.0438       |
| 3         | vib | 403.41         | 0.00             | A         | 76.1342      |
| 4         | vib | 524.81         | 0.00             | A         | 36.4897      |
| 5         | vib | 686.05         | 0.00             | A         | 15.8436      |
| 6         | vib | 845.66         | 0.00             | A         | 17.4078      |
| 7         | vib | 912.18         | 0.00             | A         | 79.4415      |
| 8         | vib | 964.96         | 0.00             | A         | 38.0493      |
| 9         | vib | 1058.14        | 0.00             | A         | 0.2519       |
| 10        | vib | 1115.71        | 0.00             | A         | 19.4621      |
| 11        | vib | 1337.70        | 0.00             | A         | 36.7319      |
| 12        | vib | 1372.16        | 0.00             | A         | 41.5928      |
| 13        | vib | 1409.80        | 0.00             | A         | 13.7547      |
| 14        | vib | 1477.54        | 0.00             | A         | 9.5018       |
| 15        | vib | 1483.10        | 0.00             | A         | 8.5371       |
| 16        | vib | 1727.06        | 0.00             | A         | 5.5489       |
| 17        | vib | 3034.91        | 0.00             | A         | 9.1719       |
| 18        | vib | 3082.02        | 0.00             | A         | 9.2816       |
| 19        | vib | 3121.49        | 0.00             | A         | 13.3239      |
| 20        | vib | 3155.85        | 0.00             | A         | 11.7398      |
| 21        | vib | 3825.56        | 0.00             | A         | 90.1905      |
| 22        | rot | 0.5819023      | -                |           |              |
| 23        | rot | 0.2195348      | -                |           |              |
| 24        | rot | 0.1641898      | -                |           |              |

| E electronic | E zpe | E electronic+E zpe |
|--------------|-------|-------------------|
| [kJ/mol] = -549306.422 | [kJ/mol] = +190.656 | [kJ/mol] = -549115.766 |
Electronic [hartrees] = -209.219738
Expe [hartrees] = +0.072617
Electronic+Expe [hartrees] = -209.147121

Thermal Correction to Energy [kJ/mol] = +203.739
Thermal Correction to Enthalpy [kJ/mol] = +206.217
Thermal Correction to Gibbs [kJ/mol] = +117.998

#120 E,E N-methyl methanimidic acid
Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

Optimized Geometry

| Center Number | Atomic Number | Type | X       | Y       | Z       |
|---------------|---------------|------|---------|---------|---------|
| 1             | 6             | 0    | -0.522801 | 0.295367 | -0.000000 |
| 2             | 6             | 0    | 1.783561  | 0.084199 | 0.000001  |
| 3             | 7             | 0    | 0.453769  | -0.485679| -0.000002 |
| 4             | 8             | 0    | -1.792928 | -0.183956| 0.000002  |
| 5             | 1             | 0    | -0.445058 | 1.390477 | 0.000001  |
| 6             | 1             | 0    | 1.797058  | 1.183109 | -0.000008 |
| 7             | 1             | 0    | 2.330166  | -0.266705| 0.877182  |
| 8             | 1             | 0    | 2.330176  | -0.266719| -0.877169 |
| 9             | 1             | 0    | -2.409862 | 0.553844 | -0.000010 |

A, B, C / GHz 49.4541231 4.3066557 4.0603883

Frequencies and Rotational Constants

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|----------|--------------|
| 1         | vib      | 205.27         | 0.00             | A        | 12.2501      |
| 2         | vib      | 281.33         | 0.00             | A        | 22.0062      |
| 3         | vib      | 328.22         | 0.00             | A        | 4.0957       |
| 4         | vib      | 403.63         | 0.00             | A        | 66.8689      |
| 5         | vib      | 605.03         | 0.00             | A        | 23.1118      |
| 6         | vib      | 972.03         | 0.00             | A        | 2.6672       |
| 7         | vib      | 1012.39        | 0.00             | A        | 17.2265      |
| 8         | vib      | 1138.19        | 0.00             | A        | 17.7691      |
| 9         | vib      | 1140.20        | 0.00             | A        | 0.0088       |
| 10        | vib      | 1192.71        | 0.00             | A        | 30.6411      |
| 11        | vib      | 1294.83        | 0.00             | A        | 309.9266     |
12  vib  1405.34  0.00  A  3.6765
13  vib  1449.86  0.00  A  13.2278
14  vib  1480.86  0.00  A  3.8487
15  vib  1507.09  0.00  A  11.3789
16  vib  1792.31  0.00  A  245.7958
17  vib  2957.15  0.00  A  63.2394
18  vib  2988.64  0.00  A  87.6228
19  vib  3052.78  0.00  A  39.1698
20  vib  3071.18  0.00  A  22.6698
21  vib  3832.60  0.00  A  74.4643
22  rot  1.6496120 -
23  rot  0.1436546 -
24  rot  0.1354400 -

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------------------------ ZPE and THERMAL CONTRIBUTIONS -------------------------

Electronic [kJ/mol] = -549409.013
Ezpe [kJ/mol] = +192.071
Eelectronic+Ezpe [kJ/mol] = -549216.942

Electronic [hartrees] = -209.258813
Ezpe [hartrees] = +0.073156
Eelectronic+Ezpe [hartrees] = -209.185657

Thermal Correction to Energy [kJ/mol] = +204.805
Thermal Correction to Enthalpy [kJ/mol] = +207.286
Thermal Correction to Gibbs [kJ/mol] = +122.107

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#123 methylene-amino-methanol

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

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---------------------- OPTIMIZED GEOMETRY ----------------------

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
| 1             | 6             | 0           | 1.719731 -0.029630 0.182019 |
| 2             | 6             | 0           | -0.521516 0.502154 -0.123120 |
| 3             | 7             | 0           | 0.630445 -0.350137 -0.365699 |
| 4             | 8             | 0           | -1.685513 -0.251800 0.107248 |
| 5             | 1             | 0           | 1.835243 0.844610 0.835675 |
| 6             | 1             | 0           | 2.605114 -0.636793 0.008870 |
| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|----------|----------|----------------|-----------------|----------|--------------|
| 1        | vib      | 98.07          | 0.00            | A        | 3.9673       |
| 2        | vib      | 251.21         | 0.00            | A        | 110.7528     |
| 3        | vib      | 389.19         | 0.00            | A        | 5.6531       |
| 4        | vib      | 530.00         | 0.00            | A        | 13.0152      |
| 5        | vib      | 714.74         | 0.00            | A        | 2.9576       |
| 6        | vib      | 949.82         | 0.00            | A        | 29.5417      |
| 7        | vib      | 1055.19        | 0.00            | A        | 76.4093      |
| 8        | vib      | 1079.49        | 0.00            | A        | 13.4927      |
| 9        | vib      | 1095.68        | 0.00            | A        | 111.0967     |
| 10       | vib      | 1217.99        | 0.00            | A        | 12.1628      |
| 11       | vib      | 1253.19        | 0.00            | A        | 18.6661      |
| 12       | vib      | 1375.41        | 0.00            | A        | 3.8079       |
| 13       | vib      | 1426.72        | 0.00            | A        | 68.5725      |
| 14       | vib      | 1491.42        | 0.00            | A        | 17.8917      |
| 15       | vib      | 1504.09        | 0.00            | A        | 3.7732       |
| 16       | vib      | 1728.95        | 0.00            | A        | 25.5795      |
| 17       | vib      | 2914.99        | 0.00            | A        | 81.3057      |
| 18       | vib      | 2979.10        | 0.00            | A        | 65.8586      |
| 19       | vib      | 3064.49        | 0.00            | A        | 19.5905      |
| 20       | vib      | 3124.93        | 0.00            | A        | 27.7784      |
| 21       | vib      | 3808.78        | 0.00            | A        | 28.0357      |
| 22       | rot      | 1.0668132      | -               |          |              |
| 23       | rot      | 0.1554530      | -               |          |              |
| 24       | rot      | 0.1490301      | -               |          |              |

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**ZPE and THERMAL CONTRIBUTIONS**

- **Electronic** [kJ/mol] = -549359.767
- **Ezpe** [kJ/mol] = +191.722
- **Eelectronic+Ezpe** [kJ/mol] = -549168.045

- **Electronic** [hartrees] = -209.240056
- **Ezpe** [hartrees] = +0.073023
- **Eelectronic+Ezpe** [hartrees] = -209.167033

- **Thermal Correction to Energy** [kJ/mol] = +204.503
- **Thermal Correction to Enthalpy** [kJ/mol] = +206.981
- **Thermal Correction to Gibbs** [kJ/mol] = +120.419
#126 O-methyl-N-oxide-formaldehyde

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

------------------------ OPTIMIZED GEOMETRY ------------------------

| Center | Atomic Number | Atomic Number | Atomic Type | X      | Y      | Z      |
|--------|---------------|---------------|-------------|--------|--------|--------|
| 1      | 6             | 0             | -1.756378   | 0.056674 | 0.000000 |
| 2      | 6             | 0             | 1.674424    | -0.132800 | 0.000000 |
| 3      | 7             | 0             | -0.601340   | -0.463859 | -0.000000 |
| 4      | 8             | 0             | 0.400375    | 0.502565  | -0.000000 |
| 5      | 1             | 0             | -2.595832   | -0.624601 | 0.000001 |
| 6      | 1             | 0             | 1.918213    | 1.131462  | 0.000001 |
| 7      | 1             | 0             | 1.804303    | -0.749090 | 0.891144 |
| 8      | 1             | 0             | 1.804300    | -0.749097 | -0.891139 |
| 9      | 1             | 0             | 2.403538    | 0.674571  | -0.000004 |

A, B, C / GHz 41.6087644 4.9177569 4.5239963

----------------------- FREQUENCIES AND ROTATIONAL CONSTANTS -----------------------

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|-------------------|----------|--------------|
| 1         | vib      | 117.85         | 0.00              | A        | 10.0503      |
| 2         | vib      | 180.15         | 0.00              | A        | 5.1622       |
| 3         | vib      | 342.09         | 0.00              | A        | 9.5740       |
| 4         | vib      | 568.54         | 0.00              | A        | 9.4396       |
| 5         | vib      | 795.41         | 0.00              | A        | 1.0315       |
| 6         | vib      | 852.90         | 0.00              | A        | 57.2137      |
| 7         | vib      | 978.61         | 0.00              | A        | 33.6008      |
| 8         | vib      | 1083.86        | 0.00              | A        | 192.1861     |
| 9         | vib      | 1175.03        | 0.00              | A        | 1.2933       |
| 10        | vib      | 1175.76        | 0.00              | A        | 3.4817       |
| 11        | vib      | 1235.24        | 0.00              | A        | 6.1762       |
| 12        | vib      | 1427.82        | 0.00              | A        | 4.5001       |
| 13        | vib      | 1466.12        | 0.00              | A        | 1.6712       |
| 14        | vib      | 1479.07        | 0.00              | A        | 5.8380       |
| 15        | vib      | 1508.39        | 0.00              | A        | 15.9020      |
| 16        | vib      | 1691.18        | 0.00              | A        | 12.0810      |
| 17        | vib      | 3020.80        | 0.00              | A        | 62.3397      |
| 18        | vib      | 3083.25        | 0.00              | A        | 39.5163      |
| 19        | vib      | 3093.53        | 0.00              | A        | 7.9600       |
|    |    |     |     |     |     |     |     |
|----|----|-----|-----|-----|-----|-----|-----|
| 20 | vib| 3126.11 | 0.00 | A | 18.7324 |
| 21 | vib| 3219.64 | 0.00 | A | 5.2558  |
| 22 | rot| 1.3879190 | - | - | - |
| 23 | rot| 0.1640387 | - | - | - |
| 24 | rot| 0.1509043 | - | - | - |

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------------------------ ZPE and THERMAL CONTRIBUTIONS -------------------------

|              | [kJ/mol]      | [kJ/mol]      | [kJ/mol]      |
|--------------|---------------|---------------|---------------|
| Electronic   | -549256.852   | +189.138      | -549067.714   |
| Zpe          |               |               |               |
| Electronic+Zpe|              |               |               |

|              | [hartrees]    | [hartrees]    | [hartrees]    |
|--------------|---------------|---------------|---------------|
| Electronic   | -209.200858   | +0.072039     | -209.128819   |
| Zpe          |               |               |               |
| Electronic+Zpe|              |               |               |

|                      | [kJ/mol]      | [kJ/mol]      | [kJ/mol]      |
|----------------------|---------------|---------------|---------------|
| Thermal Correction to Energy | +202.163        | +204.642      | +118.045      |
| Thermal Correction to Enthalpy |               |               |               |
| Thermal Correction to Gibbs     |               |               |               |

#13 Z,Z 2-imino-ethanol

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

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---------------------- OPTIMIZED GEOMETRY ----------------------

| Center Number | Atomic Number | Atomic Type | X   | Y   | Z   |
|---------------|---------------|-------------|-----|-----|-----|
| 1             | 6             | 0           | -0.777567 | 0.545945 | 0.000000 |
| 2             | 6             | 0           | 0.720336 | 0.631146 | -0.000000 |
| 3             | 7             | 0           | -1.330844 | -0.591285 | -0.000000 |
| 4             | 8             | 0           | 1.331947 | -0.629478 | 0.000000 |
| 5             | 1             | 0           | -1.319477 | 1.496550 | 0.0000002 |
| 6             | 1             | 0           | 1.031555 | 1.213759 | -0.878652 |
| 7             | 1             | 0           | 1.031556 | 1.213759 | 0.878650 |
| 8             | 1             | 0           | 0.606258 | -1.274177 | 0.000000 |
| 9             | 1             | 0           | -2.346171 | -0.537618 | 0.000000 |

A, B, C / GHz 17.9164368 6.4762261 4.9003445

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-------------------------- FREQUENCIES AND ROTATIONAL CONSTANTS --------------------------

15
| INDEX NO. | DOF TYPE | CM-1 (UNSCALED) | CM-1 (SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|-----------------|-------------------|----------|--------------|
| 1         | vib      | 220.09          | 0.00              | A        | 0.0226       |
| 2         | vib      | 307.20          | 0.00              | A        | 13.3022      |
| 3         | vib      | 442.49          | 0.00              | A        | 87.6135      |
| 4         | vib      | 654.19          | 0.00              | A        | 33.3241      |
| 5         | vib      | 725.34          | 0.00              | A        | 23.9890      |
| 6         | vib      | 882.38          | 0.00              | A        | 23.7352      |
| 7         | vib      | 1041.11         | 0.00              | A        | 22.7666      |
| 8         | vib      | 1104.93         | 0.00              | A        | 105.5312     |
| 9         | vib      | 1111.68         | 0.00              | A        | 3.1149       |
| 10        | vib      | 1177.61         | 0.00              | A        | 36.1349      |
| 11        | vib      | 1254.16         | 0.00              | A        | 3.5314       |
| 12        | vib      | 1339.05         | 0.00              | A        | 21.6070      |
| 13        | vib      | 1405.93         | 0.00              | A        | 58.2726      |
| 14        | vib      | 1460.02         | 0.00              | A        | 65.1442      |
| 15        | vib      | 1493.76         | 0.00              | A        | 13.1785      |
| 16        | vib      | 1720.43         | 0.00              | A        | 61.3411      |
| 17        | vib      | 2965.23         | 0.00              | A        | 33.6236      |
| 18        | vib      | 2976.08         | 0.00              | A        | 33.1668      |
| 19        | vib      | 3033.85         | 0.00              | A        | 61.1030      |
| 20        | vib      | 3487.41         | 0.00              | A        | 1.5254       |
| 21        | vib      | 3663.71         | 0.00              | A        | 82.7140      |
| 22        | rot      | 0.5976280       | -                 |          |              |
| 23        | rot      | 0.2160236       | -                 |          |              |
| 24        | rot      | 0.1634579       | -                 |          |              |

#130 1,2-oxazetidine

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO
### OPTIMIZED GEOMETRY

| Center Number | Atomic Number | Atomic Type | X     | Y     | Z     |
|---------------|---------------|-------------|-------|-------|-------|
| 1             | 6             | 0           | 0.578646 | 0.857869 | -0.068026 |
| 2             | 6             | 0           | -0.891394 | 0.489663 | 0.094684 |
| 3             | 7             | 0           | 0.891275  | -0.605437 | -0.046820 |
| 4             | 8             | 0           | -0.561117 | -0.904499 | -0.108466 |
| 5             | 1             | 0           | 1.041844  | 1.443752  | 0.724485 |
| 6             | 1             | 0           | 0.833505  | 1.288409  | -1.035194 |
| 7             | 1             | 0           | -1.301853 | 0.663806  | 1.095039 |
| 8             | 1             | 0           | -1.590066 | 0.859175  | -0.656543 |
| 9             | 1             | 0           | 1.143070  | -0.866279 | 0.907652 |

A, B, C / GHz 12.7347343 12.1169942 6.9643787

### FREQUENCIES AND ROTATIONAL CONSTANTS

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|----------|--------------|
| 1         | vib      | 128.38         | 0.00             | A        | 4.0720       |
| 2         | vib      | 744.84         | 0.00             | A        | 2.1893       |
| 3         | vib      | 862.98         | 0.00             | A        | 12.6503      |
| 4         | vib      | 872.84         | 0.00             | A        | 0.5614       |
| 5         | vib      | 926.30         | 0.00             | A        | 5.8405       |
| 6         | vib      | 978.21         | 0.00             | A        | 10.0613      |
| 7         | vib      | 1010.94        | 0.00             | A        | 42.1656      |
| 8         | vib      | 1050.18        | 0.00             | A        | 40.7436      |
| 9         | vib      | 1153.86        | 0.00             | A        | 3.3912       |
| 10        | vib      | 1208.47        | 0.00             | A        | 2.2385       |
| 11        | vib      | 1254.26        | 0.00             | A        | 18.3863      |
| 12        | vib      | 1311.55        | 0.00             | A        | 4.2351       |
| 13        | vib      | 1350.24        | 0.00             | A        | 0.7206       |
| 14        | vib      | 1374.39        | 0.00             | A        | 10.8328      |
| 15        | vib      | 1510.09        | 0.00             | A        | 0.3494       |
| 16        | vib      | 1531.24        | 0.00             | A        | 0.9499       |
| 17        | vib      | 2996.48        | 0.00             | A        | 75.0237      |
| 18        | vib      | 3055.66        | 0.00             | A        | 40.3332      |
| 19        | vib      | 3069.58        | 0.00             | A        | 30.9101      |
| 20        | vib      | 3103.68        | 0.00             | A        | 34.9936      |
| 21        | vib      | 3391.42        | 0.00             | A        | 3.9189       |
| 22        | rot      | 0.4247850      | -                |          |              |
| 23        | rot      | 0.4041794      | -                |          |              |
| 24        | rot      | 0.2323067      | -                |          |              |

17
# ZPE and THERMAL CONTRIBUTIONS

Electronic [kJ/mol] = \(-549176.263\)

Ezpe [kJ/mol] = \(+196.700\)

Eelectronic+Ezpe [kJ/mol] = \(-548979.563\)

Eelectronic [hartrees] = \(-209.170163\)

Ezpe [hartrees] = \(+0.074919\)

Eelectronic+Ezpe [hartrees] = \(-209.095244\)

Thermal Correction to Energy [kJ/mol] = \(+207.131\)

Thermal Correction to Enthalpy [kJ/mol] = \(+209.612\)

Thermal Correction to Gibbs [kJ/mol] = \(+127.883\)

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#131 1,3-oxazetidine

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

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**OPTIMIZED GEOMETRY**

| Center Number | Atomic Number | Atomic Type | X     | Y     | Z     |
|---------------|---------------|-------------|-------|-------|-------|
| 1             | 6             | 0           | 1.007670 | -0.026258 | 0.001683 |
| 2             | 6             | 0           | -1.007670 | -0.026258 | 0.001683 |
| 3             | 7             | 0           | -0.000000 | 1.040591  | -0.146195 |
| 4             | 8             | 0           | 0.000000  | -1.050586 | 0.030025  |
| 5             | 1             | 0           | 1.599040  | 0.010273  | 0.924490  |
| 6             | 1             | 0           | 1.674448  | -0.136850 | -0.858009 |
| 7             | 1             | 0           | -1.674448 | -0.136850 | -0.858009 |
| 8             | 1             | 0           | -1.599040 | 0.010273  | 0.924490  |
| 9             | 1             | 0           | -0.000000 | 1.688806  | 0.630002  |

A, B, C / GHz 12.9483491 12.7548106 7.1238313

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**FREQUENCIES AND ROTATIONAL CONSTANTS**

| INDEX NO. DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|--------------------|----------------|-----------------|----------|--------------|
| 1                  | vib            | 117.50          | A        | 8.0880       |
| 2                  | vib            | 773.71          | A        | 68.2324      |
| 3                  | vib            | 904.28          | A        | 97.9553      |
| 4                  | vib            | 947.77          | A        | 1.5293       |
| 5                  | vib            | 998.51          | A        | 28.6335      |
| 6                  | vib            | 1012.68         | A        | 15.7108      |
#132 3-methyl-oxaziridine

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

| Center Number | Atomic Number | Atomic Type | X   | Y   | Z   |
|--------------|---------------|-------------|-----|-----|-----|
| 1            | 6             | 0           | -0.106863 | -0.071765 | 0.474697 |
| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY) | SYMMETRY | IR-INTENSITY |
|----------|----------|----------------|-----------------|----------|--------------|
| 1        | vib      | 219.43         | 0.00            | A        | 0.1631       |
| 2        | vib      | 383.30         | 0.00            | A        | 3.9688       |
| 3        | vib      | 442.56         | 0.00            | A        | 6.8867       |
| 4        | vib      | 734.65         | 0.00            | A        | 5.8351       |
| 5        | vib      | 858.20         | 0.00            | A        | 18.4103      |
| 6        | vib      | 922.82         | 0.00            | A        | 2.3123       |
| 7        | vib      | 1005.32        | 0.00            | A        | 17.9213      |
| 8        | vib      | 1073.70        | 0.00            | A        | 20.6687      |
| 9        | vib      | 1203.13        | 0.00            | A        | 6.6033       |
| 10       | vib      | 1228.09        | 0.00            | A        | 18.5126      |
| 11       | vib      | 1287.30        | 0.00            | A        | 28.3680      |
| 12       | vib      | 1353.23        | 0.00            | A        | 25.9339      |
| 13       | vib      | 1407.36        | 0.00            | A        | 6.4557       |
| 14       | vib      | 1445.83        | 0.00            | A        | 52.2490      |
| 15       | vib      | 1479.33        | 0.00            | A        | 6.3239       |
| 16       | vib      | 1496.96        | 0.00            | A        | 5.7368       |
| 17       | vib      | 3028.50        | 0.00            | A        | 9.9813       |
| 18       | vib      | 3085.97        | 0.00            | A        | 8.7245       |
| 19       | vib      | 3090.39        | 0.00            | A        | 14.3459      |
| 20       | vib      | 3109.69        | 0.00            | A        | 39.4819      |
| 21       | vib      | 3384.67        | 0.00            | A        | 2.0840       |
| 22       | rot      | 0.6035802      | -               |         |              |
| 23       | rot      | 0.2355442      | -               |         |              |
| 24       | rot      | 0.2044763      | -               |         |              |

| Eelectronic | [kJ/mol] = -549222.503 |
| Ezpe         | [kJ/mol] = +192.840    |
| Eelectronic+ Ezpe | [kJ/mol] = -549029.663 |
| Eelectronic | [hartrees] = -209.187775 |
| Ezpe         | [hartrees] = +0.073449  |
Electronic + Hartrees = $-209.114326$

Thermal Correction to Energy [kJ/mol] = $+204.162$
Thermal Correction to Enthalpy [kJ/mol] = $+206.640$
Thermal Correction to Gibbs [kJ/mol] = $+123.816$

#133 2-methyl-oxaziridine

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

OPTIMIZED GEOMETRY

| Center Number | Atomic Number | Atomic Type | X (Å) | Y (Å) | Z (Å) |
|---------------|---------------|-------------|-------|-------|-------|
| 1             | 6             | 0           | 0.942128 | -0.599379 | 0.106111 |
| 2             | 6             | 0           | -1.415995 | -0.043907 | 0.144104 |
| 3             | 7             | 0           | -0.158829 | -0.034636 | -0.597467 |
| 4             | 8             | 0           | 0.836102  | 0.797511  | 0.151560  |
| 5             | 1             | 0           | 0.754888  | -1.119349 | 1.044482  |
| 6             | 1             | 0           | 1.746061  | -1.004933 | -0.501821 |
| 7             | 1             | 0           | -1.273549 | -0.083846 | 1.227697  |
| 8             | 1             | 0           | -1.982395 | 0.849073  | -0.114171 |
| 9             | 1             | 0           | -1.978821 | -0.918871 | -0.187690 |

A, B, C / GHz 18.8637380 7.4299514 6.5052288

FREQUENCIES AND ROTATIONAL CONSTANTS

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|----------|--------------|
| 1         | vib      | 226.70         | 0.00             | A        | 0.9645       |
| 2         | vib      | 408.19         | 0.00             | A        | 9.4253       |
| 3         | vib      | 445.88         | 0.00             | A        | 2.6378       |
| 4         | vib      | 722.80         | 0.00             | A        | 12.7739      |
| 5         | vib      | 828.95         | 0.00             | A        | 21.7495      |
| 6         | vib      | 981.66         | 0.00             | A        | 7.4185       |
| 7         | vib      | 1054.26        | 0.00             | A        | 3.6920       |
| 8         | vib      | 1126.95        | 0.00             | A        | 6.5859       |
| 9         | vib      | 1168.95        | 0.00             | A        | 1.1593       |
| 10        | vib      | 1199.55        | 0.00             | A        | 4.9118       |
| 11        | vib      | 1226.80        | 0.00             | A        | 2.9831       |
| 12        | vib      | 1315.99        | 0.00             | A        | 21.2176      |
| 13        | vib      | 1431.31        | 0.00             | A        | 3.4194       |
| 14        | vib      | 1471.96        | 0.00             | A        | 6.4583       |
# ZPE and THERMAL CONTRIBUTIONS

Electronic [kJ/mol] = -549191.801

Zepe [kJ/mol] = +191.659

Electronic+Zepe [kJ/mol] = -549000.142

Electronic [hartrees] = -209.176081

Zepe [hartrees] = +0.072999

Electronic+Zepe [hartrees] = -209.103082

Thermal Correction to Energy [kJ/mol] = +202.867

Thermal Correction to Enthalpy [kJ/mol] = +205.348

Thermal Correction to Gibbs [kJ/mol] = +122.923

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## #138 Nitrosoethane

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

### OPTIMIZED GEOMETRY

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
| 1             | 6             | 0           | 0.417227 0.602291 -0.010447 |
| 2             | 6             | 0           | 1.631551 -0.317890 -0.088462 |
| 3             | 7             | 0           | -0.753266 -0.180783 0.470113 |
| 4             | 8             | 0           | -1.697742 -0.155490 -0.270476 |
| 5             | 1             | 0           | 0.172897 1.076036 -0.962696 |
| 6             | 1             | 0           | 0.574566 1.365754 0.757153 |
| 7             | 1             | 0           | 2.523458 0.259789 -0.328131 |
| 8             | 1             | 0           | 1.794420 -0.824780 0.862195 |
| 9             | 1             | 0           | 1.496784 -1.073803 -0.862051 |
| INDEX NO. | DOF | TYPE | CM-1 (UNSCALED) | CM-1 (SCALED BY ) | SYMMETRY | IR-INTENSITY |
|----------|-----|------|----------------|-------------------|----------|-------------|
| 1        | vib | 79.40| 0.00           | A                 | 0.0184   |
| 2        | vib | 205.14| 0.00          | A                 | 0.4162   |
| 3        | vib | 374.10| 0.00          | A                 | 4.4297   |
| 4        | vib | 563.39| 0.00          | A                 | 1.5243   |
| 5        | vib | 776.12| 0.00          | A                 | 20.5473  |
| 6        | vib | 850.70| 0.00          | A                 | 9.5389   |
| 7        | vib | 989.90| 0.00          | A                 | 2.4258   |
| 8        | vib | 1040.25| 0.00         | A                 | 5.7739   |
| 9        | vib | 1172.52| 0.00         | A                 | 12.3543  |
| 10       | vib | 1254.81| 0.00         | A                 | 5.5744   |
| 11       | vib | 1327.44| 0.00         | A                 | 3.0053   |
| 12       | vib | 1409.23| 0.00         | A                 | 2.1296   |
| 13       | vib | 1465.42| 0.00         | A                 | 4.1679   |
| 14       | vib | 1493.82| 0.00         | A                 | 8.6307   |
| 15       | vib | 1504.95| 0.00         | A                 | 7.2162   |
| 16       | vib | 1656.05| 0.00         | A                 | 93.3781  |
| 17       | vib | 3017.51| 0.00         | A                 | 11.6852  |
| 18       | vib | 3041.12| 0.00         | A                 | 17.5099  |
| 19       | vib | 3076.90| 0.00         | A                 | 9.0755   |
| 20       | vib | 3108.84| 0.00         | A                 | 18.9555  |
| 21       | vib | 3112.99| 0.00         | A                 | 19.9702  |
| 22       | rot | 0.8960503| -           |                   |           |
| 23       | rot | 0.1573449| -           |                   |           |
| 24       | rot | 0.1518506| -           |                   |           |

| INDEX NO. | DOF | TYPE | CM-1 (UNSCALED) | CM-1 (SCALED BY ) | SYMMETRY | IR-INTENSITY |
|----------|-----|------|----------------|-------------------|----------|-------------|
| 1        | vib | 79.40| 0.00           | A                 | 0.0184   |
| 2        | vib | 205.14| 0.00          | A                 | 0.4162   |
| 3        | vib | 374.10| 0.00          | A                 | 4.4297   |
| 4        | vib | 563.39| 0.00          | A                 | 1.5243   |
| 5        | vib | 776.12| 0.00          | A                 | 20.5473  |
| 6        | vib | 850.70| 0.00          | A                 | 9.5389   |
| 7        | vib | 989.90| 0.00          | A                 | 2.4258   |
| 8        | vib | 1040.25| 0.00         | A                 | 5.7739   |
| 9        | vib | 1172.52| 0.00         | A                 | 12.3543  |
| 10       | vib | 1254.81| 0.00         | A                 | 5.5744   |
| 11       | vib | 1327.44| 0.00         | A                 | 3.0053   |
| 12       | vib | 1409.23| 0.00         | A                 | 2.1296   |
| 13       | vib | 1465.42| 0.00         | A                 | 4.1679   |
| 14       | vib | 1493.82| 0.00         | A                 | 8.6307   |
| 15       | vib | 1504.95| 0.00         | A                 | 7.2162   |
| 16       | vib | 1656.05| 0.00         | A                 | 93.3781  |
| 17       | vib | 3017.51| 0.00         | A                 | 11.6852  |
| 18       | vib | 3041.12| 0.00         | A                 | 17.5099  |
| 19       | vib | 3076.90| 0.00         | A                 | 9.0755   |
| 20       | vib | 3108.84| 0.00         | A                 | 18.9555  |
| 21       | vib | 3112.99| 0.00         | A                 | 19.9702  |
| 22       | rot | 0.8960503| -           |                   |           |
| 23       | rot | 0.1573449| -           |                   |           |
| 24       | rot | 0.1518506| -           |                   |           |

ZPE and THERMAL CONTRIBUTIONS

- Electronic [kJ/mol] = -549236.07
- ZPE [kJ/mol] = +188.535
- Electronic + ZPE [kJ/mol] = -549047.535

- Electronic [hartrees] = -209.192942
- ZPE [hartrees] = +0.071809
- Electronic + ZPE [hartrees] = -209.121133

- Thermal Correction to Energy [kJ/mol] = +201.570
- Thermal Correction to Enthalpy [kJ/mol] = +204.049
- Thermal Correction to Gibbs [kJ/mol] = +116.360
#15 cis 2-aziridinol

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

----------------------------------------- OPTIMIZED GEOMETRY -----------------------------------------

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
| 1             | 6             | 0           | 0.211182 -0.021230 0.487094 |
| 2             | 6             | 0           | -0.964671 -0.662937 -0.144074 |
| 3             | 7             | 0           | -0.847593 0.810445 -0.022555 |
| 4             | 8             | 0           | 1.414178 0.029147 -0.228674 |
| 5             | 1             | 0           | 0.332316 -0.011293 1.56666 |
| 6             | 1             | 0           | -0.798648 -1.109413 -1.116385 |
| 7             | 1             | 0           | -1.749845 -1.111384 0.451316 |
| 8             | 1             | 0           | -0.553280 1.210261 -0.908157 |
| 9             | 1             | 0           | 1.910114 -0.779466 -0.064284 |

A, B, C / GHz 18.2513624 7.1913381 6.2700414

----------------------------------------- FREQUENCIES AND ROTATIONAL CONSTANTS -----------------------------------------

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|-------------------|----------|--------------|
| 1         | vib      | 214.79         | 0.00              | A        | 111.9950     |
| 2         | vib      | 426.92         | 0.00              | A        | 13.7633      |
| 3         | vib      | 460.58         | 0.00              | A        | 14.0688      |
| 4         | vib      | 760.78         | 0.00              | A        | 49.1489      |
| 5         | vib      | 946.92         | 0.00              | A        | 18.9792      |
| 6         | vib      | 964.73         | 0.00              | A        | 20.6272      |
| 7         | vib      | 1026.60        | 0.00              | A        | 17.3604      |
| 8         | vib      | 1110.63        | 0.00              | A        | 21.2169      |
| 9         | vib      | 1136.85        | 0.00              | A        | 3.1975       |
| 10        | vib      | 1210.15        | 0.00              | A        | 20.3363      |
| 11        | vib      | 1243.15        | 0.00              | A        | 25.8477      |
| 12        | vib      | 1263.52        | 0.00              | A        | 91.7286      |
| 13        | vib      | 1321.81        | 0.00              | A        | 47.5409      |
| 14        | vib      | 1414.33        | 0.00              | A        | 27.9438      |
| 15        | vib      | 1501.58        | 0.00              | A        | 9.2617       |
| 16        | vib      | 3097.04        | 0.00              | A        | 39.6044      |
| 17        | vib      | 3105.19        | 0.00              | A        | 20.0166      |
| 18        | vib      | 3191.16        | 0.00              | A        | 16.7486      |
| 19        | vib      | 3501.78        | 0.00              | A        | 5.9581       |
| 20        | vib      | 3803.92        | 0.00              | A        | 32.2970      |
| 21        | rot      | 0.6087999      | -                 |         |              |
| 22        | rot      | 0.2398772      | -                 |         |              |
| 23        | rot      | 0.2091461      | -                 |         |              |

24
#156 Figure 17s

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

Optimized Geometry

| Center Number | Atomic Number | Atomic Type | X (Angstroms) | Y (Angstroms) | Z (Angstroms) |
|---------------|---------------|-------------|---------------|---------------|---------------|
| 1             | 6             | 0           | -1.856243     | 0.028724      | -0.044216     |
| 2             | 6             | 0           | 0.553913      | 0.473367      | 0.089176      |
| 3             | 7             | 0           | -0.550914     | -0.258072     | 0.042032      |
| 4             | 8             | 0           | 1.737638      | -0.208216     | -0.144827     |
| 5             | 1             | 0           | -2.552725     | -0.780171     | 0.065956      |
| 6             | 1             | 0           | -2.168798     | 1.056965      | -0.086246     |
| 7             | 1             | 0           | 0.506079      | 1.539581      | -0.073089     |
| 8             | 1             | 0           | -0.333575     | -1.249201     | 0.071712      |
| 9             | 1             | 0           | 2.318292      | -0.107489     | 0.616292      |

A, B, C / GHz 46.3967009 4.3773934 4.0542576

Frequencies and Rotational Constants

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|--------------|----------|--------------|
| 1         | vib      | 164.16         | 0.00         | A        | 2.1852       |
| 2         | vib      | 317.53         | 0.00         | A        | 27.0958      |
| 3         | vib      | 360.44         | 0.00         | A        | 174.1150     |
|   | vib  |       |       | A   |       |
|---|------|-------|-------|-----|-------|
| 4 | vib  | 394.10| 0.00  | A   | 139.8587|
| 5 | vib  | 502.40| 0.00  | A   | 77.9148  |
| 6 | vib  | 588.88| 0.00  | A   | 4.7373   |
| 7 | vib  | 608.94| 0.00  | A   | 58.3677  |
| 8 | vib  | 937.69| 0.00  | A   | 74.9143  |
| 9 | vib  | 1030.04| 0.00  | A   | 47.9665  |
|10 | vib  | 1145.66| 0.00  | A   | 228.3569 |
|11 | vib  | 1228.09| 0.00  | A   | 30.6505  |
|12 | vib  | 1307.09| 0.00  | A   | 22.1916  |
|13 | vib  | 1363.54| 0.00  | A   | 36.8541  |
|14 | vib  | 1407.20| 0.00  | A   | 166.1979 |
|15 | vib  | 1499.52| 0.00  | A   | 17.3043  |
|16 | vib  | 1645.80| 0.00  | A   | 82.2508  |
|17 | vib  | 3192.08| 0.00  | A   | 18.0472  |
|18 | vib  | 3198.12| 0.00  | A   | 17.3219  |
|19 | vib  | 3316.63| 0.00  | A   | 4.9792   |
|20 | vib  | 3522.81| 0.00  | A   | 29.8867  |
|21 | vib  | 3764.62| 0.00  | A   | 58.3570  |
|22 | rot  | 1.5476274| -    |     |         |
|23 | rot  | 0.1460141| -    |     |         |
|24 | rot  | 0.1352355| -    |     |         |

#163 Figure 17t
Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

| Center | Atomic | Atomic Coordinates (Angstroms) |
### Frequencies and Rotational Constants

| INDEX NO. | DOF | TYPE | CM-1(UNSCALED) | CM-1(SCALED BY) | SYMMETRY | IR-INTENSITY |
|-----------|-----|------|----------------|-----------------|----------|--------------|
| 1         | vib | 223.77 | 0.00           | A               | 7.2230   |
| 2         | vib | 310.82 | 0.00           | A               | 4.1834   |
| 3         | vib | 406.96 | 0.00           | A               | 8.7446   |
| 4         | vib | 645.78 | 0.00           | A               | 0.0898   |
| 5         | vib | 659.31 | 0.00           | A               | 16.5090  |
| 6         | vib | 672.39 | 0.00           | A               | 57.9360  |
| 7         | vib | 915.87 | 0.00           | A               | 49.2066  |
| 8         | vib | 989.37 | 0.00           | A               | 61.0471  |
| 9         | vib | 1022.99 | 0.00         | A               | 0.2090   |
| 10        | vib | 1128.14 | 0.00          | A               | 11.0356  |
| 11        | vib | 1356.45 | 0.00          | A               | 43.5479  |
| 12        | vib | 1408.91 | 0.00          | A               | 8.8114   |
| 13        | vib | 1460.03 | 0.00          | A               | 10.1278  |
| 14        | vib | 1466.28 | 0.00          | A               | 10.5587  |
| 15        | vib | 1488.94 | 0.00          | A               | 26.0509  |
| 16        | vib | 1544.61 | 0.00          | A               | 26.2505  |
| 17        | vib | 2969.20 | 0.00          | A               | 9.4773   |
| 18        | vib | 2995.90 | 0.00          | A               | 17.2619  |
| 19        | vib | 3130.06 | 0.00          | A               | 5.5065   |
| 20        | vib | 3213.65 | 0.00          | A               | 4.6210   |
| 21        | vib | 3337.45 | 0.00          | A               | 31.5346  |
| 22        | rot | 0.6240102 | -            |                |
| 23        | rot | 0.2146016 | -            |                |
| 24        | rot | 0.1645353 | -            |                |

### ZPE and Thermal Contributions

- Electronic Energy [kJ/mol] = -549092.071
- Vibrational Energy [kJ/mol] = +187.495
- Electronic + Vibrational Energy [kJ/mol] = -548904.576
Eelectronic [hartrees] = -209.138096
Expe [hartrees] = +0.071413
Eelectronic+Expe [hartrees] = -209.066683
Thermal Correction to Energy [kJ/mol] = +199.677
Thermal Correction to Enthalpy [kJ/mol] = +202.156
Thermal Correction to Gibbs [kJ/mol] = +117.685

#176 H−¨C−O−CH₂−NH₂
Charge = 0 Multiplicity = 1 Stoichiometry C₂H₅NO

------------------------------ OPTIMIZED GEOMETRY -------------------------------

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

|   |   |     |     |   |   |   |
|---|---|-----|-----|---|---|---|
|1  |6  |0    |1.387918| -0.636398| 0.145748|
|2  |6  |0    |-0.633174| 0.631840  | 0.146647|
|3  |7  |0    |-1.402671| -0.519933| -0.030496|
|4  |8  |0    |0.862133 | 0.484672  | -0.192705|
|5  |1  |0    |2.453582 | -0.522490 | -0.157260|
|6  |1  |0    |-0.616152| 0.953106  | 1.184535|
|7  |1  |0    |-0.942260| 1.440943  | -0.507207|
|8  |1  |0    |-1.008056| -1.299433 | 0.483663|
|9  |1  |0    |-1.493940| -0.782621 | -1.002991|

A, B, C / GHz 18.8215263 6.1632786 5.0156982

---------------------------- FREQUENCIES AND ROTATIONAL CONSTANTS -------------------------------

INDEX NO. DOF TYPE CM-1(UNSCALED) CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
|   |   |     |     |     |     |
|---|---|-----|-----|-----|-----|
|1  |vib| 63.73 | 0.00 | A | 8.2596|
|2  |vib| 312.36| 0.00 | A | 29.4337|
|3  |vib| 418.04| 0.00 | A | 28.9446|
|4  |vib| 564.06| 0.00 | A | 77.9112|
|5  |vib| 639.27| 0.00 | A | 31.0641|
|6  |vib| 735.85| 0.00 | A | 61.1085|
|7  |vib| 832.19| 0.00 | A | 330.3172|
|8  |vib| 941.15| 0.00 | A | 2.5783|
|9  |vib| 1193.29| 0.00 | A | 22.4249|
|10 |vib| 1225.54| 0.00 | A | 3.7146|
|11 |vib| 1304.29| 0.00 | A | 48.2502|
| Number | Type | X     | Y     | Z     |
|--------|------|-------|-------|-------|
| 1      | 6    | 1.334455 | -0.691701 | -0.045638 |
| 2      | 6    | -1.341916 | 0.516882  | 0.040039  |
| 3      | 8    | -0.980363 | 0.699870  | -0.109194 |
| 4      | 8    | 0.900220  | 0.494725  | 0.051320  |
| 5      | 1    | 2.423425  | -0.537639 | 0.109194  |
| 6      | 1    | -1.106670 | -1.022738 | 0.981658  |
| INDEX NO. | TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|------|----------------|------------------|-----------|-------------|
| 1         | vib  | 155.45         | 0.00             | A         | 7.3941      |
| 2         | vib  | 236.43         | 0.00             | A         | 4.7047      |
| 3         | vib  | 354.70         | 0.00             | A         | 7.7697      |
| 4         | vib  | 523.49         | 0.00             | A         | 51.5762     |
| 5         | vib  | 623.25         | 0.00             | A         | 22.9240     |
| 6         | vib  | 814.39         | 0.00             | A         | 47.0799     |
| 7         | vib  | 937.64         | 0.00             | A         | 28.6607     |
| 8         | vib  | 1006.45        | 0.00             | A         | 5.7883      |
| 9         | vib  | 1144.56        | 0.00             | A         | 0.2005      |
| 10        | vib  | 1197.83        | 0.00             | A         | 18.0685     |
| 11        | vib  | 1334.51        | 0.00             | A         | 11.8023     |
| 12        | vib  | 1361.15        | 0.00             | A         | 11.8483     |
| 13        | vib  | 1422.75        | 0.00             | A         | 4.8308      |
| 14        | vib  | 1452.46        | 0.00             | A         | 7.9972      |
| 15        | vib  | 1472.52        | 0.00             | A         | 4.5512      |
| 16        | vib  | 1516.22        | 0.00             | A         | 11.2763     |
| 17        | vib  | 2870.40        | 0.00             | A         | 122.0037    |
| 18        | vib  | 3005.49        | 0.00             | A         | 25.3710     |
| 19        | vib  | 3081.81        | 0.00             | A         | 13.4670     |
| 20        | vib  | 3136.09        | 0.00             | A         | 6.0947      |
| 21        | vib  | 3492.74        | 0.00             | A         | 3.4460      |
| 22        | rot  | 0.6269669      | -                |           |             |
| 23        | rot  | 0.2173917      | -                |           |             |
| 24        | rot  | 0.1692771      | -                |           |             |

| Eelectronic [kJ/mol] | = -549027.014 |
| Ezpe [kJ/mol] | = +186.261 |
| Eelectronic+Ezpe [kJ/mol] | = -548840.753 |

| Eelectronic [hartrees] | = -209.113317 |
| Ezpe [hartrees] | = +0.070943 |
| Eelectronic+Ezpe [hartrees] | = -209.042374 |

| Thermal Correction to Energy [kJ/mol] | = +199.176 |
| Thermal Correction to Enthalpy [kJ/mol] | = +201.657 |
| Thermal Correction to Gibbs [kJ/mol] | = +115.454 |
**Figure 17d**

Charge = 0  Multiplicity = 1  Stoichiometry  C2H5NO

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**OPTIMIZED GEOMETRY**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|--------------|-------------|-------------------------|
| 1             | 6            | 0           | -0.586277 0.953212 -0.003374 |
| 2             | 6            | 0           | 0.710824 0.646464 0.003263 |
| 3             | 7            | 0           | -1.358006 -0.410567 -0.011651 |
| 4             | 8            | 0           | 1.228754 -0.670117 0.051434 |
| 5             | 1            | 0           | 1.466642 1.422198 0.011308 |
| 6             | 1            | 0           | -2.081338 -0.360041 -0.720813 |
| 7             | 1            | 0           | -1.820859 -0.528020 0.885400 |
| 8             | 1            | 0           | -0.748692 -1.220475 -0.181915 |
| 9             | 1            | 0           | 2.112976 -0.676811 -0.323232 |

A, B, C / GHz  16.2515812  6.5794330  4.8161930

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**FREQUENCIES AND ROTATIONAL CONSTANTS**

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|----------|--------------|
| 1         | vib      | 158.54         | 0.00             | A        | 5.6651       |
| 2         | vib      | 220.74         | 0.00             | A        | 119.0212     |
| 3         | vib      | 305.97         | 0.00             | A        | 48.1793      |
| 4         | vib      | 454.07         | 0.00             | A        | 23.9043      |
| 5         | vib      | 623.21         | 0.00             | A        | 13.1708      |
| 6         | vib      | 689.80         | 0.00             | A        | 6.7764       |
| 7         | vib      | 802.02         | 0.00             | A        | 19.1323      |
| 8         | vib      | 960.46         | 0.00             | A        | 4.8321       |
| 9         | vib      | 974.14         | 0.00             | A        | 10.1114      |
| 10        | vib      | 1001.95        | 0.00             | A        | 136.8915     |
| 11        | vib      | 1211.66        | 0.00             | A        | 75.0958      |
| 12        | vib      | 1303.31        | 0.00             | A        | 16.4750      |
| 13        | vib      | 1348.83        | 0.00             | A        | 72.5557      |
| 14        | vib      | 1635.68        | 0.00             | A        | 27.3293      |
| 15        | vib      | 1646.77        | 0.00             | A        | 30.3204      |
| 16        | vib      | 1660.00        | 0.00             | A        | 47.6515      |
| 17        | vib      | 3161.60        | 0.00             | A        | 20.9302      |
| 18        | vib      | 3306.85        | 0.00             | A        | 42.2000      |
| 19        | vib      | 3497.74        | 0.00             | A        | 48.0917      |


#2 acetamide

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

Optimized Geometry

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z
8 -0.363513000 1.328263000 0.001128000
6 -0.076498000 0.147236000 -0.007334000
6 1.361187000 -0.337360000 -0.000701000
1 1.469685000 -1.382458000 -0.288918000
1 1.940982000 0.287773000 -0.675802000
1 1.768768000 -0.207675000 1.002709000
7 -1.027074000 -0.831302000 -0.006501000
1 -1.993598000 -0.557102000 0.034355000
1 -0.796341000 -1.806778000 0.012353000

Rotational constants (GHz): 10.8737276 9.2791366 5.1663717

25.6342 4.6659
155.8186 181.4092
- Thermochemistry -  

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.073013 (Hartree/Particle)  
Thermal correction to Energy= 0.078367  
Thermal correction to Enthalpy= 0.079311  
Thermal correction to Gibbs Free Energy= 0.044303  
Sum of electronic and zero-point Energies= -209.229887  
Sum of electronic and thermal Energies= -209.224533  
Sum of electronic and thermal Enthalpies= -209.223589  
Sum of electronic and thermal Free Energies= -209.258597  

#21 Figure 17e

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

---------------------------------------------------------------------  
---------------------- OPTIMIZED GEOMETRY ---------------------------  
---------------------------------------------------------------------

| Center | Atomic Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------|---------------|---------------|-------------|-------------------------|
| 1      | 6             | 0             | -0.930091   | -0.753240               | 0.031379                 |
| 2      | 6             | 0             | -0.719104   | 0.738921                | -0.145670               |
| 3      | 7             | 0             | 0.763984    | 0.524753                | 0.169157                |
| 4      | 8             | 0             | 0.628006    | -0.846913               | -0.216839               |
| 5      | 1             | 0             | -0.990186   | -0.943123               | 1.118380                |
| 6      | 1             | 0             | -1.218029   | 1.462725                | 0.499449                |
| INDEX NO. | TYPE  | CM-1 UNSCALED | CM-1 SCALED BY | SYMMETRY | IR-INTENSITY |
|----------|-------|----------------|----------------|----------|--------------|
| 1        | vib   | 306.29         | 0.00           | A        | 6.5470       |
| 2        | vib   | 422.82         | 0.00           | A        | 22.1436      |
| 3        | vib   | 642.14         | 0.00           | A        | 2.5380       |
| 4        | vib   | 743.43         | 0.00           | A        | 20.2463      |
| 5        | vib   | 854.09         | 0.00           | A        | 3.6770       |
| 6        | vib   | 913.68         | 0.00           | A        | 3.2914       |
| 7        | vib   | 922.45         | 0.00           | A        | 75.0711      |
| 8        | vib   | 968.36         | 0.00           | A        | 26.7227      |
| 9        | vib   | 1157.74        | 0.00           | A        | 35.6997      |
| 10       | vib   | 1178.68        | 0.00           | A        | 3.8621       |
| 11       | vib   | 1221.45        | 0.00           | A        | 9.7483       |
| 12       | vib   | 1280.48        | 0.00           | A        | 1.1273       |
| 13       | vib   | 1307.82        | 0.00           | A        | 21.7885      |
| 14       | vib   | 1316.13        | 0.00           | A        | 20.5849      |
| 15       | vib   | 1490.98        | 0.00           | A        | 3.7745       |
| 16       | vib   | 1576.10        | 0.00           | A        | 20.2543      |
| 17       | vib   | 2888.95        | 0.00           | A        | 143.7573     |
| 18       | vib   | 3006.30        | 0.00           | A        | 73.1048      |
| 19       | vib   | 3082.21        | 0.00           | A        | 35.7808      |
| 20       | vib   | 3197.13        | 0.00           | A        | 222.5227     |
| 21       | vib   | 3311.15        | 0.00           | A        | 3.9138       |
| 22       | rot   | 0.4222528      | -              |          |              |
| 23       | rot   | 0.3908269      | -              |          |              |
| 24       | rot   | 0.2359327      | -              |          |              |

### ZPE and THERMAL CONTRIBUTIONS

|                  | [kJ/mol]   | [hartrees]  |
|------------------|------------|-------------|
| Electronic       | -548872.561| -209.054489 |
| ZPE              | +190.136   | +0.072419   |
| Electronic+ZPE   | -548682.425| -208.982070 |

|                  | [kJ/mol]   | [hartrees]  |
|------------------|------------|-------------|
| Electronic       | -209.054489| -208.982070 |
| ZPE              | +190.136   | +0.072419   |
| Electronic+ZPE   | -208.982070| -208.982070 |

|                  | [kJ/mol]   |
|------------------|------------|
| Thermal Correction to Energy | +200.822   |
| Thermal Correction to Enthalpy | +203.300   |
| Thermal Correction to Gibbs    | +122.136    |
#23 amino-acetaldehyde

Charge = 0  Multiplicity = 1  Stoichiometry  C2H5NO

| Center | Atomic Number | Atomic Number | Type | X        | Y        | Z        |
|--------|---------------|---------------|------|----------|----------|----------|
| 1      | 6             | 0             | -0.758674 | -0.313659 | 0.195571 |
| 2      | 6             | 0             | 0.495113  | 0.531152  | 0.085855 |
| 3      | 7             | 0             | 1.676233  | -0.312513 | -0.057763|
| 4      | 8             | 0             | -1.846030 | 0.034373  | -0.183081|
| 5      | 1             | 0             | 0.572015  | 1.071164  | 1.035845 |
| 6      | 1             | 0             | 0.338117  | 1.281816  | -0.696649|
| 7      | 1             | 0             | 2.519101  | 0.192351  | 0.178712 |
| 8      | 1             | 0             | 1.779434  | -0.636665 | -1.010904|
| 9      | 1             | 0             | -0.592687 | -1.301024 | 0.673426 |

A, B, C / GHz  33.4719497  4.2840339  4.0540002

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|-------------------|----------|--------------|
| 1         | vib      | 88.37          | 0.00              | A        | 9.0922       |
| 2         | vib      | 245.80         | 0.00              | A        | 41.5304      |
| 3         | vib      | 346.61         | 0.00              | A        | 11.7967      |
| 4         | vib      | 531.97         | 0.00              | A        | 4.7939       |
| 5         | vib      | 729.74         | 0.00              | A        | 9.5399       |
| 6         | vib      | 816.50         | 0.00              | A        | 147.7441     |
| 7         | vib      | 991.65         | 0.00              | A        | 8.3809       |
| 8         | vib      | 1061.72        | 0.00              | A        | 24.1080      |
| 9         | vib      | 1095.80        | 0.00              | A        | 3.3616       |
| 10        | vib      | 1190.55        | 0.00              | A        | 0.4725       |
| 11        | vib      | 1305.25        | 0.00              | A        | 13.1691      |
| 12        | vib      | 1371.53        | 0.00              | A        | 0.1742       |
| 13        | vib      | 1405.70        | 0.00              | A        | 8.0414       |
| 14        | vib      | 1468.71        | 0.00              | A        | 8.5116       |
| 15        | vib      | 1668.83        | 0.00              | A        | 21.5177      |
| 16        | vib      | 1813.03        | 0.00              | A        | 168.1661     |
| 17        | vib      | 2886.46        | 0.00              | A        | 95.4388      |
| 18        | vib      | 2993.07        | 0.00              | A        | 37.8506      |
| 19        | vib      | 3033.56        | 0.00              | A        | 16.8028      |
#24 aziridine-N-oxide

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO
| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|----------|-------------|
| 1         | vib      | 409.31         | 0.00             | A        | 5.5345      |
| 2         | vib      | 426.21         | 0.00             | A        | 14.8352     |
| 3         | vib      | 678.94         | 0.00             | A        | 23.3610     |
| 4         | vib      | 754.95         | 0.00             | A        | 2.6058      |
| 5         | vib      | 818.50         | 0.00             | A        | 1.3924      |
| 6         | vib      | 919.28         | 0.00             | A        | 1.0002      |
| 7         | vib      | 1020.33        | 0.00             | A        | 55.0317     |
| 8         | vib      | 1099.90        | 0.00             | A        | 4.6449      |
| 9         | vib      | 1101.77        | 0.00             | A        | 65.3671     |
| 10        | vib      | 1128.46        | 0.00             | A        | 3.3484      |
| 11        | vib      | 1154.38        | 0.00             | A        | 45.1894     |
| 12        | vib      | 1207.59        | 0.00             | A        | 2.2562      |
| 13        | vib      | 1227.21        | 0.00             | A        | 10.6212     |
| 14        | vib      | 1431.24        | 0.00             | A        | 7.2294      |
| 15        | vib      | 1454.95        | 0.00             | A        | 5.0311      |
| 16        | vib      | 1482.55        | 0.00             | A        | 2.8219      |
| 17        | vib      | 3131.97        | 0.00             | A        | 8.3453      |
| 18        | vib      | 3136.49        | 0.00             | A        | 6.4125      |
| 19        | vib      | 3242.62        | 0.00             | A        | 1.3381      |
| 20        | vib      | 3254.28        | 0.00             | A        | 0.0312      |
| 21        | vib      | 3309.80        | 0.00             | A        | 22.5508     |
| 22        | rot      | 0.5964125      | -                | -        | -           |
| 23        | rot      | 0.2490444      | -                | -        | -           |
| 24        | rot      | 0.2131933      | -                | -        | -           |

#28 Figure 17f

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO
### OPTIMIZED GEOMETRY

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | -0.490737  | 0.693024   | -0.000000   |
| 2             | 6             | 0           | -1.469375  | -0.421058  | 0.000000    |
| 3             | 7             | 0           | 0.785993   | 0.442198   | 0.000000    |
| 4             | 8             | 0           | 1.343774   | -0.694280  | -0.000000   |
| 5             | 1             | 0           | -0.766469  | 1.736617   | -0.000000   |
| 6             | 1             | 0           | -1.322720  | -1.062180  | -0.873196   |
| 7             | 1             | 0           | -2.489016  | -0.043099  | 0.000006    |
| 8             | 1             | 0           | -1.322712  | -1.062186  | 0.873190    |
| 9             | 1             | 0           | 1.409446   | 1.257904   | 0.000000    |

### FREQUENCIES AND ROTATIONAL CONSTANTS

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|----------|--------------|
| 1         | vib      | 82.07          | 0.00             | A        | 1.4272       |
| 2         | vib      | 265.06         | 0.00             | A        | 12.8322      |
| 3         | vib      | 455.92         | 0.00             | A        | 32.4121      |
| 4         | vib      | 714.49         | 0.00             | A        | 30.2512      |
| 5         | vib      | 739.04         | 0.00             | A        | 10.9527      |
| 6         | vib      | 928.06         | 0.00             | A        | 21.4763      |
| 7         | vib      | 963.50         | 0.00             | A        | 3.7587       |
| 8         | vib      | 1045.22        | 0.00             | A        | 0.6838       |
| 9         | vib      | 1121.41        | 0.00             | A        | 5.2622       |
| 10        | vib      | 1156.95        | 0.00             | A        | 65.6837      |
| 11        | vib      | 1389.19        | 0.00             | A        | 87.1052      |
| 12        | vib      | 1425.84        | 0.00             | A        | 44.5414      |
| 13        | vib      | 1465.61        | 0.00             | A        | 11.0437      |
| 14        | vib      | 1479.65        | 0.00             | A        | 1.8831       |
| 15        | vib      | 1540.88        | 0.00             | A        | 4.5401       |
| 16        | vib      | 1656.76        | 0.00             | A        | 90.8264      |
| 17        | vib      | 3020.23        | 0.00             | A        | 11.2330      |
| 18        | vib      | 3057.13        | 0.00             | A        | 10.5878      |
| 19        | vib      | 3124.45        | 0.00             | A        | 13.0179      |
| 20        | vib      | 3206.95        | 0.00             | A        | 5.3028       |
| 21        | vib      | 3317.36        | 0.00             | A        | 13.1439      |
| 22        | rot      | 0.6343483      | -                |          |              |
| 23        | rot      | 0.2104639      | -                |          |              |
| 24        | rot      | 0.1627208      | -                |          |              |

| A, B, C / GHz | 19.0172843 | 6.3095501 | 4.8782482 |

---
# ZPE and THERMAL CONTRIBUTIONS

Electronic [kJ/mol] = -549271.461  
E_xpe [kJ/mol] = +192.334  
Electronic+E_zpe [kJ/mol] = -549079.127

Electronic [hartrees] = -209.206422  
E_xpe [hartrees] = +0.073256  
Electronic+E_zpe [hartrees] = -209.133166

Thermal Correction to Energy [kJ/mol] = +204.750  
Thermal Correction to Enthalpy [kJ/mol] = +207.228  
Thermal Correction to Gibbs [kJ/mol] = +120.823

---

#3 Figure 17u

Charge = 0  Multiplicity = 1  Stoichiometry  C2H5NO

---

## OPTIMIZED GEOMETRY

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
| 1             | 6             | 0           | 1.148005 0.729945 0.027460 |
| 2             | 6             | 0           | -1.415479 0.062127 -0.179207 |
| 3             | 7             | 0           | -0.103201 0.011607 0.459789 |
| 4             | 8             | 0           | 0.852039 -0.756290 -0.228487 |
| 5             | 1             | 0           | 0.816504 1.200049 -0.918177 |
| 6             | 1             | 0           | -1.259094 0.263869 -1.234200 |
| 7             | 1             | 0           | -1.933267 -0.888389 -0.048817 |
| 8             | 1             | 0           | -1.993594 0.867229 0.274460 |
| 9             | 1             | 0           | -0.119610 -0.226120 1.446589 |

A, B, C / GHz  18.4161009  7.2307510  6.2978684

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## FREQUENCIES AND ROTATIONAL CONSTANTS

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|-----------|-------------|
| 1         | vib      | 214.06         | 0.00             | A         | 0.4782      |
| 2         | vib      | 352.04         | 0.00             | A         | 2.5650      |
| 3         | vib      | 438.61         | 0.00             | A         | 11.5038     |
| 4         | vib      | 542.32         | 0.00             | A         | 24.8650     |
| 5         | vib      | 818.38         | 0.00             | A         | 17.0138     |
| 6         | vib      | 914.95         | 0.00             | A         | 8.2722      |
7 vib 1022.32 0.00 A 25.9313
8 vib 1108.19 0.00 A 15.2134
9 vib 1158.63 0.00 A 12.2823
10 vib 1189.54 0.00 A 24.9718
11 vib 1220.51 0.00 A 2.0051
12 vib 1343.96 0.00 A 8.8798
13 vib 1443.78 0.00 A 4.5665
14 vib 1488.81 0.00 A 6.2342
15 vib 1480.86 0.00 A 7.8903
16 vib 1493.77 0.00 A 11.4611
17 vib 2878.46 0.00 A 123.6950
18 vib 3039.95 0.00 A 24.7136
19 vib 3108.38 0.00 A 11.8710
20 vib 3157.71 0.00 A 2.7970
21 vib 3493.27 0.00 A 25.3059
22 rot 0.6142950 -
23 rot 0.2411919 -
24 rot 0.2100743 -

------------------------ ZPE and THERMAL CONTRIBUTIONS ------------------------

Eelectronic [kJ/mol] = -548964.246
Ezpe [kJ/mol] = +190.617
Eelectronic+Ezpe [kJ/mol] = -548773.629

Eelectronic [hartrees] = -209.089410
Ezpe [hartrees] = +0.072602
Eelectronic+Ezpe [hartrees] = -209.016808

Thermal Correction to Energy [kJ/mol] = +202.342
Thermal Correction to Enthalpy [kJ/mol] = +204.821
Thermal Correction to Gibbs [kJ/mol] = +121.432

#30 N-methylene-N-oxide-methanamine
Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

---------------------- OPTIMIZED GEOMETRY ----------------------

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

1 6 0 1.084109 -0.819874 0.000000
| INDEX NO. | DOF TYPE | CM-1 (UNSCALED) | CM-1 (SCALED BY) | SYMMETRY | IR-INTENSITY |
|-----------|----------|-----------------|------------------|----------|--------------|
| 1         | vib      | 166.72          | 0.00             | A        | 1.3754       |
| 2         | vib      | 472.80          | 0.00             | A        | 4.1795       |
| 3         | vib      | 530.02          | 0.00             | A        | 0.6341       |
| 4         | vib      | 558.88          | 0.00             | A        | 16.6874      |
| 5         | vib      | 689.90          | 0.00             | A        | 14.5976      |
| 6         | vib      | 805.04          | 0.00             | A        | 51.9664      |
| 7         | vib      | 861.91          | 0.00             | A        | 0.1330       |
| 8         | vib      | 1083.25         | 0.00             | A        | 6.3376       |
| 9         | vib      | 1124.42         | 0.00             | A        | 58.9842      |
| 10        | vib      | 1146.96         | 0.00             | A        | 0.0038       |
| 11        | vib      | 1354.48         | 0.00             | A        | 44.8107      |
| 12        | vib      | 1426.38         | 0.00             | A        | 1.5281       |
| 13        | vib      | 1458.16         | 0.00             | A        | 48.3732      |
| 14        | vib      | 1469.99         | 0.00             | A        | 10.2608      |
| 15        | vib      | 1497.52         | 0.00             | A        | 5.3039       |
| 16        | vib      | 1639.55         | 0.00             | A        | 144.5555     |
| 17        | vib      | 3065.16         | 0.00             | A        | 11.0412      |
| 18        | vib      | 3149.03         | 0.00             | A        | 3.5341       |
| 19        | vib      | 3157.27         | 0.00             | A        | 9.1216       |
| 20        | vib      | 3184.54         | 0.00             | A        | 1.0894       |
| 21        | vib      | 3309.35         | 0.00             | A        | 0.3986       |
| 22        | rot      | 0.3771036       |                  |          |              |
| 23        | rot      | 0.3355891       |                  |          |              |
| 24        | rot      | 0.1836836       |                  |          |              |

**ZPE and THERMAL CONTRIBUTIONS**

- **Electronic [kJ/mol]** = -549248.075
- **Ezpe [kJ/mol]** = +192.307
- **Electronic+Ezpe [kJ/mol]** = -549055.768

- **Electronic [hartrees]** = -209.197515
- **Ezpe [hartrees]** = +0.073246
Electronic Energy [hartrees] = -209.124269

Thermal Correction to Energy [kJ/mol] = +203.965
Thermal Correction to Enthalpy [kJ/mol] = +206.443
Thermal Correction to Gibbs [kJ/mol] = +122.666

#31 Figure 17g
Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

---------------------- OPTIMIZED GEOMETRY ---------------------------

| Center | Atomic Number | Atomic Type | X     | Y     | Z     |
|--------|---------------|--------------|-------|-------|-------|
| 1      | 6             | 0            | -0.742638 | -0.263711 | 0.000000 |
| 2      | 6             | 0            | 0.380421   | 0.553262   | 0.000000 |
| 3      | 7             | 0            | 1.673886   | -0.153405  | -0.000000|
| 4      | 8             | 0            | -1.935350  | 0.024290   | -0.000000|
| 5      | 1             | 0            | 0.432556   | 1.626873   | -0.000000|
| 6      | 1             | 0            | 2.258615   | 0.017374   | -0.823364|
| 7      | 1             | 0            | 1.432337   | -1.153362  | 0.000000 |
| 8      | 1             | 0            | 2.258615   | 0.017374   | 0.823363 |
| 9      | 1             | 0            | -0.443230  | -1.366049  | 0.000000 |

A, B, C / GHz 41.8042728 4.1760206 3.8763336

-------------------------- FREQUENCIES AND ROTATIONAL CONSTANTS --------------------------

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY) | SYMMETRY | IR-INTENSITY |
|------------|----------|----------------|-----------------|----------|--------------|
| 1          | vib      | 123.28         | 46.9134         | A        |              |
| 2          | vib      | 329.16         | 5.3501          | A        |              |
| 3          | vib      | 339.45         | 26.6554         | A        |              |
| 4          | vib      | 484.58         | 68.1236         | A        |              |
| 5          | vib      | 584.31         | 27.5182         | A        |              |
| 6          | vib      | 939.15         | 43.2559         | A        |              |
| 7          | vib      | 974.81         | 0.0253          | A        |              |
| 8          | vib      | 1029.52        | 31.8717         | A        |              |
| 9          | vib      | 1070.31        | 10.7232         | A        |              |
| 10         | vib      | 1202.58        | 51.6364         | A        |              |
| 11         | vib      | 1359.14        | 28.9410         | A        |              |
| 12         | vib      | 1446.70        | 41.0979         | A        |              |
| 13         | vib      | 1463.41        | 22.5385         | A        |              |
| 14         | vib      | 1619.75        | 20.8719         | A        |              |
15  vib  1676.80  0.00  A  61.1915
16  vib  1733.88  0.00  A  509.8741
17  vib  2523.68  0.00  A  338.6961
18  vib  3253.47  0.00  A   1.1473
19  vib  3300.17  0.00  A   73.7720
20  vib  3319.53  0.00  A  14.0941
21  vib  3354.36  0.00  A  22.0630
22  rot  1.3944404 -
23  rot  0.1392971 -
24  rot  0.1293006 -

------------------------------- ZPE and THERMAL CONTRIBUTIONS -----------------------------

\[
\text{Eelectronic [kJ/mol]} = -549248.393 \\
\text{Ezpe [kJ/mol]} = +192.168 \\
\text{Eelectronic+Ezpe [kJ/mol]} = -549056.225
\]

\[
\text{Eelectronic [hartrees]} = -209.197636 \\
\text{Ezpe [hartrees]} = +0.073193 \\
\text{Eelectronic+Ezpe [hartrees]} = -209.124443
\]

\[
\text{Thermal Correction to Energy [kJ/mol]} = +204.978 \\
\text{Thermal Correction to Enthalpy [kJ/mol]} = +207.457 \\
\text{Thermal Correction to Gibbs [kJ/mol]} = +121.366
\]

#32 Figure 17h

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

------------------------------- OPTIMIZED GEOMETRY -----------------------------

| Center | Atomic Number | Atomic Number | Type | Coordinates (Angstroms) |
|--------|---------------|---------------|------|------------------------|
| 1      | 6             | 0             |      | 0.795012 0.261114 0.432436 |
| 2      | 6             | 0             |      | 1.680713 -0.367903 -0.327977 |
| 3      | 7             | 0             |      | -0.491723 0.473990 -0.284474 |
| 4      | 8             | 0             |      | -1.570171 -0.401902 0.113045 |
| 5      | 1             | 0             |      | 2.632317 -0.548717 0.179496 |
| 6      | 1             | 0             |      | -0.224883 0.260146 -1.258242 |
| 7      | 1             | 0             |      | 0.737564 0.654160 1.445656 |
| 8      | 1             | 0             |      | -0.906742 1.402017 -0.189731 |
| 9      | 1             | 0             |      | -1.089175 -1.229595 0.283028 |

43
| INDEX NO. | DOF  | CM-1 (UNSCALED) | CM-1 (SCALED BY) | SYMMETRY | IR-INTENSITY |
|-----------|------|----------------|-----------------|----------|--------------|
| 1         | vib  | 124.39         | 0.00            | A        | 20.2659      |
| 2         | vib  | 361.30         | 0.00            | A        | 58.4192      |
| 3         | vib  | 411.92         | 0.00            | A        | 50.7386      |
| 4         | vib  | 459.69         | 0.00            | A        | 60.5557      |
| 5         | vib  | 690.40         | 0.00            | A        | 55.3764      |
| 6         | vib  | 747.21         | 0.00            | A        | 13.9752      |
| 7         | vib  | 879.50         | 0.00            | A        | 144.2405     |
| 8         | vib  | 921.23         | 0.00            | A        | 26.9276      |
| 9         | vib  | 976.93         | 0.00            | A        | 10.2216      |
| 10        | vib  | 1099.34        | 0.00            | A        | 42.2318      |
| 11        | vib  | 1247.64        | 0.00            | A        | 19.5633      |
| 12        | vib  | 1276.67        | 0.00            | A        | 29.3268      |
| 13        | vib  | 1320.41        | 0.00            | A        | 40.1902      |
| 14        | vib  | 1475.20        | 0.00            | A        | 47.0581      |
| 15        | vib  | 1542.75        | 0.00            | A        | 20.0480      |
| 16        | vib  | 1576.79        | 0.00            | A        | 48.1657      |
| 17        | vib  | 1635.46        | 0.00            | A        | 45.0803      |
| 18        | vib  | 3094.43        | 0.00            | A        | 55.6135      |
| 19        | vib  | 3252.80        | 0.00            | A        | 35.0562      |
| 20        | vib  | 3439.95        | 0.00            | A        | 10.7490      |
| 21        | vib  | 3677.96        | 0.00            | A        | 42.5882      |
| 22        | rot  | 0.7969969      | -               |          |              |
| 23        | rot  | 0.1642802      | -               |          |              |
| 24        | rot  | 0.1584387      | -               |          |              |

| ZPE and THERMAL CONTRIBUTIONS |

Eelectronic [kJ/mol] = -548974.708
Expe [kJ/mol] = +189.188
Eelectronic+Expe [kJ/mol] = -548785.520

Eelectronic [hartrees] = -209.093395
Expe [hartrees] = +0.072058
Eelectronic+Expe [hartrees] = -209.021337

Thermal Correction to Energy [kJ/mol] = +201.946
Thermal Correction to Enthalpy [kJ/mol] = +204.424
Thermal Correction to Gibbs [kJ/mol] = +118.365
#38 CH$_3$–C–NH–OH

Charge = 0  Multiplicity = 1  Stoichiometry  C$_2$H$_5$NO

---------------------------------------------------------------------
---------------------- OPTIMIZED GEOMETRY ----------------------------
---------------------------------------------------------------------
Center       Atomic  Atomic  Coordinates (Angstroms)
Number  Number   Type    X         Y         Z
---------------------------------------------------------------------
  1   6        0   -0.655138  0.779004  0.016341
  2   6        0   -1.516829 -0.434368 -0.017239
  3   7        0    0.596054  0.658967  0.015318
  4   8        0   1.437800 -0.616945 -0.109763
  5   1        0  -2.355396 -0.263154 -0.691925
  6   1        0  -1.959619 -0.550553  0.976352
  7   1        0  -1.000266 -1.357232 -0.289760
  8   1        0   1.265452  1.411856 -0.000379
  9   1        0   1.406856 -0.985951  0.781974

A, B, C / GHz   17.4296096  5.7895608  4.5251913

---------------------------------------------------------------------
----------------------- FREQUENCIES AND ROTATIONAL CONSTANTS -----------------------
---------------------------------------------------------------------
INDEX NO. DOF TYPE CM-1(UNSCALED) CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
  1  vib   71.18     0.00   A     7.2801
  2  vib  170.78     0.00   A    98.2329
  3  vib  248.22     0.00   A   38.0843
  4  vib  433.14     0.00   A   12.7307
  5  vib  496.71     0.00   A  186.7947
  6  vib  684.24     0.00   A   74.0894
  7  vib  693.25     0.00   A   92.9353
  8  vib  934.94     0.00   A  37.3441
  9  vib 1026.25     0.00   A   5.4962
 10  vib 1087.38     0.00   A   6.4332
 11  vib 1209.77     0.00   A   28.6818
 12  vib 1341.32     0.00   A  10.5432
 13  vib 1381.84     0.00   A   9.9192
 14  vib 1457.91     0.00   A   8.1179
 15  vib 1487.12     0.00   A   9.0238
 16  vib 1602.58     0.00   A  55.5368
 17  vib 3012.76     0.00   A  14.9435
 18  vib 3070.69     0.00   A  13.6897
 19  vib 3095.99     0.00   A   6.8775
 20  vib 3603.14     0.00   A  51.1137
 21  vib 3776.49     0.00   A  36.6740
 22  rot   0.5813892  -     -      -
 23  rot   0.1931190  -     -      -
### ZPE and THERMAL CONTRIBUTIONS

- **Electronic [kJ/mol]** = -549141.992
- **Ezpe [kJ/mol]** = +184.738
- **Eelectronic+Ezpe [kJ/mol]** = -548957.254

- **Electronic [hartrees]** = -209.157110
- **Ezpe [hartrees]** = +0.070363
- **Eelectronic+Ezpe [hartrees]** = -209.086747

- **Thermal Correction to Energy [kJ/mol]** = +199.480
- **Thermal Correction to Enthalpy [kJ/mol]** = +201.959
- **Thermal Correction to Gibbs [kJ/mol]** = +110.833

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### #39 CH$_3$–NH–C$\ddot{\text{c}}$–OH

Charge = 0 Multiplicity = 1 Stoichiometry C$2$H$5$NO

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### OPTIMIZED GEOMETRY

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
| 1             | 6             | 0           | -0.866438 0.698687 -0.000046 |
| 2             | 6             | 0           | 1.377928 -0.472603 0.000009 |
| 3             | 7             | 0           | 0.467359 0.679467 0.000017 |
| 4             | 8             | 0           | -1.417995 -0.518712 -0.000001 |
| 5             | 1             | 0           | 2.400600 -0.106141 -0.002581 |
| 6             | 1             | 0           | 1.242919 -1.094167 -0.887925 |
| 7             | 1             | 0           | 1.246317 -1.091769 0.890128 |
| 8             | 1             | 0           | 0.895767 1.588403 0.000262 |
| 9             | 1             | 0           | -0.782094 -1.259395 0.000225 |

A, B, C / GHz 18.4542809 6.4334075 4.9183080

---

### FREQUENCIES AND ROTATIONAL CONSTANTS

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|---------------|------------------|----------|--------------|
| 1         | vib      | 112.35        | 0.00             | A        | 0.3823       |
| 2         | vib      | 309.85        | 0.00             | A        | 3.7905       |
### ZPE and THERMAL CONTRIBUTIONS

| Term                      | Value        |
|---------------------------|--------------|
| Electronic [kJ/mol]       | -549292.827  |
| ZPE [kJ/mol]              | +192.016     |
| Electronic + ZPE [kJ/mol] | -549100.811  |
| Electronic [hartrees]     | -209.214560  |
| ZPE [hartrees]            | +0.073135    |
| Electronic + ZPE [hartrees]| -209.141425 |
| Thermal Correction to Energy [kJ/mol] | +204.855 |
| Thermal Correction to Enthalpy [kJ/mol] | +207.333 |
| Thermal Correction to Gibbs [kJ/mol] | +120.844 |

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**#4 2-oxiranamine**

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

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**OPTIMIZED GEOMETRY**

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47
| Center Atomic | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X          | Y          | Z          |
| 1             | 6             | 0           | 0.196306   | -0.068390 | 0.464592   |
| 2             | 6             | 0           | -1.007645  | 0.606315  | 0.001108   |
| 3             | 7             | 0           | 1.468649   | 0.204618  | -0.085542  |
| 4             | 8             | 0           | -0.798783  | -0.782123 | -0.307082  |
| 5             | 1             | 0           | -0.937300  | 1.284408  | -0.845288  |
| 6             | 1             | 0           | -1.821016  | 0.819488  | 0.687660   |
| 7             | 1             | 0           | 0.246979   | -0.394562 | 1.497618   |
| 8             | 1             | 0           | 1.407016   | 0.485909  | -1.055711  |
| 9             | 1             | 0           | 2.082072   | -0.598136 | -0.023033  |

A, B, C / GHz
19.1566184
6.9732212
6.1726644

INDEX NO. DOF TYPE CM-1(UNSCALED) CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
1 vib 301.29     0.00 A  37.7357
2 vib 425.60     0.00 A  32.6433
3 vib 455.32     0.00 A  39.9036
4 vib 745.25     0.00 A  16.1936
5 vib 814.40     0.00 A  235.6671
6 vib 839.89     0.00 A  10.3847
7 vib 960.22     0.00 A  19.6202
8 vib 1054.36    0.00 A  19.7710
9 vib 1107.92    0.00 A  16.7802
10 vib 1147.96   0.00 A  7.4523
11 vib 1174.99   0.00 A  2.6403
12 vib 1267.95   0.00 A  22.4978
13 vib 1311.43   0.00 A  8.0545
14 vib 1466.65   0.00 A  25.2097
15 vib 1540.73   0.00 A  21.6145
16 vib 1663.78   0.00 A  36.3417
17 vib 3070.61   0.00 A  31.0018
18 vib 3131.31   0.00 A  11.8951
19 vib 3151.74   0.00 A  38.9269
20 vib 3505.49   0.00 A  2.0277
21 vib 3587.31   0.00 A  4.6978
22 rot 0.6389960 -
23 rot 0.2326016 -
24 rot 0.2058979 -

Eelectronic [kJ/mol] = -549337.713
Ezpe [kJ/mol] = +195.734

48
Electronic+Ezpe \[kJ/mol\] = -549141.979

Electronic \[hartrees\] = -209.231656

Ezpe \[hartrees\] = +0.074551

Electronic+Ezpe \[hartrees\] = -209.157105

Thermal Correction to Energy \[kJ/mol\] = +206.774

Thermal Correction to Enthalpy \[kJ/mol\] = +209.255

Thermal Correction to Gibbs \[kJ/mol\] = +127.234

#40 H–\(\overset{\text{C}}{\text{C}}\)–N(OH)CH\(_3\)

Charge = 0 Multiplicity = 1 Stoichiometry \(\text{C}_2\text{H}_5\text{NO}\)

---------------------------------------------------------------------

Optimized Geometry

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z

1 6 0 -0.706263 1.299944 0.000016
2 6 0 1.368106 0.007594 0.000033
3 7 0 -0.075404 0.206794 -0.000081
4 8 0 -0.648385 -1.162386 -0.000044
5 1 0 -1.792395 1.134340 0.000003
6 1 0 1.835575 0.984646 -0.000033
7 1 0 1.650595 -0.558289 -0.885856
8 1 0 1.650502 -0.558103 0.886076
9 1 0 -1.600427 -0.996291 0.000435

---------------------------------------------------------------------

A, B, C / GHz 10.5478988 9.8038906 5.2481133

---------------------------------------------------------------------

Frequencies and Rotational Constants

---------------------------------------------------------------------

INDEX NO. DOF TYPE CM-1(UNSCALED) CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
1 vib 180.28 0.00 A 5.8498
2 vib 267.13 0.00 A 82.4781
3 vib 421.00 0.00 A 5.6288
4 vib 430.59 0.00 A 4.4120
5 vib 494.09 0.00 A 77.8968
6 vib 648.33 0.00 A 164.5176
7 vib 900.53 0.00 A 30.3370
8 vib 958.81 0.00 A 34.0119
9 vib 1108.95 0.00 A 46.3708
10 vib 1160.88 0.00 A 1.6265
|   |  |    |       |       |       |
|---|---|-----|-------|-------|-------|
| 11| vib| 1195.34 | 0.00 | A | 97.3185 |
| 12| vib| 1307.82 | 0.00 | A | 14.0740 |
| 13| vib| 1437.97 | 0.00 | A | 1.0178  |
| 14| vib| 1482.10 | 0.00 | A | 10.6454 |
| 15| vib| 1494.11 | 0.00 | A | 9.5295  |
| 16| vib| 1654.77 | 0.00 | A | 37.9277 |
| 17| vib| 3002.83 | 0.00 | A | 49.2715 |
| 18| vib| 3059.31 | 0.00 | A | 14.5948 |
| 19| vib| 3122.11 | 0.00 | A | 9.9665  |
| 20| vib| 3182.21 | 0.00 | A | 1.8523  |
| 21| vib| 3763.16 | 0.00 | A | 26.5837 |
| 22| rot| 0.3518400 | - |   |       |
| 23| rot| 0.3270226 | - |   |       |
| 24| rot| 0.1750582 | - |   |       |

______________________________

------------------------ ZPE and THERMAL CONTRIBUTIONS -------------------------

| Electronic [kJ/mol] | = -549119.555 |
| Ezpe [kJ/mol]       | = +187.051    |
| Electronic+Ezpe [kJ/mol] | = -548932.504 |
|                      |               |
| Electronic [hartrees] | = -209.148564 |
| Ezpe [hartrees]      | = +0.071244   |
| Electronic+Ezpe [hartrees] | = -209.077320 |

Thermal Correction to Energy [kJ/mol] = +200.202
Thermal Correction to Enthalpy [kJ/mol] = +202.681
Thermal Correction to Gibbs [kJ/mol] = +116.297

#41 H₂N–C−CH₂OH

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

---------------------------------------------------------------------

---------------------- OPTIMIZED GEOMETRY -----------------------------

| Center | Atomic Number | Atomic Number | Type | X     | Y     | Z     |
|--------|--------------|---------------|------|-------|-------|-------|
| 1      | 6            | 0             |      | 0.825266 | 0.746866 | 0.050258 |
| 2      | 6            | 0             |      | -0.665376 | 0.667915 | -0.017384 |
| 3      | 7            | 0             |      | 1.370636 | -0.434761 | -0.002896 |
| 4      | 8            | 0             |      | -1.261987 | -0.647562 | -0.097350 |
| 5      | 1            | 0             |      | -1.073762 | 1.231011 | 0.826293  |

50
| INDEX NO. | DOF  | TYPE | CM-1 (UNSCALED) | CM-1 (SCALED BY) | SYMMETRY | IR-INTENSITY |
|----------|------|------|----------------|-----------------|----------|-------------|
| 1        | vib  | 157.21 | 0.00          | A              | 82.7279   |
| 2        | vib  | 269.46 | 0.00          | A              | 48.5616   |
| 3        | vib  | 312.78 | 0.00          | A              | 13.0221   |
| 4        | vib  | 648.95 | 0.00          | A              | 1.5934    |
| 5        | vib  | 680.59 | 0.00          | A              | 6.5765    |
| 6        | vib  | 787.92 | 0.00          | A              | 134.3252  |
| 7        | vib  | 907.78 | 0.00          | A              | 1.9113    |
| 8        | vib  | 963.97 | 0.00          | A              | 126.9905  |
| 9        | vib  | 978.56 | 0.00          | A              | 28.0510   |
| 10       | vib  | 1183.65| 0.00          | A              | 27.6856   |
| 11       | vib  | 1230.43| 0.00          | A              | 2.9771    |
| 12       | vib  | 1334.89| 0.00          | A              | 17.7218   |
| 13       | vib  | 1353.78| 0.00          | A              | 1.4525    |
| 14       | vib  | 1428.50| 0.00          | A              | 23.4072   |
| 15       | vib  | 1483.40| 0.00          | A              | 0.6499    |
| 16       | vib  | 1641.50| 0.00          | A              | 47.8045   |
| 17       | vib  | 3022.05| 0.00          | A              | 19.0792   |
| 18       | vib  | 3054.45| 0.00          | A              | 11.2219   |
| 19       | vib  | 3357.44| 0.00          | A              | 13.6836   |
| 20       | vib  | 3592.60| 0.00          | A              | 35.5192   |
| 21       | vib  | 3841.84| 0.00          | A              | 36.6458   |
| 22       | rot  | 0.5767990|           |                |           |
| 23       | rot  | 0.2137805|           |                |           |
| 24       | rot  | 0.1628415|           |                |           |

**ZPE and THERMAL CONTRIBUTIONS**

Electronic [kJ/mol] = -549260.494

Expe [kJ/mol] = +192.788

Electronic+Expe [kJ/mol] = -549067.706

Electronic [hartrees] = -209.202245

Expe [hartrees] = +0.073429

Electronic+Expe [hartrees] = -209.128816

Thermal Correction to Energy [kJ/mol] = +205.564

Thermal Correction to Enthalpy [kJ/mol] = +208.045
Thermal Correction to Gibbs [kJ/mol] = +121.962

#43 H₂N—C—O—CH₃

Charge = 0 Multiplicity = 1 Stoichiometry C₂H₅NO

| Center Number | Atomic Number | Atomic Type | X (Å)       | Y (Å)       | Z (Å)  |
|---------------|---------------|-------------|-------------|-------------|--------|
| 1             | 6             | 0           | -0.555394   | 0.542666   | -0.000280 |
| 2             | 6             | 0           | 1.743333    | 0.077080   | 0.000228  |
| 3             | 7             | 0           | -1.732672   | -0.070649  | 0.000252  |
| 4             | 8             | 0           | 0.395233    | -0.398005  | -0.000413 |
| 5             | 1             | 0           | 2.246661    | -0.310599  | -0.885013 |
| 6             | 1             | 0           | 2.242379    | -0.298598  | 0.893094  |
| 7             | 1             | 0           | 1.748671    | 1.164885   | -0.006882 |
| 8             | 1             | 0           | -1.832185   | -1.082133  | 0.000569  |
| 9             | 1             | 0           | -2.566318   | 0.486544   | 0.000083  |

A, B, C / GHz 46.9864232 4.6143622 4.3160730

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|----------|--------------|
| 1         | vib      | 72.26          | 0.00             | A        | 0.5102       |
| 2         | vib      | 214.16         | 0.00             | A        | 23.7398      |
| 3         | vib      | 349.05         | 0.00             | A        | 21.5968      |
| 4         | vib      | 502.63         | 0.00             | A        | 157.8730     |
| 5         | vib      | 587.56         | 0.00             | A        | 9.5058       |
| 6         | vib      | 742.76         | 0.00             | A        | 5.8235       |
| 7         | vib      | 923.15         | 0.00             | A        | 5.5832       |
| 8         | vib      | 1145.50        | 0.00             | A        | 145.7734     |
| 9         | vib      | 1183.60        | 0.00             | A        | 1.0982       |
| 10        | vib      | 1185.64        | 0.00             | A        | 12.3193      |
| 11        | vib      | 1289.51        | 0.00             | A        | 153.0959     |
| 12        | vib      | 1357.40        | 0.00             | A        | 115.2288     |
| 13        | vib      | 1468.50        | 0.00             | A        | 11.8629      |
| 14        | vib      | 1495.13        | 0.00             | A        | 3.1792       |
| 15        | vib      | 1506.32        | 0.00             | A        | 9.0608       |
| 16        | vib      | 1629.90        | 0.00             | A        | 98.1243      |
| 17        | vib      | 3034.19        | 0.00             | A        | 62.3475      |
| 18        | vib      | 3102.07        | 0.00             | A        | 29.6250      |
|   | Type | Eelectronic | Ezpe | Eelectronic+Ezpe |
|---|------|-------------|------|------------------|
| 19 | vib  | 3126.68     | 0.00 | A 11.9052        |
| 20 | vib  | 3443.52     | 0.00 | A 3.0240         |
| 21 | vib  | 3697.23     | 0.00 | A 70.0940        |
| 22 | rot  | 1.5672984   | -    |                  |
| 23 | rot  | 0.1539186   | -    |                  |
| 24 | rot  | 0.1439687   | -    |                  |

---

**ZPE and THERMAL CONTRIBUTIONS**

|                  | [kJ/mol]      | [kJ/mol] | [kJ/mol]      |
|------------------|---------------|----------|---------------|
| Eelectronic      | -549305.12    | +191.743 | -549113.377   |
| Ezpe             | +205.272      | +207.751 | +119.786      |
| Eelectronic+Ezpe |               |          |               |

**#44 H−C−NH−OCH₃**

Charge = 0 Multiplicity = 1 Stoichiometry C₂H₅N₀

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**OPTIMIZED GEOMETRY**

| Center Number | Atomic Number | Atomic Type | X      | Y      | Z      |
|---------------|---------------|-------------|--------|--------|--------|
| 1             | 6             | 0           | -1.871976 | -0.021466 | 0.248691 |
| 2             | 6             | 0           | 1.581688 | 0.114965  | 0.240392 |
| 3             | 7             | 0           | -0.742452 | 0.350711  | -0.169745 |
| 4             | 8             | 0           | 0.453908 | -0.499641 | -0.364238 |
| 5             | 1             | 0           | -1.841027 | -1.081474 | 0.526741  |
| 6             | 1             | 0           | 1.754060 | 1.124109  | -0.153225 |
| 7             | 1             | 0           | 2.437890 | -0.505027 | -0.018808 |
| 8             | 1             | 0           | 1.480733 | 0.164499  | 1.328192  |
| 9             | 1             | 0           | -0.524031 | 1.279049  | -0.515279 |

**A, B, C / GHz**

A 30.6992326 B 4.8617169 C 4.6598569
| INDEX NO. | DOF TYPE | CM-1 (UNSCALED) | CM-1 (SCALED BY ) | SYMMETRY | IR-INTENSITY |
|---------|----------|----------------|------------------|--------|-------------|
| 1       | vib      | 65.40          | 0.00             | A      | 1.4333      |
| 2       | vib      | 199.25         | 0.00             | A      | 0.7056      |
| 3       | vib      | 347.88         | 0.00             | A      | 5.1656      |
| 4       | vib      | 470.73         | 0.00             | A      | 105.6103    |
| 5       | vib      | 665.23         | 0.00             | A      | 34.1485     |
| 6       | vib      | 703.59         | 0.00             | A      | 143.4272    |
| 7       | vib      | 1006.23        | 0.00             | A      | 117.5112    |
| 8       | vib      | 1057.21        | 0.00             | A      | 127.6162    |
| 9       | vib      | 1139.21        | 0.00             | A      | 65.1101     |
| 10      | vib      | 1171.39        | 0.00             | A      | 2.1533      |
| 11      | vib      | 1199.99        | 0.00             | A      | 6.3978      |
| 12      | vib      | 1394.68        | 0.00             | A      | 17.8753     |
| 13      | vib      | 1464.58        | 0.00             | A      | 1.9012      |
| 14      | vib      | 1482.10        | 0.00             | A      | 8.9146      |
| 15      | vib      | 1505.71        | 0.00             | A      | 14.0382     |
| 16      | vib      | 1570.15        | 0.00             | A      | 30.5765     |
| 17      | vib      | 2979.12        | 0.00             | A      | 60.3245     |
| 18      | vib      | 3040.29        | 0.00             | A      | 49.2273     |
| 19      | vib      | 3042.59        | 0.00             | A      | 15.7524     |
| 20      | vib      | 3113.18        | 0.00             | A      | 13.8110     |
| 21      | vib      | 3504.04        | 0.00             | A      | 12.2118     |
| 22      | rot      | 1.0240162      | -                |        |             |
| 23      | rot      | 0.1621694      | -                |        |             |
| 24      | rot      | 0.1554361      | -                |        |             |

| Eelectronic [kJ/mol] | = -549090.669 |
| Ezpe [kJ/mol]       | = +186.153    |
| Eelectronic+Ezpe [kJ/mol] | = -548904.516 |

| Eelectronic [hartrees] | = -209.137562 |
| Ezpe [hartrees]       | = +0.070902   |
| Eelectronic+Ezpe [hartrees] | = -209.066660 |

| Thermal Correction to Energy [kJ/mol] | = +199.795 |
| Thermal Correction to Enthalpy [kJ/mol] | = +202.274 |
| Thermal Correction to Gibbs [kJ/mol] | = +113.506 |
#46 H–C–NH–CH₂OH
Charge = 0 Multiplicity = 1 Stoichiometry C₂H₅NO

---------------------------- OPTIMIZED GEOMETRY -----------------------------

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
| 1             | 6             | 0           | 1.868897 -0.029467 -0.300427 |
| 2             | 6             | 0           | -0.520125 -0.377475 0.400608 |
| 3             | 7             | 0           | 0.730437 0.373015 0.195629 |
| 4             | 8             | 0           | -1.559691 0.064630 -0.435002 |
| 5             | 1             | 0           | 1.738713 -1.103284 -0.544736 |
| 6             | 1             | 0           | -0.800935 -0.310932 1.456193 |
| 7             | 1             | 0           | -0.302444 -1.411880 0.143388 |
| 8             | 1             | 0           | 0.666698 1.348824 0.471245 |
| 9             | 1             | 0           | -2.030192 0.790777 -0.016564 |

A, B, C / GHz 27.0798970 4.6483254 4.5972423

---------------------------- FREQUENCIES AND ROTATIONAL CONSTANTS -----------------------------

| INDEX NO. DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|---------------------|----------------|------------------|-----------|--------------|
| 1                   | vib            | 64.07            | A         | 10.8927      |
| 2                   | vib            | 243.71           | A         | 103.3526     |
| 3                   | vib            | 384.26           | A         | 5.1888       |
| 4                   | vib            | 498.26           | A         | 11.5426      |
| 5                   | vib            | 658.00           | A         | 4.4514       |
| 6                   | vib            | 938.01           | A         | 40.2045      |
| 7                   | vib            | 1035.73          | A         | 20.1762      |
| 8                   | vib            | 1066.67          | A         | 206.3126     |
| 9                   | vib            | 1093.31          | A         | 18.2770      |
| 10                  | vib            | 1206.16          | A         | 61.1230      |
| 11                  | vib            | 1310.95          | A         | 11.7404      |
| 12                  | vib            | 1388.35          | A         | 15.8916      |
| 13                  | vib            | 1411.36          | A         | 43.0043      |
| 14                  | vib            | 1466.52          | A         | 10.1161      |
| 15                  | vib            | 1495.64          | A         | 0.2911       |
| 16                  | vib            | 1540.29          | A         | 16.3644      |
| 17                  | vib            | 2887.84          | A         | 98.0604      |
| 18                  | vib            | 3009.83          | A         | 53.1223      |
| 19                  | vib            | 3111.95          | A         | 12.9211      |
| 20                  | vib            | 3465.41          | A         | 5.9727       |
| 21                  | vib            | 3828.86          | A         | 48.3890      |
| 22                  | rot            | 0.9032881        | -         |              |
| 23                  | rot            | 0.1550514        | -         |              |
ZPE and THERMAL CONTRIBUTIONS

Electronic [kJ/mol] = -549209.058
Ezpe [kJ/mol] = +192.032
Electronic+Ezpe [kJ/mol] = -549017.026

Electronic [hartrees] = -209.182654
Ezpe [hartrees] = +0.073141
Electronic+Ezpe [hartrees] = -209.109513

Thermal Correction to Energy [kJ/mol] = +205.170
Thermal Correction to Enthalpy [kJ/mol] = +207.651
Thermal Correction to Gibbs [kJ/mol] = +119.576

#5 Figure 17a

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

Optimized Geometry

| Center Atomic | Atomic Coordinates (Angstroms) |
|---------------|-------------------------------|
| Number Number | X Y Z                          |
| 1 6 0         | -0.581519 -0.448888 -0.000008 |
| 2 6 0         | 0.371345 0.501192 0.000007    |
| 3 7 0         | 1.721524 -0.137769 0.000005   |
| 4 8 0         | -1.894236 -0.097063 -0.000008 |
| 5 1 0         | 0.390839 1.587455 0.000021    |
| 6 1 0         | 1.412156 -1.130913 -0.000008  |
| 7 1 0         | 2.288506 0.051025 0.828375    |
| 8 1 0         | 2.288512 0.051044 -0.828357   |
| 9 1 0         | -2.015750 0.868456 0.000003   |

A, B, C / GHz 43.0426143 4.1242515 3.8427924

Frequencies and Rotational Constants

| Index NO. DDF Type | CM-1(UNSCALED) | CM-1(SCALED BY ) | Symmetry | IR-Intensity |
|--------------------|----------------|------------------|----------|--------------|
| 1 vib              | 252.50 0.00    | A 58.0323        |
| 2 vib              | 301.89 0.00    | A 88.2824        |
| 3 | vib | 378.74 | 0.00 | A | 29.4702 |
|---|-----|--------|------|---|---------|
| 4 | vib | 527.12 | 0.00 | A | 9.5829  |
| 5 | vib | 534.81 | 0.00 | A | 1.6535  |
| 6 | vib | 645.31 | 0.00 | A | 93.7235 |
| 7 | vib | 891.35 | 0.00 | A | 0.2328  |
| 8 | vib | 1013.12| 0.00 | A | 0.4648  |
| 9 | vib | 1067.42| 0.00 | A | 5.3776  |
| 10| vib | 1104.39| 0.00 | A | 100.3752|
| 11| vib | 1238.27| 0.00 | A | 93.7691 |
| 12| vib | 1320.72| 0.00 | A | 4.5273  |
| 13| vib | 1365.79| 0.00 | A | 147.6443|
| 14| vib | 1510.33| 0.00 | A | 39.8165 |
| 15| vib | 1610.56| 0.00 | A | 16.5456 |
| 16| vib | 1642.93| 0.00 | A | 16.8005 |
| 17| vib | 3103.51| 0.00 | A | 61.8325 |
| 18| vib | 3137.59| 0.00 | A | 160.2336|
| 19| vib | 3381.45| 0.00 | A | 8.0938  |
| 20| vib | 3419.77| 0.00 | A | 13.8187 |
| 21| vib | 3567.56| 0.00 | A | 67.3999 |
| 22| rot | 1.4357471| -  |   |         |
| 23| rot | 0.1375702| -  |   |         |
| 24| rot | 0.1281818| -  |   |         |

------------------------------- ZPE and THERMAL CONTRIBUTIONS -----------------------------

| Eelectronic   | [kJ/mol]    | = -549119.809 |
| Ezpe          | [kJ/mol]    | = +191.493    |
| Eelectronic+Ezpe| [kJ/mol]    | = -548928.316 |

| Eelectronic   | [hartrees]  | = -209.148661 |
| Ezpe          | [hartrees]  | = +0.072936   |
| Eelectronic+Ezpe| [hartrees]  | = -209.075725 |

Thermal Correction to Energy [kJ/mol] = +204.075
Thermal Correction to Enthalpy [kJ/mol] = +206.553
Thermal Correction to Gibbs [kJ/mol] = +121.726

#51 N-methyl-formamide

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

------------------------------- OPTIMIZED GEOMETRY -----------------------------

57
| Center Atomic | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               | X           | Y                      | Z                      |
| 1             | 6             | 0           | -1.451949              | -0.431750              | 0.000019               |
| 2             | 6             | 0           | 0.866168               | 0.426163               | -0.000034              |
| 3             | 7             | 0           | -0.473590              | 0.640457               | -0.000089              |
| 4             | 8             | 0           | 1.408394               | -0.658767              | 0.000016               |
| 5             | 1             | 0           | -2.080047              | -0.392409              | 0.891338               |
| 6             | 1             | 0           | 1.433421               | 1.373519               | 0.000242               |
| 7             | 1             | 0           | -0.791729              | 1.594209               | 0.000673               |
| 8             | 1             | 0           | -2.090041              | -0.382384              | -0.883574              |
| 9             | 1             | 0           | -0.908942              | -1.372478              | -0.008101              |

A, B, C / GHz  20.1092105  6.0935137  4.8180080

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---- FREQUENCIES AND ROTATIONAL CONSTANTS ----
--------------------------------------------------------------------------------

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|----------|--------------|
| 1         | vib      | 66.73          | 0.00             | A        | 0.0826       |
| 2         | vib      | 269.36         | 0.00             | A        | 65.3388      |
| 3         | vib      | 295.94         | 0.00             | A        | 13.5206      |
| 4         | vib      | 537.56         | 0.00             | A        | 39.1007      |
| 5         | vib      | 768.62         | 0.00             | A        | 0.6517       |
| 6         | vib      | 951.93         | 0.00             | A        | 17.2895      |
| 7         | vib      | 1022.28        | 0.00             | A        | 0.0035       |
| 8         | vib      | 1154.30        | 0.00             | A        | 0.8934       |
| 9         | vib      | 1161.15        | 0.00             | A        | 22.8437      |
| 10        | vib      | 1218.41        | 0.00             | A        | 82.4316      |
| 11        | vib      | 1422.49        | 0.00             | A        | 5.4770       |
| 12        | vib      | 1443.62        | 0.00             | A        | 20.2832      |
| 13        | vib      | 1493.19        | 0.00             | A        | 33.3830      |
| 14        | vib      | 1502.88        | 0.00             | A        | 6.4416       |
| 15        | vib      | 1555.93        | 0.00             | A        | 91.8433      |
| 16        | vib      | 1781.88        | 0.00             | A        | 325.4093     |
| 17        | vib      | 2935.19        | 0.00             | A        | 115.7132     |
| 18        | vib      | 3028.74        | 0.00             | A        | 44.6153      |
| 19        | vib      | 3076.04        | 0.00             | A        | 29.1941      |
| 20        | vib      | 3143.31        | 0.00             | A        | 0.9929       |
| 21        | vib      | 3631.65        | 0.00             | A        | 22.6070      |
| 22        | rot      | 0.6707711      | -                |          |              |
| 23        | rot      | 0.2032577      | -                |          |              |
| 24        | rot      | 0.1607114      | -                |          |              |

--------------------------------------------------------------------------------

-- ZPE and THERMAL CONTRIBUTIONS --

| Electronic [kJ/mol] | = -549483.859 |
| Zpe [kJ/mol]        | = +194.161    |

58
Electronic + Ezpe [kJ/mol] = -549289.698
Electronic [hartrees] = -209.287320
Ezpe [hartrees] = +0.073952
Electronic + Ezpe [hartrees] = -209.213368
Thermal Correction to Energy [kJ/mol] = +207.197
Thermal Correction to Enthalpy [kJ/mol] = +209.678
Thermal Correction to Gibbs [kJ/mol] = +121.784

#52 Figure 17j
Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

---------------------------------------------------------------------------------------------------------
# OPTIMIZED GEOMETRY #
---------------------------------------------------------------------------------------------------------
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X   | Y   | Z   |
|---------------|---------------|-------------|-------------------------|-----|-----|-----|
| 1             | 6             | 0           |                         | 1.320282 | -0.393653 | -0.017033 |
| 2             | 6             | 0           |                         | -1.052372 | -0.865609 | 0.045925  |
| 3             | 7             | 0           |                         | 0.038476  | -0.103197 | -0.009242 |
| 4             | 8             | 0           |                         | -0.208607 | 1.293253  | -0.062924 |
| 5             | 1             | 0           |                         | 1.604403  | -1.397163 | -0.276813 |
| 6             | 1             | 0           |                         | -1.926813 | -0.523332 | -0.481425 |
| 7             | 1             | 0           |                         | -0.915298 | -1.895069 | 0.326261  |
| 8             | 1             | 0           |                         | 2.016030  | 0.353387  | 0.317380  |
| 9             | 1             | 0           |                         | -0.986261 | 1.394102  | 0.509331  |

---------------------------------------------------------------------------------------------------------
| A, B, C / GHz | 10.8727464 | 10.5170096 | 5.4443874 |

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# FREQUENCIES AND ROTATIONAL CONSTANTS #
---------------------------------------------------------------------------------------------------------
| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|----------|--------------|
| 1         | vib      | 392.91         | 0.00             | A        | 11.5470      |
| 2         | vib      | 429.21         | 0.00             | A        | 108.5356     |
| 3         | vib      | 512.88         | 0.00             | A        | 4.8584       |
| 4         | vib      | 517.48         | 0.00             | A        | 30.4160      |
| 5         | vib      | 569.82         | 0.00             | A        | 310.8011     |
| 6         | vib      | 583.49         | 0.00             | A        | 126.5943     |
| 7         | vib      | 623.54         | 0.00             | A        | 53.7688      |
| 8         | vib      | 673.05         | 0.00             | A        | 32.8650      |
| 9         | vib      | 826.31         | 0.00             | A        | 58.3113      |
| 10        | vib      | 1084.84        | 0.00             | A        | 16.9439      |

---------------------------------------------------------------------------------------------------------
11 vib 1098.22 0.00 A 8.7985
12 vib 1300.90 0.00 A 41.9159
13 vib 1347.75 0.00 A 87.8008
14 vib 1447.58 0.00 A 9.4911
15 vib 1488.21 0.00 A 10.4303
16 vib 1665.95 0.00 A 282.5780
17 vib 3172.99 0.00 A 2.9226
18 vib 3196.27 0.00 A 5.4024
19 vib 3295.73 0.00 A 2.2599
20 vib 3321.84 0.00 A 0.1941
21 vib 3684.02 0.00 A 10.6147
22 rot 0.3626758 -
23 rot 0.3508097 -
24 rot 0.1816052 -

ZPE and THERMAL CONTRIBUTIONS

\[
\begin{align*}
\text{E}_{\text{electronic}} \ [\text{kJ/mol}] &= -549114.761 \\
\text{E}_{\text{zpe}} \ [\text{kJ/mol}] &= +186.815 \\
\text{E}_{\text{electronic}} + \text{E}_{\text{zpe}} \ [\text{kJ/mol}] &= -548927.946 \\
\text{E}_{\text{electronic}} \ [\text{hartrees}] &= -209.146738 \\
\text{E}_{\text{zpe}} \ [\text{hartrees}] &= +0.071154 \\
\text{E}_{\text{electronic}} + \text{E}_{\text{zpe}} \ [\text{hartrees}] &= -209.075584 \\
\text{Thermal Correction to Energy} \ [\text{kJ/mol}] &= +198.976 \\
\text{Thermal Correction to Enthalpy} \ [\text{kJ/mol}] &= +201.455 \\
\text{Thermal Correction to Gibbs} \ [\text{kJ/mol}] &= +117.709
\end{align*}
\]

#54 HO–\(\ddot{\text{C}}\)–CH\(_2\)–NH\(_2\)
Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

OPTIMIZED GEOMETRY

\[
\begin{align*}
\text{Center} & \quad \text{Atomic Number} & \quad \text{Atomic Number} & \quad \text{Type} & \quad X & \quad Y & \quad Z \\
1 & 6 & 0 & -0.643635 & -0.578962 & 0.191018 \\
2 & 6 & 0 & 0.466248 & 0.434842 & 0.155903 \\
3 & 7 & 0 & 1.803218 & -0.062983 & -0.134443 \\
4 & 8 & 0 & -1.794893 & -0.054025 & -0.116735 \\
5 & 1 & 0 & 0.463811 & 0.870745 & 1.165759
\end{align*}
\]
| INDEX NO. | DOF | TYPE | CM-1(UNSCALED) | CM-1(SCALED BY A) | SYMMETRY | IR-INTENSITY |
|-----------|-----|------|----------------|-------------------|----------|--------------|
| 1         | vib | 77.52| 0.00          | A                 | 5.7934   |
| 2         | vib | 210.90| 0.00         | A                 | 79.7206  |
| 3         | vib | 342.03| 0.00         | A                 | 69.7291  |
| 4         | vib | 522.70| 0.00         | A                 | 3.5080   |
| 5         | vib | 682.23| 0.00         | A                 | 38.6986  |
| 6         | vib | 878.75| 0.00         | A                 | 112.4156 |
| 7         | vib | 894.71| 0.00         | A                 | 41.0109  |
| 8         | vib | 970.15| 0.00         | A                 | 37.1332  |
| 9         | vib | 1129.20| 0.00       | A                 | 1.1492   |
| 10        | vib | 1134.33| 0.00       | A                 | 6.3563   |
| 11        | vib | 1312.86| 0.00       | A                 | 60.2647  |
| 12        | vib | 1331.89| 0.00       | A                 | 71.6940  |
| 13        | vib | 1364.26| 0.00       | A                 | 43.2619  |
| 14        | vib | 1384.18| 0.00       | A                 | 55.5899  |
| 15        | vib | 1413.78| 0.00       | A                 | 4.2346   |
| 16        | vib | 1670.63| 0.00       | A                 | 22.7675  |
| 17        | vib | 2891.35| 0.00       | A                 | 78.4473  |
| 18        | vib | 2982.87| 0.00       | A                 | 13.2531  |
| 19        | vib | 3311.95| 0.00       | A                 | 109.3975 |
| 20        | vib | 3486.19| 0.00       | A                 | 0.3787   |
| 21        | vib | 3559.28| 0.00       | A                 | 2.1325   |
| 22        | rot | 1.1479653| -         |                   |          |
| 23        | rot | 0.1406150| -         |                   |          |
| 24        | rot | 0.1339456| -         |                   |          |

| ZPE and THERMAL CONTRIBUTIONS |
|--------------------------------|

- **Eelectronic** [kJ/mol] = -549183.074
- **Ezpe** [kJ/mol] = +188.721
- **Eelectronic+Ezpe** [kJ/mol] = -548994.353

- **Eelectronic** [hartrees] = -209.172757
- **Ezpe** [hartrees] = +0.071880
- **Eelectronic+Ezpe** [hartrees] = -209.100877

- **Thermal Correction to Energy** [kJ/mol] = +202.108
- **Thermal Correction to Enthalpy** [kJ/mol] = +204.587
Thermal Correction to Gibbs [kJ/mol] = +116.367

#58 Figure 17k

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

----------------------------------------------- OPTIMIZED GEOMETRY -----------------------------------------------

| Center | Atomic Number | Atomic Type | X  | Y  | Z   |
|--------|---------------|-------------|----|----|-----|
| 1      | 6             | 0           | 1.460732 | 0.494475 | -0.115409 |
| 2      | 6             | 0           | -0.621063 | -0.621954 | 0.034411 |
| 3      | 7             | 0           | -1.341053 | 0.532659 | -0.077537 |
| 4      | 8             | 0           | 0.653210  | -0.611126 | 0.020682 |
| 5      | 1             | 0           | 2.447351  | 0.257008 | 0.252043 |
| 6      | 1             | 0           | -1.103082 | -1.583557 | -0.015699 |
| 7      | 1             | 0           | -2.326980 | 0.451747 | 0.108060 |
| 8      | 1             | 0           | -0.919547 | 1.364627 | 0.314205 |
| 9      | 1             | 0           | 1.025935  | 1.435444 | 0.204682 |

A, B, C / GHz 20.5098700 6.5343526 4.9982893

----------------------------------------------- FREQUENCIES AND ROTATIONAL CONSTANTS -----------------------------------------------

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|----------|--------------|
| 1         | vib      | 185.40         | 0.00             | A        | 127.7461     |
| 2         | vib      | 308.89         | 0.00             | A        | 1.2925       |
| 3         | vib      | 380.13         | 0.00             | A        | 10.6015      |
| 4         | vib      | 460.41         | 0.00             | A        | 250.0262     |
| 5         | vib      | 545.11         | 0.00             | A        | 54.6033      |
| 6         | vib      | 616.99         | 0.00             | A        | 22.9475      |
| 7         | vib      | 640.62         | 0.00             | A        | 154.0560     |
| 8         | vib      | 673.77         | 0.00             | A        | 126.0867     |
| 9         | vib      | 995.87         | 0.00             | A        | 7.1935       |
| 10        | vib      | 1077.15        | 0.00             | A        | 67.8656      |
| 11        | vib      | 1244.10        | 0.00             | A        | 2.4867       |
| 12        | vib      | 1275.98        | 0.00             | A        | 71.6452      |
| 13        | vib      | 1402.05        | 0.00             | A        | 14.3136      |
| 14        | vib      | 1480.93        | 0.00             | A        | 7.3210       |
| 15        | vib      | 1600.65        | 0.00             | A        | 14.9374      |
| 16        | vib      | 1646.52        | 0.00             | A        | 122.1893     |
| 17        | vib      | 3089.41        | 0.00             | A        | 32.4832      |
| 18        | vib      | 3225.56        | 0.00             | A        | 24.9424      |
19  vib  3242.88  0.00    A  14.8553
20  vib  3511.46  0.00    A  4.8506
21  vib  3655.43  0.00    A  54.2484
22  rot  0.6841356  -       
23  rot  0.2179625  -       
24  rot  0.1667250  -       

------------------------ ZPE and THERMAL CONTRIBUTIONS -------------------------

Eelectronic [kJ/mol] = -549166.317
Ezpe [kJ/mol] = +186.972
Eelectronic+Ezpe [kJ/mol] = -548979.345

Eelectronic [hartrees] = -209.166375
Ezpe [hartrees] = +0.071214
Eelectronic+Ezpe [hartrees] = -209.095161

Thermal Correction to Energy [kJ/mol] = +200.431
Thermal Correction to Enthalpy [kJ/mol] = +202.909
Thermal Correction to Gibbs [kJ/mol] = +116.520

#59 Figure 17l
Charge = 0 Multiplicity = 1 Stoichiometry  C2H5NO

---------------------- OPTIMIZED GEOMETRY ---------------------------

| Center Number | Atomic Number | Atomic Type | X     | Y     | Z     |
|---------------|---------------|-------------|-------|-------|-------|
| 1             | 6             | 0           | 1.424781 | 0.079208 | 0.177387 |
| 2             | 6             | 0           | -1.224017 | 0.727517 | -0.081199 |
| 3             | 7             | 0           | -0.852766 | -0.620099 | 0.356694 |
| 4             | 8             | 0           | 0.207801  | -0.122004 | -0.563135 |
| 5             | 1             | 0           | 1.900458  | -0.889044 | 0.324805 |
| 6             | 1             | 0           | 2.044346  | 0.726827  | -0.439684 |
| 7             | 1             | 0           | -0.727280 | 1.366882  | 0.672520  |
| 8             | 1             | 0           | -1.328206 | -1.278231 | -0.261203 |
| 9             | 1             | 0           | 1.213054  | 0.549949  | 1.134657  |

A, B, C / GHz  19.0264740  6.8370916  6.1531051
### Frequencies and Rotational Constants

| INDEX NO. | DOF TYPE | CM-1 (UNSCALED) | CM-1 (SCALED BY) | SYMMETRY | IR-INTENSITY |
|-----------|----------|-----------------|------------------|---------|--------------|
| 1         | vib      | 129.48          | 0.00             | A       | 1.8569       |
| 2         | vib      | 271.55          | 0.00             | A       | 11.4349      |
| 3         | vib      | 319.72          | 0.00             | A       | 8.6145       |
| 4         | vib      | 413.57          | 0.00             | A       | 3.8023       |
| 5         | vib      | 753.05          | 0.00             | A       | 6.2988       |
| 6         | vib      | 951.98          | 0.00             | A       | 17.9890      |
| 7         | vib      | 1005.60         | 0.00             | A       | 62.0641      |
| 8         | vib      | 1050.66         | 0.00             | A       | 75.0131      |
| 9         | vib      | 1146.89         | 0.00             | A       | 20.6428      |
| 10        | vib      | 1182.91         | 0.00             | A       | 11.6830      |
| 11        | vib      | 1190.08         | 0.00             | A       | 8.8823       |
| 12        | vib      | 1368.10         | 0.00             | A       | 39.4218      |
| 13        | vib      | 1395.88         | 0.00             | A       | 4.8629       |
| 14        | vib      | 1456.83         | 0.00             | A       | 6.5591       |
| 15        | vib      | 1480.54         | 0.00             | A       | 6.8928       |
| 16        | vib      | 1485.91         | 0.00             | A       | 8.0957       |
| 17        | vib      | 2893.42         | 0.00             | A       | 109.8225     |
| 18        | vib      | 3043.20         | 0.00             | A       | 27.8481      |
| 19        | vib      | 3128.77         | 0.00             | A       | 11.6747      |
| 20        | vib      | 3138.54         | 0.00             | A       | 8.7681       |
| 21        | vib      | 3415.59         | 0.00             | A       | 2.6944       |
| 22        | rot      | 0.6346549       | -                |         |              |
| 23        | rot      | 0.2280608       | -                |         |              |
| 24        | rot      | 0.2052455       | -                |         |              |

### ZPE and Thermal Contributions

- Electronic [kJ/mol] = -548879.498
- ZPE [kJ/mol] = +186.752
- Electronic + ZPE [kJ/mol] = -548692.746

- Electronic [hartrees] = -209.057131
- ZPE [hartrees] = +0.071130
- Electronic + ZPE [hartrees] = -208.986001

- Thermal Correction to Energy [kJ/mol] = +199.756
- Thermal Correction to Enthalpy [kJ/mol] = +202.237
- Thermal Correction to Gibbs [kJ/mol] = +115.947
#6 N-hydroxy-ethenamine

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

OPTIMIZED GEOMETRY

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X       | Y       | Z       |
|---------------|---------------|-------------|-------------------------|---------|---------|---------|
| 1             | 6             | 0           | -1.477669               | -0.539280 | -0.004319 |
| 2             | 6             | 0           | -0.730751               | 0.559891  | 0.003154  |
| 3             | 7             | 0           | 0.660144                | 0.640990  | 0.135668  |
| 4             | 8             | 0           | 1.324976                | -0.587059 | -0.138758 |
| 5             | 1             | 0           | -2.552654               | -0.455986 | -0.040396 |
| 6             | 1             | 0           | 1.175585                | 1.548699  | -0.031786 |
| 7             | 1             | 0           | -1.038196               | -1.524091 | 0.021816  |
| 8             | 1             | 0           | 1.064758                | 1.330485  | -0.486928 |
| 9             | 1             | 0           | 1.731375                | -0.813237 | 0.704670  |

A, B, C / GHz 18.5667767 6.2240864 4.7701222

FREQUENCIES AND ROTATIONAL CONSTANTS

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|----------|-------------|
| 1         | vib      | 254.40         | 0.00             | A        | 1.3317      |
| 2         | vib      | 304.01         | 0.00             | A        | 3.5143      |
| 3         | vib      | 317.77         | 0.00             | A        | 75.3234     |
| 4         | vib      | 610.88         | 0.00             | A        | 43.9594     |
| 5         | vib      | 677.26         | 0.00             | A        | 78.2010     |
| 6         | vib      | 772.01         | 0.00             | A        | 130.8712    |
| 7         | vib      | 865.50         | 0.00             | A        | 55.8269     |
| 8         | vib      | 979.55         | 0.00             | A        | 36.7125     |
| 9         | vib      | 996.44         | 0.00             | A        | 16.8513     |
| 10        | vib      | 1018.07        | 0.00             | A        | 5.9553      |
| 11        | vib      | 1168.69        | 0.00             | A        | 30.9414     |
| 12        | vib      | 1325.52        | 0.00             | A        | 0.8944      |
| 13        | vib      | 1377.64        | 0.00             | A        | 57.7575     |
| 14        | vib      | 1444.66        | 0.00             | A        | 4.7583      |
| 15        | vib      | 1480.80        | 0.00             | A        | 7.7782      |
| 16        | vib      | 1711.80        | 0.00             | A        | 83.2422     |
| 17        | vib      | 3149.25        | 0.00             | A        | 8.5457      |
| 18        | vib      | 3171.28        | 0.00             | A        | 5.9261      |
| 19        | vib      | 3257.50        | 0.00             | A        | 5.1679      |
| 20        | vib      | 3506.56        | 0.00             | A        | 7.8986      |
| 21        | vib      | 3792.63        | 0.00             | A        | 50.5938     |
| 22        | rot      | 0.6193210      | -                |         |             |
| 23        | rot      | 0.2076132      | -                |         |             |
| 24        | rot      | 0.1591141      | -                |         |             |
ZPE and THERMAL CONTRIBUTIONS

Electronic [kJ/mol] = -549248.803
Ezpe [kJ/mol] = +192.491
Eelectronic+Ezpe [kJ/mol] = -549056.312

Electronic [hartrees] = -209.197792
Ezpe [hartrees] = +0.073316
Eelectronic+Ezpe [hartrees] = -209.124476

Thermal Correction to Energy [kJ/mol] = +204.868
Thermal Correction to Enthalpy [kJ/mol] = +207.346
Thermal Correction to Gibbs [kJ/mol] = +122.508

#60 Figure 17m
Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

OPTIMIZED GEOMETRY

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X          | Y          | Z          |
| 1             | 6             | 0           | 0.634711   | -0.547786 | 0.195625   |
| 2             | 6             | 0           | 1.806102   | 0.007017  | -0.108781  |
| 3             | 7             | 0           | -0.480108  | 0.480636  | 0.123435   |
| 4             | 8             | 0           | -1.700452  | -0.198058 | -0.155773  |
| 5             | 1             | 0           | 1.966729   | 1.054488  | -0.386628  |
| 6             | 1             | 0           | 2.699000   | -0.604813 | -0.092966  |
| 7             | 1             | 0           | -0.386478  | 1.192799  | -0.608510  |
| 8             | 1             | 0           | -0.602615  | 0.939923  | 1.025743   |
| 9             | 1             | 0           | -1.357139  | -1.117789 | -0.082561  |

A, B, C / GHz 33.0901035 4.6032611 4.2292622

FREQUENCIES AND ROTATIONAL CONSTANTS

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|----------|--------------|
| 1         | vib      | 76.55          | 0.00             | A        | 2.6477       |
| 2         | vib      | 308.41         | 0.00             | A        | 19.8722      |
| 3         | vib      | 498.01         | 0.00             | A        | 19.8069      |
#69 Figure 17n

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

---------------------------- OPTIMIZED GEOMETRY -----------------------------

| Center | Atomic | Atomic Coordinates (Angstroms) | Coordinates (Angstroms) |
|--------|--------|--------------------------------|-------------------------|
| 4      | vib    | 559.08                         | 0.00                    |
| 5      | vib    | 634.07                         | 0.00                    |
| 6      | vib    | 688.93                         | 0.00                    |
| 7      | vib    | 909.36                         | 0.00                    |
| 8      | vib    | 951.95                         | 0.00                    |
| 9      | vib    | 978.81                         | 0.00                    |
| 10     | vib    | 1075.23                        | 0.00                    |
| 11     | vib    | 1245.92                        | 0.00                    |
| 12     | vib    | 1284.47                        | 0.00                    |
| 13     | vib    | 1415.96                        | 0.00                    |
| 14     | vib    | 1489.61                        | 0.00                    |
| 15     | vib    | 1620.51                        | 0.00                    |
| 16     | vib    | 1634.35                        | 0.00                    |
| 17     | vib    | 3012.79                        | 0.00                    |
| 18     | vib    | 3174.15                        | 0.00                    |
| 19     | vib    | 3324.08                        | 0.00                    |
| 20     | vib    | 3445.91                        | 0.00                    |
| 21     | vib    | 3459.34                        | 0.00                    |
| 22     | rot    | 1.1037670                      |                         |
| 23     | rot    | 0.1535483                      |                         |
| 24     | rot    | 0.1410730                      |                         |

---------------------------- ZPE and THERMAL CONTRIBUTIONS ------------------------------

Electronic [kJ/mol] = -549012.269
Ezpe [kJ/mol] = +190.131
Electronic+Ezpe [kJ/mol] = -548822.138

Electronic [hartrees] = -209.107701
Ezpe [hartrees] = +0.072417
Electronic+Ezpe [hartrees] = -209.035284

Thermal Correction to Energy [kJ/mol] = +202.996
Thermal Correction to Enthalpy [kJ/mol] = +205.474
Thermal Correction to Gibbs [kJ/mol] = +118.589
| Number | Type | X       | Y       | Z       |
|--------|------|---------|---------|---------|
| 1      | 6    | -2.097347 | 0.189229 | -0.009052 |
| 2      | 6    | 0.502102  | 0.537256 | 0.016937 |
| 3      | 7    | -0.764008 | -0.379246 | -0.026236 |
| 4      | 8    | 1.687067  | -0.190019 | -0.109633 |
| 5      | 1    | 0.400724  | 1.116726 | 0.932899 |
| 6      | 1    | 0.395817  | 1.183263 | -0.849117 |
| 7      | 1    | -0.844001 | -0.867581 | 0.877829 |
| 8      | 1    | -0.525493 | -1.141147 | -0.703635 |
| 9      | 1    | 1.995945  | -0.475293 | 0.755438 |

\[A, B, C / \text{GHz} \quad 33.5443144 \quad 4.2663460 \quad 4.0020678\]

------------ FREQUENCIES AND ROTATIONAL CONSTANTS -------------

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|------------|----------|----------------|------------------|----------|--------------|
| 1          | vib      | 109.18         | 0.00             | A        | 48.1185      |
| 2          | vib      | 259.06         | 0.00             | A        | 32.2999      |
| 3          | vib      | 354.23         | 0.00             | A        | 114.1004     |
| 4          | vib      | 394.01         | 0.00             | A        | 0.7441       |
| 5          | vib      | 572.48         | 0.00             | A        | 24.9511      |
| 6          | vib      | 707.87         | 0.00             | A        | 11.4008      |
| 7          | vib      | 857.58         | 0.00             | A        | 13.4471      |
| 8          | vib      | 959.49         | 0.00             | A        | 17.1733      |
| 9          | vib      | 1063.66        | 0.00             | A        | 207.8317     |
| 10         | vib      | 1071.62        | 0.00             | A        | 0.4530       |
| 11         | vib      | 1217.39        | 0.00             | A        | 43.5811      |
| 12         | vib      | 1304.28        | 0.00             | A        | 6.0264       |
| 13         | vib      | 1358.33        | 0.00             | A        | 18.0495      |
| 14         | vib      | 1390.87        | 0.00             | A        | 18.5995      |
| 15         | vib      | 1467.53        | 0.00             | A        | 41.0995      |
| 16         | vib      | 1493.77        | 0.00             | A        | 6.1794       |
| 17         | vib      | 2900.18        | 0.00             | A        | 255.6710     |
| 18         | vib      | 3069.76        | 0.00             | A        | 18.1503      |
| 19         | vib      | 3155.61        | 0.00             | A        | 10.2596      |
| 20         | vib      | 3355.14        | 0.00             | A        | 46.8752      |
| 21         | vib      | 3819.43        | 0.00             | A        | 55.6872      |
| 22         | rot      | 1.1189179      |                |          |              |
| 23         | rot      | 0.1423100      |                |          |              |
| 24         | rot      | 0.1334946      |                |          |              |

------------ ZPE and THERMAL CONTRIBUTIONS -------------

\[\text{Eelectronic} \quad [\text{kJ/mol}] = -548763.474\]
\[\text{Ezpe} \quad [\text{kJ/mol}] = +184.712\]
\[\text{Eelectronic+Ezpe} \quad [\text{kJ/mol}] = -548578.762\]
Electronic [hartrees] = -209.012940
Expe [hartrees] = +0.070353
Electronic+Expe [hartrees] = -208.942587

Thermal Correction to Energy [kJ/mol] = +198.359
Thermal Correction to Enthalpy [kJ/mol] = +200.838
Thermal Correction to Gibbs [kJ/mol] = +112.991

#77 Figure 17o

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

OPTIMIZED GEOMETRY

| Center | Atomic Number | Atomic Type | X       | Y       | Z       |
|--------|---------------|-------------|---------|---------|---------|
| 1      | 6             | 0           | 1.576948| -0.639695| -0.135120|
| 2      | 6             | 0           | 0.818139| 0.539735 | 0.128553 |
| 3      | 7             | 0           | -0.728317| 0.500968 | -0.150198|
| 4      | 8             | 0           | -1.280715| -0.683372| 0.128198 |
| 5      | 1             | 0           | 0.833719 | -1.450396| -0.248752|
| 6      | 1             | 0           | 1.234967 | 1.505491 | -0.171701|
| 7      | 1             | 0           | 0.892860 | 0.461437 | 1.233046 |
| 8      | 1             | 0           | -1.143674| 1.272911 | 0.392641 |
| 9      | 1             | 0           | -0.844460| 0.770520 | -1.140028|

A, B, C / GHz 16.7464126 6.2623874 4.9183681

FREQUENCIES AND ROTATIONAL CONSTANTS

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|----------|--------------|
| 1         | vib      | 123.45         | 0.00             | A        | 27.7248      |
| 2         | vib      | 279.79         | 0.00             | A        | 26.9927      |
| 3         | vib      | 431.17         | 0.00             | A        | 12.0304      |
| 4         | vib      | 546.07         | 0.00             | A        | 22.0065      |
| 5         | vib      | 618.66         | 0.00             | A        | 2.3876       |
| 6         | vib      | 762.60         | 0.00             | A        | 66.7543      |
| 7         | vib      | 950.91         | 0.00             | A        | 42.0112      |
| 8         | vib      | 1017.69        | 0.00             | A        | 43.1860      |
| 9         | vib      | 1061.82        | 0.00             | A        | 18.2564      |
| 10        | vib      | 1135.32        | 0.00             | A        | 20.9029      |
| 11        | vib      | 1218.71        | 0.00             | A        | 9.2287       |
12 vib 1275.67 0.00 A 14.5505
13 vib 1300.45 0.00 A 25.6985
14 vib 1338.02 0.00 A 43.1518
15 vib 1402.87 0.00 A 5.4007
16 vib 1651.48 0.00 A 3.0401
17 vib 2921.38 0.00 A 19.5585
18 vib 2962.40 0.00 A 5.4184
19 vib 3042.87 0.00 A 23.5453
20 vib 3202.76 0.00 A 41.2018
21 vib 3224.12 0.00 A 7.0340
22 rot 0.5586002 - -
23 rot 0.2088908 - -
24 rot 0.1640591 - -

------------------------ ZPE and THERMAL CONTRIBUTIONS -------------------------

Electronic [kJ/mol] = -548820.985
Ezpe [kJ/mol] = +182.241
Electronic+Ezpe [kJ/mol] = -548638.744

Electronic [hartrees] = -209.034845
Ezpe [hartrees] = +0.069412
Electronic+Ezpe [hartrees] = -208.965433

Thermal Correction to Energy [kJ/mol] = +195.027
Thermal Correction to Enthalpy [kJ/mol] = +197.506
Thermal Correction to Gibbs [kJ/mol] = +111.166

#79 Figure 17p
Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

---------------------- OPTIMIZED GEOMETRY ---------------------------
| INDEX NO. | DOF | TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|-----|------|----------------|------------------|----------|--------------|
| 1         | vib | 127.26 | 0.00 | A | 3.6984 |
| 2         | vib | 186.95 | 0.00 | A | 47.2864 |
| 3         | vib | 308.82 | 0.00 | A | 29.4832 |
| 4         | vib | 619.25 | 0.00 | A | 11.7454 |
| 5         | vib | 631.18 | 0.00 | A | 0.0086 |
| 6         | vib | 742.00 | 0.00 | A | 8.5395 |
| 7         | vib | 805.66 | 0.00 | A | 2.1099 |
| 8         | vib | 1015.24 | 0.00 | A | 63.9424 |
| 9         | vib | 1048.94 | 0.00 | A | 42.1000 |
| 10        | vib | 1148.51 | 0.00 | A | 28.3125 |
| 11        | vib | 1214.97 | 0.00 | A | 14.8401 |
| 12        | vib | 1271.36 | 0.00 | A | 65.8084 |
| 13        | vib | 1398.76 | 0.00 | A | 21.3430 |
| 14        | vib | 1398.76 | 0.00 | A | 60.3219 |
| 15        | vib | 1434.57 | 0.00 | A | 7.5314 |
| 16        | vib | 1528.66 | 0.00 | A | 20.2653 |
| 17        | vib | 2938.23 | 0.00 | A | 10.2404 |
| 18        | vib | 2942.91 | 0.00 | A | 0.4608 |
| 19        | vib | 3128.63 | 0.00 | A | 36.0092 |
| 20        | vib | 3131.17 | 0.00 | A | 15.5309 |
| 21        | vib | 3155.24 | 0.00 | A | 9.1515 |
| 22        | rot | 0.5685529 | - | - | - |
| 23        | rot | 0.2219137 | - | - | - |
| 24        | rot | 0.1683439 | - | - | - |

ZPE and THERMAL CONTRIBUTIONS

- **Electronic** [kJ/mol] = -548885.576
- **ZPE** [kJ/mol] = +179.926
- **Electronic+ZPE** [kJ/mol] = -548705.650

- **Electronic** [hartrees] = -209.059446
- **ZPE** [hartrees] = +0.068530
- **Electronic+ZPE** [hartrees] = -208.990916

- **Thermal Correction to Energy** [kJ/mol] = +193.363
- **Thermal Correction to Enthalpy** [kJ/mol] = +195.841
- **Thermal Correction to Gibbs** [kJ/mol] = +108.218
# 8 Z 2-amino-ethenol

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

Optimized Geometry

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X | Y | Z |
|---------------|---------------|-------------|-------------------------|---|---|---|
| 1             | 6             | 0           | -0.575379               | 0.699459 | -0.000000 |
| 2             | 6             | 0           | 0.752953                | 0.585561 | 0.000001  |
| 3             | 7             | 0           | -1.349236               | -0.512339 | -0.000000 |
| 4             | 8             | 0           | 1.400782                | -0.600562 | -0.000000 |
| 5             | 1             | 0           | -1.046201               | 1.675217  | -0.000000 |
| 6             | 1             | 0           | 1.418925                | 1.436724  | 0.000001  |
| 7             | 1             | 0           | -1.947501               | -0.579852 | 0.814871  |
| 8             | 1             | 0           | 0.695244                | -1.271495 | -0.000004 |
| 9             | 1             | 0           | -1.947511               | -0.579846 | -0.814864 |

A, B, C / GHz 18.0964688 6.3036178 4.7938224

Frequencies and Rotational Constants

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|-------------------|-----------|--------------|
| 1         | vib      | 197.11         | 0.00              | A         | 16.9927      |
| 2         | vib      | 267.34         | 0.00              | A         | 3.6363       |
| 3         | vib      | 481.74         | 0.00              | A         | 0.0000       |
| 4         | vib      | 702.91         | 0.00              | A         | 141.2077     |
| 5         | vib      | 735.88         | 0.00              | A         | 68.0399      |
| 6         | vib      | 752.32         | 0.00              | A         | 0.2139       |
| 7         | vib      | 883.12         | 0.00              | A         | 74.1197      |
| 8         | vib      | 953.64         | 0.00              | A         | 7.4076       |
| 9         | vib      | 1018.07        | 0.00              | A         | 22.3498      |
| 10        | vib      | 1121.62        | 0.00              | A         | 127.9884     |
| 11        | vib      | 1200.29        | 0.00              | A         | 3.3242       |
| 12        | vib      | 1234.60        | 0.00              | A         | 87.2743      |
| 13        | vib      | 1372.40        | 0.00              | A         | 5.0837       |
| 14        | vib      | 1428.77        | 0.00              | A         | 43.7776      |
| 15        | vib      | 1634.39        | 0.00              | A         | 13.7260      |
| 16        | vib      | 1730.10        | 0.00              | A         | 99.6606      |
| 17        | vib      | 3144.58        | 0.00              | A         | 19.6393      |
| 18        | vib      | 3205.40        | 0.00              | A         | 16.2805      |
| 19        | vib      | 3485.92        | 0.00              | A         | 0.4391       |
| Number | Type | X         | Y         | Z         |
|--------|------|-----------|-----------|-----------|
| 1      | 6    | 0.858179  | -0.745010 | -0.141695 |
| 2      | 6    | 0.855792  | 0.745894  | -0.141627 |
| 3      | 7    | -0.317475 | 0.000077  | 0.410090  |
| 4      | 8    | -1.483192 | -0.000831 | -0.204529 |
| 5      | 1    | 1.481533  | 1.272964  | 0.566929  |
| 6      | 1    | 0.594663  | 1.261912  | -1.050384 |
| 7      | 1    | 1.478515  | 1.276251  | 0.565753  |
| 8      | 1    | 1.261343  | 1.261343  | -1.050736 |
| 9      | 1    | -0.341482 | -0.000841 | 1.433962  |

A, B, C / GHz 17.8798095 7.4682673 6.3936097
| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|----------|--------------|
| 1         | vib      | 409.71         | 0.00             | A        | 5.5757       |
| 2         | vib      | 426.24         | 0.00             | A        | 14.8442      |
| 3         | vib      | 679.28         | 0.00             | A        | 23.2803      |
| 4         | vib      | 755.30         | 0.00             | A        | 2.6169       |
| 5         | vib      | 818.27         | 0.00             | A        | 1.4672       |
| 6         | vib      | 919.88         | 0.00             | A        | 1.0088       |
| 7         | vib      | 1019.91        | 0.00             | A        | 55.1834      |
| 8         | vib      | 1099.62        | 0.00             | A        | 8.4921       |
| 9         | vib      | 1101.76        | 0.00             | A        | 61.2077      |
| 10        | vib      | 1128.70        | 0.00             | A        | 3.3251       |
| 11        | vib      | 1154.34        | 0.00             | A        | 45.0661      |
| 12        | vib      | 1207.56        | 0.00             | A        | 2.2749       |
| 13        | vib      | 1227.20        | 0.00             | A        | 10.1090      |
| 14        | vib      | 1431.05        | 0.00             | A        | 7.2269       |
| 15        | vib      | 1454.72        | 0.00             | A        | 5.0470       |
| 16        | vib      | 1482.33        | 0.00             | A        | 2.8228       |
| 17        | vib      | 3132.33        | 0.00             | A        | 8.3512       |
| 18        | vib      | 3136.88        | 0.00             | A        | 6.4665       |
| 19        | vib      | 3243.27        | 0.00             | A        | 1.3379       |
| 20        | vib      | 3254.91        | 0.00             | A        | 0.0287       |
| 21        | vib      | 3309.30        | 0.00             | A        | 22.5367      |
| 22        | rot      | 0.5964062      | -                |          |              |
| 23        | rot      | 0.2491146      | -                |          |              |
| 24        | rot      | 0.2132679      | -                |          |              |

------------------------ ZPE and THERMAL CONTRIBUTIONS ------------------------

|                      | [kJ/mol]       | [hartrees]        | [kJ/mol]      | [hartrees]        | [kJ/mol]      |
|----------------------|----------------|------------------|---------------|------------------|---------------|
| Electronic           | -549101.88     | -209.141832      | -548908.129   | -209.068036      |
| Zpe                  | +193.751       | +0.073796        | +204.067      | +206.545         |
| Electronic+Zpe       | -548909.139    | -209.141832      | -548908.129   | -209.068036      |
| Thermal Correction to Energy | +204.067  | +204.067         | +206.545      | +206.545         |
| Thermal Correction to Enthalpy | +125.801     | +125.801         | +125.801      | +125.801         |

#85 O-ethenyl-hydroxylamine

Charge = 0  Multiplicity = 1  Stoichiometry  C2H5N0
### OPTIMIZED GEOMETRY

| Center Atomic Number | Atomic Number | Type | X   | Y   | Z    |
|----------------------|---------------|------|-----|-----|------|
| 1                    | 6             | 0    | -0.609356 | 0.364178 | -0.000000 |
| 2                    | 6             | 0    | -1.860130 | -0.075200 | 0.000000  |
| 3                    | 7             | 0    | 1.700433  | 0.227774  | 0.000000  |
| 4                    | 8             | 0    | 0.454225  | -0.494558 | -0.000001 |
| 5                    | 1             | 0    | -2.095461 | -1.129695 | 0.000000  |
| 6                    | 1             | 0    | -2.670980 | 0.635756  | 0.000000  |
| 7                    | 1             | 0    | 2.187744  | -0.143420 | -0.811885 |
| 8                    | 1             | 0    | 2.187742  | -0.143419 | 0.811887  |
| 9                    | 1             | 0    | 2.187742  | -0.143419 | -0.811885 |

A, B, C / GHz 44.5110312 4.4938650 4.1712904

### FREQUENCIES AND ROTATIONAL CONSTANTS

| INDEX NO. | DOF TYPE | CM-1(UNSCALED) | CM-1(SCALED BY ) | SYMMETRY | IR-INTENSITY |
|-----------|----------|----------------|------------------|----------|--------------|
| 1         | vib      | 59.10          | 0.00             | A        | 5.2525       |
| 2         | vib      | 223.44         | 0.00             | A        | 45.8597      |
| 3         | vib      | 345.17         | 0.00             | A        | 3.9069       |
| 4         | vib      | 550.43         | 0.00             | A        | 3.9069       |
| 5         | vib      | 695.83         | 0.00             | A        | 6.3031       |
| 6         | vib      | 850.83         | 0.00             | A        | 57.5419      |
| 7         | vib      | 866.98         | 0.00             | A        | 7.9262       |
| 8         | vib      | 996.67         | 0.00             | A        | 49.9241      |
| 9         | vib      | 996.67         | 0.00             | A        | 20.4491      |
| 10        | vib      | 1141.11        | 0.00             | A        | 64.2882      |
| 11        | vib      | 1271.24        | 0.00             | A        | 143.7806     |
| 12        | vib      | 1317.88        | 0.00             | A        | 3.5018       |
| 13        | vib      | 1327.86        | 0.00             | A        | 1.5394       |
| 14        | vib      | 1424.90        | 0.00             | A        | 7.8375       |
| 15        | vib      | 1657.65        | 0.00             | A        | 21.0955      |
| 16        | vib      | 1697.04        | 0.00             | A        | 155.9041     |
| 17        | vib      | 3161.62        | 0.00             | A        | 1.6310       |
| 18        | vib      | 3185.44        | 0.00             | A        | 5.2834       |
| 19        | vib      | 3254.38        | 0.00             | A        | 5.3587       |
| 20        | vib      | 3436.52        | 0.00             | A        | 0.2065       |
| 21        | vib      | 3517.67        | 0.00             | A        | 1.9937       |
| 22        | rot      | 1.4847282      | -                |          |              |
| 23        | rot      | 0.1498992      | -                |          |              |
| 24        | rot      | 0.1391393      | -                |          |              |

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ZPE and THERMAL CONTRIBUTIONS

Electronic [kJ/mol] = -549234.759
EzpE [kJ/mol] = +191.231
Electronic+EzpE [kJ/mol] = -549043.528

Electronic [hartrees] = -209.192443
EzpE [hartrees] = +0.072836
Electronic+EzpE [hartrees] = -209.119607

Thermal Correction to Energy [kJ/mol] = +204.650
Thermal Correction to Enthalpy [kJ/mol] = +207.128
Thermal Correction to Gibbs [kJ/mol] = +118.859

#24 aziridine N-oxide Cs

Charge = 0 Multiplicity = 1 Stoichiometry C2H5NO

OPTIMIZED GEOMETRY

Center Atomic Atomic Coordinates (Angstroms)
Number Number Type X Y Z
1 6 0 -0.235967 -0.836187 0.745505
2 6 0 -0.235967 -0.836187 -0.745505
3 7 0 -0.235967 0.461677 -0.000000
4 8 0 0.815001 1.256235 -0.000000
5 1 0 -1.141358 -1.098465 1.275632
6 1 0 0.699372 -0.984314 1.261034
7 1 0 0.699372 -0.984314 -1.261034
8 1 0 -1.141358 -1.098465 -1.275632
9 1 0 -1.152670 0.918182 -0.000000

A, B, C / GHz 17.8799931 7.4661638 6.3913741

FREQUENCIES AND ROTATIONAL CONSTANTS

INDEX NO. DOF TYPE CM-1(UNSCALED) CM-1(SCALED BY ) SYMMETRY IR-INTENSITY
1 vib 409.32 0.00 A" 5.5343
2 vib 426.21 0.00 A' 14.8347
3 vib 678.94 0.00 A" 23.3611
4 vib 754.95 0.00 A' 2.6062
5 vib 818.51 0.00 A' 1.3925
6 vib 919.28 0.00 A" 1.0005

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|   | vib |          |    | A'   | vib |          |    | A''  |
|---|-----|----------|----|------|-----|----------|----|------|
| 7 | vib | 1020.34  | 0.00|      | A'   | 55.0306 |
| 8 | vib | 1099.91  | 0.00|      | A''  | 4.6432  |
| 9 | vib | 1101.77  | 0.00|      | A'   | 65.3571 |
| 10| vib | 1128.46  | 0.00|      | A''  | 3.3502  |
| 11| vib | 1154.38  | 0.00|      | A'   | 45.1983 |
| 12| vib | 1207.59  | 0.00|      | A''  | 2.2558  |
| 13| vib | 1227.21  | 0.00|      | A'   | 10.6216 |
| 14| vib | 1431.23  | 0.00|      | A'   | 7.2299  |
| 15| vib | 1454.96  | 0.00|      | A''  | 5.0312  |
| 16| vib | 1482.55  | 0.00|      | A'   | 2.8218  |
| 17| vib | 1311.97  | 0.00|      | A''  | 8.3453  |
| 18| vib | 3136.49  | 0.00|      | A'   | 6.4124  |
| 19| vib | 3242.61  | 0.00|      | A''  | 1.3381  |
| 20| vib | 3254.27  | 0.00|      | A'   | 0.0312  |
| 21| vib | 3309.80  | 0.00|      | A'   | 22.5509 |
| 22| vib | 409.32   | 0.00|      | A''  | 5.5343  |
| 23| vib | 426.21   | 0.00|      | A'   | 14.8347 |
| 24| vib | 678.94   | 0.00|      | A''  | 23.3611 |
| 25| vib | 754.95   | 0.00|      | A'   | 2.6062  |
| 26| vib | 818.51   | 0.00|      | A''  | 1.3925  |
| 27| vib | 919.28   | 0.00|      | A'   | 1.0005  |
| 28| vib | 1020.34  | 0.00|      | A'   | 55.0306 |
| 29| vib | 1099.91  | 0.00|      | A''  | 4.6432  |
| 30| vib | 1101.77  | 0.00|      | A'   | 65.3571 |
| 31| vib | 1128.46  | 0.00|      | A''  | 3.3502  |
| 32| vib | 1154.38  | 0.00|      | A'   | 45.1983 |
| 33| vib | 1207.59  | 0.00|      | A''  | 2.2558  |
| 34| vib | 1227.21  | 0.00|      | A'   | 10.6216 |
| 35| vib | 1431.23  | 0.00|      | A'   | 7.2299  |
| 36| vib | 1454.96  | 0.00|      | A''  | 5.0312  |
| 37| vib | 1482.55  | 0.00|      | A'   | 2.8218  |
| 38| vib | 3131.97  | 0.00|      | A''  | 8.3453  |
| 39| vib | 3136.49  | 0.00|      | A'   | 6.4124  |
| 40| vib | 3242.61  | 0.00|      | A''  | 1.3381  |
| 41| vib | 3254.27  | 0.00|      | A'   | 0.0312  |
| 42| vib | 3309.80  | 0.00|      | A'   | 22.5509 |
| 43| rot | 0.5964124|      |      |      |         |
| 44| rot | 0.2490444|      |      |      |         |
| 45| rot | 0.2131933|      |      |      |         |

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**ZPE and THERMAL CONTRIBUTIONS**

- Electronic [kJ/mol] = -549101.877
- Ezpe [kJ/mol] = +193.738
- Electronic+Ezpe [kJ/mol] = -548908.139

- Electronic [hartrees] = -209.141831
- Ezpe [hartrees] = +0.073791

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Electronic+Ezpe [hartrees] = -209.068040

Thermal Correction to Energy [kJ/mol] = +204.059
Thermal Correction to Enthalpy [kJ/mol] = +206.538
Thermal Correction to Gibbs [kJ/mol] = +125.788

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