Supplement of

The role of organic acids in new particle formation from methanesulfonic acid and methylamine

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Selection of Boundary Clusters

In ACDC simulation, the boundary clusters are ones allowed to flux out the simulation box for further growth, therefore, these clusters are required to have favorable compositions for the stability. In the studied MSA-MA-ForA system, the binary (MSA)\(_z\)(MA)\(_z\) (\(z = 1\) - 3) and (MSA)\(_{z+1}\)(MA)\(_z\) (\(z = 1\) - 2) clusters have relatively lower evaporation rates than other binary MSA-MA clusters at all considered temperature conditions (238.15-298.15 K). For ForA-containing clusters, the effective evaporation rates (as described in the main manuscript) of small (MSA)\(_1\)(ForA)\(_1\) and (MSA)\(_1\)(MA)\(_1\)(ForA)\(_1\) cluster are lower than those of corresponding binary MSA-MA clusters. However, effective evaporation rates for clusters with larger size are much higher than those of corresponding binary MSA-MA clusters. Therefore, ForA-containing clusters can not be selected as the boundary clusters and only possibly stable (MSA)\(_4\)(MA)\(_3\) and (MSA)\(_4\)(MA)\(_4\) clusters are chosen as boundary clusters for ACDC simulation in this study.
Table S1. Atmospheric concentrations (molecules cm⁻³) and acid dissociation constants (pKₐ) of organic acids and MSA.

| Organic Acids | Concentration (molecules cm⁻³) | pKₐ₁ | pKₐ₂ |
|---------------|-------------------------------|------|------|
| ForA          | (2.50 × 10⁹-3.75 × 10¹¹)⁹ⁱ⁷      | 3.75⁵⁶ | -    |
| AceA          | (7.50 × 10⁹-4.00 × 10¹¹)⁹ⁱ⁷      | 4.76⁵⁶ | -    |
| GlyA          | (1.00 × 10⁸-7.71 × 10⁶)²⁴      | 3.18⁵⁶ | -    |
| OxaA          | (1.01 × 10⁹-9.61 × 10⁹)²⁴      | 1.25⁵⁶ | 3.81⁵⁶ |
| PyrA          | (9.64 × 10⁶-6.10 × 10⁷)³⁴      | 2.39⁵⁶ | -    |
| MalA          | (5.96 × 10⁷-6.42 × 10⁸)³⁴      | 2.85⁵⁶ | 5.70⁵⁶ |
| MaleA         | (1.35 × 10⁷-1.38 × 10⁸)³⁴      | 1.92⁵⁶ | 6.23⁵⁶ |
| SucA          | (1.07 × 10⁸-9.94 × 10⁸)³⁴      | 4.21⁵⁶ | 5.64⁵⁶ |
| GluA          | (4.11 × 10⁷-2.06 × 10⁸)³⁴      | 4.32⁵⁶ | 5.42⁵⁶ |
| AdiA          | (2.13 × 10⁷-1.35 × 10⁸)³⁴      | 4.41⁵⁶ | 5.41⁵⁶ |
| BenA          | (5.47 × 10⁷-1.05 × 10⁹)⁴¹      | 4.20⁵⁶ | -    |
| PinA          | (3.64 × 10⁷-3.19 × 10⁸)⁵⁶      | 4.72⁵⁶ | -    |
| MSA           | (1.00 × 10⁵-1.00 × 10⁷)⁷⁷      | -1.86⁸⁸ | -    |

[1] (Khwaja, 1995); [2] (Haynes et al., 2016); [3] (Ho et al., 2007); [4] (Ho et al., 2010); [5] (Kavouras et al., 1998); [6] (Kolodziejczyk et al., 2019); [7] (Chen and Finlayson-Pitts, 2017); [8] (NIST Database, 2013).
Table S2. Calculated (effective) evaporation rates of the (MSA)$_x$(MA)$_y$(ForA)$_z$ (0 ≤ $y$ ≤ $x+z$ ≤ 3) clusters at 238.15, 258.15, 278.15 and 298.15 K.

| Clusters | (Effective) Evaporation rates (s$^{-1}$) |
|----------|----------------------------------------|
|          | 298.15 K | 278.15 K | 258.15 K | 238.15 K |
| (MSA)$_1$(MA)$_1$ | 1.67 × 10$^6$ | 2.44 × 10$^5$ | 2.62 × 10$^4$ | 1.94 × 10$^3$ |
| (MA)$_1$(ForA)$_1$ | 1.41 × 10$^6$ | 3.63 × 10$^5$ | 7.52 × 10$^4$ | 1.19 × 10$^4$ |
| (MSA)$_2$(MA)$_1$ | 2.50 × 10$^0$ | 1.26 × 10$^{-1}$ | 4.01 × 10$^{-3}$ | 7.20 × 10$^{-5}$ |
| (MSA)$_1$(MA)$_1$(ForA)$_1$ | 6.29 × 10$^{-1}$ | 5.59 × 10$^{-2}$ | 3.41 × 10$^{-3}$ | 1.29 × 10$^{-4}$ |
| (MA)$_1$(ForA)$_2$ | 8.60 × 10$^6$ | 2.74 × 10$^6$ | 7.38 × 10$^5$ | 1.59 × 10$^5$ |
| (MA)$_1$(MSA)$_3$ | 8.29 × 10$^1$ | 5.79 × 10$^0$ | 2.67 × 10$^{-1}$ | 7.31 × 10$^{-3}$ |
| (MSA)$_2$(MA)$_1$(ForA)$_1$ | 2.80 × 10$^2$ | 3.59 × 10$^1$ | 3.59 × 10$^0$ | 2.09 × 10$^{-1}$ |
| (MSA)$_1$(MA)$_1$(ForA)$_2$ | 1.37 × 10$^2$ | 1.40 × 10$^1$ | 1.00 × 10$^0$ | 4.61 × 10$^{-2}$ |
| (MA)$_1$(ForA)$_3$ | 6.36 × 10$^3$ | 1.02 × 10$^3$ | 1.17 × 10$^2$ | 1.05 × 10$^1$ |
| (MSA)$_2$(MA)$_2$ | 4.33 × 10$^{-1}$ | 2.41 × 10$^{-2}$ | 8.52 × 10$^{-4}$ | 1.72 × 10$^{-5}$ |
| (MSA)$_1$(MA)$_2$(ForA)$_1$ | 4.89 × 10$^5$ | 9.15 × 10$^4$ | 1.32 × 10$^4$ | 1.36 × 10$^3$ |
| (MA)$_2$(ForA)$_2$ | 4.09 × 10$^7$ | 1.43 × 10$^7$ | 4.21 × 10$^6$ | 1.01 × 10$^6$ |
| (MSA)$_3$(MA)$_2$ | 7.67 × 10$^1$ | 4.18 × 10$^0$ | 1.45 × 10$^{-1}$ | 2.84 × 10$^{-3}$ |
| (MSA)$_2$(MA)$_2$(ForA)$_1$ | 3.33 × 10$^3$ | 4.21 × 10$^2$ | 3.86 × 10$^1$ | 2.37 × 10$^0$ |
| (MSA)$_1$(MA)$_2$(ForA)$_2$ | 1.93 × 10$^5$ | 3.67 × 10$^4$ | 5.39 × 10$^3$ | 5.72 × 10$^2$ |
| (MA)$_2$(ForA)$_3$ | 1.40 × 10$^7$ | 3.50 × 10$^6$ | 7.04 × 10$^5$ | 1.78 × 10$^5$ |
| (MSA)$_3$(MA)$_3$ | 9.86 × 10$^0$ | 5.04 × 10$^{-1}$ | 1.62 × 10$^{-2}$ | 2.90 × 10$^{-4}$ |
| (MSA)$_2$(MA)$_3$(ForA)$_1$ | 3.43 × 10$^3$ | 5.10 × 10$^2$ | 5.64 × 10$^1$ | 4.29 × 10$^0$ |
| (MSA)$_1$(MA)$_3$(ForA)$_2$ | 8.11 × 10$^3$ | 1.45 × 10$^3$ | 1.98 × 10$^2$ | 1.92 × 10$^1$ |
| (MA)$_3$(ForA)$_3$ | 3.13 × 10$^6$ | 6.60 × 10$^5$ | 1.09 × 10$^5$ | 1.33 × 10$^4$ |
| (MSA)$_2$ | 6.29 × 10$^4$ | 6.01 × 10$^3$ | 3.97 × 10$^2$ | 1.66 × 10$^1$ |
| (MSA)$_1$(ForA)$_1$ | 2.08 × 10$^3$ | 2.91 × 10$^2$ | 2.99 × 10$^1$ | 2.10 × 10$^0$ |
|        |       |       |       |       |
|--------|-------|-------|-------|-------|
| (ForA)$_2$ | $6.57 \times 10^3$ | $1.11 \times 10^3$ | $1.41 \times 10^2$ | $1.27 \times 10^1$ |
| (MSA)$_3$   | $7.63 \times 10^6$ | $1.10 \times 10^6$ | $1.18 \times 10^5$ | $8.59 \times 10^3$ |
| (MSA)$_2$(ForA)$_1$ | $3.45 \times 10^8$ | $1.30 \times 10^8$ | $4.25 \times 10^7$ | $1.15 \times 10^7$ |
| (MSA)$_1$(ForA)$_2$ | $8.55 \times 10^7$ | $3.08 \times 10^7$ | $9.51 \times 10^6$ | $2.41 \times 10^6$ |
| (ForA)$_3$   | $4.75 \times 10^7$ | $2.33 \times 10^7$ | $1.02 \times 10^7$ | $3.86 \times 10^6$ |
Table S3. The calculated mean concentrations of (SA)\textsubscript{i}(amine)\textsubscript{j}(OAs)\textsubscript{k} based on the mass balance equation, reported concentrations of precursors and energetic data of the (SA)\textsubscript{i}(amine)\textsubscript{j}(OAs)\textsubscript{k} clusters.*

| Clusters | $\Delta G$ (kcal mol\textsuperscript{-1}) (amine=MA) | Concentration (amine=MA) (molecules cm\textsuperscript{-3}) | $\Delta G$ (kcal mol\textsuperscript{-1}) (amine=DMA) | Concentration (amine=DMA) (molecules cm\textsuperscript{-3}) |
|----------|---------------------------------|------------------|---------------------------------|------------------|
| (SA)\textsubscript{i}(amine)\textsubscript{j}(ForA)\textsubscript{k} | -21.00 | $1.98 \times 10^3$ | -22.02 | $1.11 \times 10^4$ |
| (SA)\textsubscript{i}(amine)\textsubscript{j}(AceA)\textsubscript{k} | -18.21 | $1.92 \times 10^1$ | -22.29 | $1.88 \times 10^4$ |
| (SA)\textsubscript{i}(amine)\textsubscript{j}(OxaA)\textsubscript{k} | -18.91 | $1.63 \times 10^0$ | -21.25 | $8.48 \times 10^1$ |
| (SA)\textsubscript{i}(amine)\textsubscript{j}(PyrA)\textsubscript{k} | -16.19 | $1.10 \times 10^{-4}$ | -20.94 | $3.34 \times 10^1$ |
| (SA)\textsubscript{i}(amine)\textsubscript{j}(MalA)\textsubscript{k} | -17.63 | $1.24 \times 10^{-2}$ | -22.12 | $2.43 \times 10^1$ |
| (SA)\textsubscript{i}(amine)\textsubscript{j}(MaleA)\textsubscript{k} | -22.11 | $5.17 \times 10^{-2}$ | -26.50 | $8.57 \times 10^3$ |
| (SA)\textsubscript{i}(amine)\textsubscript{j}(SucA)\textsubscript{k} | -18.00 | $3.63 \times 10^{-2}$ | -22.33 | $5.44 \times 10^1$ |
| (SA)\textsubscript{i}(amine)\textsubscript{j}(GluA)\textsubscript{k} | -21.81 | $5.07 \times 10^{-2}$ | -22.75 | $2.48 \times 10^1$ |
| (SA)\textsubscript{i}(amine)\textsubscript{j}(AdiA)\textsubscript{k} | -21.17 | $1.09 \times 10^{-2}$ | -23.02 | $2.48 \times 10^1$ |
| (SA)\textsubscript{i}(amine)\textsubscript{j}(BenA)\textsubscript{k} | -18.74 | $1.27 \times 10^{-1}$ | -20.65 | $3.19 \times 10^0$ |
| (SA)\textsubscript{i}(amine)\textsubscript{j}(PinA)\textsubscript{k} | -18.15 | $1.51 \times 10^{-2}$ | -22.44 | $2.12 \times 10^1$ |

*Binding free energy ($\Delta G$) (kcal mol\textsuperscript{-1}) of (SA)\textsubscript{i}(amine)\textsubscript{j}(OAs)\textsubscript{k} was calculated by the equation: $\Delta G = \Delta G_{R1} + \Delta G_{R2}$, $R1$ presents the reaction $SA + amine \rightarrow (SA)\textsubscript{i}(amine)\textsubscript{j}$ and $R2$ for reaction $(SA)\textsubscript{i}(amine)\textsubscript{j} + OA \rightarrow (SA)\textsubscript{i}(amine)\textsubscript{j}(OA)\textsubscript{k}$. (Li et al., 2020). Concentrations of precursors are from Table S1. [amine] and [SA] were set to be $2.5 \times 10^8$ molecules cm\textsuperscript{-3} (~10ppt) and $10^7$ molecules cm\textsuperscript{-3} in the calculations, respectively.
Figure S1. Lowest Gibbs free energy conformations of MaleA and (MSA)_{1}(MA)_{1}(MaleA)_{1} cluster at the ωB97X-D/6-31++G(d,p) level of theory. The red balls represent oxygen atoms, blue ones for nitrogen atoms, gray ones for carbon atoms, and white ones for hydrogen atoms.
Figure S2. Lowest Gibbs free energy conformations of the organic acid monomers at the oB97X-D/6-31++G(d,p) level of theory. The red balls represent oxygen atoms, blue ones for nitrogen atoms, gray ones for carbon atoms, and white ones for hydrogen atoms. Dashed red lines indicate hydrogen bonds.
Figure S3. Lowest Gibbs free energy conformations of ForA-containing clusters at the ωB97X-D/6-31++G(d,p) level of theory. The red balls represent oxygen atoms, blue ones for nitrogen atoms, gray ones for carbon atoms, and white ones for hydrogen atoms. Dashed red lines indicate hydrogen bonds.
Figure S4. Formation free energy (ΔG) (kcal mol⁻¹) of (MSA)ₓ(MA)ᵧ(ForA)ₓ (0 ≤ y ≤ x+² ≤ 3) clusters calculated at the DLPNO-CCSD(T)/aug-cc-pVTZ//ωB97X-D/6-31++G(d,p) level of theory, at 298.15 K and 1 atm. a) without ForA monomer, b) containing 1 ForA monomer, c) containing 2 ForA monomers, and d) containing 3 ForA monomers.
Figure S5. Variation of the enhancing coefficient ($R$) with coagulation sink coefficient ($s^{-1}$) at $[\text{MA}] = 10$ ppt, $[\text{MSA}] = 10^7$ cm$^{-3}$, $[\text{ForA}] = 10^{11}$ cm$^{-3}$ and $T = 258.15$ K.
Figure S6. Main cluster formation pathways for the ternary MA-MSA-ForA system at two different [MA] (1 ppt (a) and 100 ppt (b)), $T = 258.15$ K, [MSA] = $10^7$ cm$^{-3}$, and [ForA] = $10^{11}$ cm$^{-3}$.
Figure S7. Main cluster formation pathways for the ternary MA-MSA-ForA system at two different [MSA] (10^5 cm\(^{-3}\) (a) and 10^8 cm\(^{-3}\) (b)), \(T = 258.15\) K, [MA] = 10 ppt, and [ForA] = 10^{11} cm\(^{-3}\).
Figure S8. Main cluster formation pathways for the ternary MA-MSA-ForA system at two different coagulation sink coefficients ($2 \times 10^{-4}$ s$^{-1}$ (a) and $2 \times 10^{-3}$ s$^{-1}$ (b)), $T = 258.15$ K, $[\text{MA}] = 10$ ppt, $[\text{MSA}] = 10^7$ cm$^{-3}$ and $[\text{ForA}] = 10^{11}$ cm$^{-3}$.
### Coordinates of all optimized organic acids and clusters

#### ForA

|   |          |          |               |
|---|----------|----------|---------------|
|   | C        | O        | H             |
| O | 1.113654 | -0.091447| 0.000001      |
| C | -0.131480| 0.401285 | 0.000000      |
| O | -1.133493| -0.264478| 0.000000      |
| H | 1.050917 | -1.058312| -0.000003     |
| H | -0.103328| 1.498008 | -0.000001     |

#### AceA

|   |          |          |               |
|---|----------|----------|---------------|
|   | C        | O        | H             |
| C | 1.055277 | -0.917024| 0.000000      |
| C | 0.000000 | 0.151467 | 0.000000      |
| O | 0.196381 | 1.344113 | 0.000000      |
| H | 2.040634 | -0.454362| 0.000000      |
| H | 0.937609 | -1.552060| 0.881829      |
| H | 0.937609 | -1.552060| -0.881829     |
| O | -1.244280| -0.371530| 0.000000      |
| H | -1.864320| 0.371157 | 0.000000      |

#### GlyA

|   |          |          |               |
|---|----------|----------|---------------|
|   | C        | O        | H             |
| C | -0.746216| -0.761242| 0.000000      |
| C | 0.000000 | 0.579543 | 0.000000      |
| O | 1.323966 | 0.459917 | 0.000000      |
| O | -0.591134| 1.626184 | 0.000000      |
| O | -0.136040| -1.802595| 0.000000      |
| H | -1.845623| -0.691929| 0.000000      |
| H | 1.548590 | -0.485932| 0.000000      |

#### OxaA

|   |          |          |               |
|---|----------|----------|---------------|
|   | C        | O        | H             |
| C | 0.754712 | 0.164430 | 0.000111      |
| C | -0.754717| -0.164438| 0.000075      |
| O | -1.529126| 0.902788 | -0.000162     |
| O | 1.529139 | -0.902775| -0.000162     |
| H | -0.957238| 1.690766 | -0.000218     |
| H | 0.957292 | -1.690791| -0.000228     |
| O | 1.139986 | 1.306770 | 0.000114      |
| O | -1.140002| -1.306774| 0.000127      |

#### PyrA

|   |          |          |               |
|---|----------|----------|---------------|
| C | 0.767813 | -0.279635| 0.000019      |
| C      | 1.008278 | -1.458435 | 0.000056 |
|--------|----------|-----------|----------|
| O      | -1.693077| 0.673528  | 0.00008  |
| H      | 1.229743 | 1.530264  | -0.00024 |
| C      | -0.677199| 0.280943  | -0.00020 |
| C      | -1.793986| -0.709227 | -0.00006 |
| H      | -2.751467| -0.189685 | -0.00062 |
| H      | -1.706445| -1.360020 | -0.87531 |
| H      | -1.706501| -1.359927 | 0.875377 |
| O      | -0.806993| 1.488268  | -0.00056 |

**MalA**

| C      | 0.000279 | -0.023685 | 0.959207 |
|--------|----------|-----------|----------|
| C      | 1.268432 | 0.033674  | 0.134554 |
| C      | -1.268353| -0.040237 | 0.133528 |
| O      | 1.217344 | 1.013785  | -0.78364 |
| O      | 2.230493 | -0.675810 | 0.292731 |
| O      | -1.219242| -0.976417 | -0.82954 |
| O      | -2.228795| 0.663313  | 0.324582 |
| H      | 0.042990 | -0.927835 | 1.570040 |
| H      | -0.041702| 0.848483  | 1.614903 |
| H      | 2.054870 | 1.004334  | -1.26873 |
| H      | -2.056703| -0.942459 | -1.31328 |

**MaleA**

| C      | 1.558612 | 0.056128  | -0.000185 |
|--------|----------|-----------|----------|
| O      | 1.252519 | 1.238358  | 0.000001 |
| O      | 2.834226 | -0.333031 | -0.000138 |
| H      | 3.389080 | 0.460593  | -0.000132 |
| C      | 0.639117 | -1.100777 | 0.000085 |
| H      | 1.141080 | -2.062929 | 0.000215 |
| C      | -0.701849| -1.088279 | 0.000197 |
| H      | -1.197425| -2.054438 | 0.000419 |
| C      | -1.737644| 0.013262  | -0.000027 |
| O      | -2.901702| -0.317275 | 0.000164 |
| O      | -1.371213| 1.284454  | -0.000104 |
| H      | -0.392790| 1.394721  | -0.000298 |

**SucA**

| C      | 1.922376 | -0.101722 | -0.000013 |
|--------|----------|-----------|----------|
| O      | 2.162315 | -1.287411 | -0.000114 |
|   |   |   |
|---|---|---|
| O | 2.893452 | 0.830879 |
| H | 3.740410 | 0.363163 |
| C | 0.552009 | 0.522705 |
| H | 0.474301 | 1.181835 |
| H | 0.474291 | 1.181955 |
| C | -0.552009 | -0.522705 |
| H | -0.474295 | -1.181840 |
| H | -0.474297 | -1.181950 |
| C | -1.922376 | 0.101722 |
| O | -2.162315 | 1.287411 |
| O | -2.893452 | -0.830879 |
| H | -3.740410 | -0.363163 |

### GluA

|   |   |   |
|---|---|---|
| C | -1.017098 | -0.784553 |
| C | 0.000003 | -0.001322 |
| C | 1.017025 | 0.783436 |
| C | 1.955695 | -0.085230 |
| H | 0.520544 | 1.479046 |
| H | -1.641170 | -1.407371 |
| H | -0.520649 | -1.479044 |
| H | -0.528923 | 0.704235 |
| O | 2.767814 | 0.647692 |
| C | -1.955689 | 0.085541 |
| O | -2.018834 | 1.294254 |
| O | -2.767800 | -0.645926 |
| H | 3.346786 | 0.029006 |
| H | 1.641033 | 1.405233 |
| H | -3.346752 | -0.026404 |
| H | 0.529013 | -0.708061 |
| O | 2.018882 | -1.294004 |

### AdiA

|   |   |   |
|---|---|---|
| C | -0.714848 | 1.296432 |
| C | 0.368757 | 0.254083 |
| C | 1.721658 | 0.683007 |
| C | -2.085803 | 0.884131 |
| C | 2.828058 | -0.292482 |
| C | -2.709709 | -0.253714 |
| O | 3.987298 | 0.061944 |
|       |       |       |
|-------|-------|-------|
| O     | 2.737188 | -1.277367 | -0.766851 |
| O     | -3.759099 | -0.786924 | -0.454469 |
| O     | -2.359810 | -0.652667 | 1.287912  |
| H     | -0.789142 | 1.477289  | 1.037782  |
| H     | -0.437288 | 2.248605  | -0.508065 |
| H     | 0.085575  | -0.704319 | 0.127632  |
| H     | 0.457898  | 0.085720  | -1.397387 |
| H     | 1.680935  | 0.812101  | -1.324952 |
| H     | 2.027306  | 1.656160  | -0.168100 |
| H     | -2.041397 | 0.602592  | -1.627249 |
| H     | -2.794887 | 1.718849  | -0.509068 |
| H     | 4.647136  | -0.600668 | 0.273555  |
| H     | -4.122959 | -1.484953 | 0.108816  |

**BenA**

|       |       |       |
|-------|-------|-------|
| C     | -0.217545 | 0.029809 | 0.000005 |
| C     | 2.564772  | -0.043411 | -0.000003 |
| C     | 0.512148  | 1.221527  | 0.000093 |
| C     | 0.446946  | -1.199814 | -0.000084 |
| C     | 1.837935  | -1.232805 | -0.000099 |
| C     | 1.901776  | 1.183270  | 0.000097 |
| C     | -1.701749 | 0.119638  | -0.000020 |
| O     | -2.308412 | -1.084734 | 0.000227 |
| H     | 3.260368  | -0.916164 | 0.000068 |
| H     | -0.023426 | 2.164855  | 0.000151 |
| H     | 2.467595  | 2.109251  | 0.000176 |
| H     | 3.650077  | -0.072706 | -0.000008 |
| H     | 2.354962  | -2.186858 | -0.000185 |
| H     | 0.124149  | -2.121220 | -0.000149 |
| O     | -2.332883 | 1.153929  | -0.000225 |

**PinA**

|       |       |       |
|-------|-------|-------|
| O     | -2.957415 | -1.438942 | 0.687771 |
| O     | 2.978084  | 1.098032  | -0.281856 |
| O     | 3.970771  | -0.643755 | 0.713927 |
| C     | 0.592799  | -0.408779 | -0.835215 |
| C     | -0.331045 | 0.596522  | -0.070653 |
| C     | -1.549224 | -0.148150 | -0.746416 |
| C     | -0.622947 | -1.331880 | -1.059223 |
| C     | -0.294853 | 0.416642  | 1.446667 |
| C       | -0.175599 | 2.065047 | -0.441196 |
|---------|-----------|----------|-----------|
| C       | -2.769288 | -0.385445 | 0.109942  |
| C       | -3.731554 | 0.773832 | 0.238571  |
| C       | 1.806462  | -1.024115 | -0.160875 |
| C       | 2.942802  | -0.061164 | 0.063763  |
| H       | 0.903679  | 0.053118 | -1.778535 |
| H       | -1.842401 | 0.399583 | -1.649941 |
| H       | -0.727283 | -1.803877 | -2.038889 |
| H       | -0.713805 | -2.099959 | -0.284788 |
| H       | 0.668424  | 0.752937 | 1.845146  |
| H       | -1.073896 | 1.019517 | 1.926301  |
| H       | -0.454208 | -0.622589 | 1.749833  |
| H       | -0.984324 | 2.665449 | -0.007165 |
| H       | -0.197914 | 2.201169 | -1.527527 |
| H       | 0.779564  | 2.453166 | -0.076692 |
| H       | -4.477755 | 0.563807 | 1.005424  |
| H       | -3.190538 | 1.695646 | 0.478498  |
| H       | -4.231681 | 0.939161 | -0.722393 |
| H       | 2.194306  | -1.849644 | -0.770859 |
| H       | 1.550130  | -1.472025 | 0.805652  |
| H       | 4.660865  | 0.026797 | 0.814971  |

(MSA)\textsubscript{1}(MA)\textsubscript{1}(ForA)\textsubscript{1}

| N | 1.139107 | 1.719249 | 0.000203 |
| H | 0.486508 | 1.629418 | -0.800794 |
| H | 1.706188 | 0.845109 | -0.000211 |
| C | 1.959672 | 2.943036 | -0.000008 |
| H | 2.588597 | 2.954246 | -0.889954 |
| H | 1.307824 | 3.816561 | 0.000728  |
| H | 2.589943 | 2.953705 | 0.888990  |
| S | -1.463822 | -0.040312 | -0.000059 |
| O | -0.980346 | -1.447880 | -0.001385 |
| O | -1.076705 | 0.700946 | -1.230781 |
| O | -1.075784 | 0.698949 | 1.231565  |
| H | 0.487372 | 1.629115 | 0.801811  |
| C | -3.240262 | -0.158332 | 0.000462  |
| H | -3.542310 | -0.697548 | -0.897325 |
| H | -3.541669 | -0.699047 | 0.897565  |
| H | -3.647806 | 0.852585 | 0.001463  |
| C | 2.444384 | -1.853859 | 0.000114  |
|     | (MSA)₁(MA)₁(AceA)₁ |     |     |     |
|-----|-------------------|-----|-----|-----|
|     |                   |     |     |     |
| N   | 0.012601          | 2.096751 | 0.009713 |
| H   | -0.591836         | 1.776897 | -0.771126 |
| H   | 0.866069          | 1.495982 | -0.025672 |
| C   | 0.318973          | 3.537516 | 0.006008 |
| H   | 0.860761          | 3.786724 | -0.906113 |
| H   | -0.610051         | 4.105987 | 0.048333 |
| H   | 0.936951          | 3.777321 | 0.871064 |
| S   | -1.720226         | -0.511519 | -0.000902 |
| O   | -0.714199         | -1.602743 | -0.091697 |
| O   | -1.721303         | 0.370129 | -1.200376 |
| O   | -1.604818         | 0.273691 | 1.257816 |
| H   | -0.525466         | 1.766838 | 0.830808 |
| C   | -3.301652         | -1.329389 | 0.038761 |
| H   | -3.410536         | -1.896399 | -0.885719 |
| H   | -3.318076         | -1.991737 | 0.904241 |
| H   | -4.075547         | -0.565991 | 0.118333 |
| C   | 4.101790          | -0.993169 | 0.037596 |
| C   | 2.636737          | -0.655382 | -0.015780 |
| O   | 2.235381          | 0.507387 | -0.047757 |
| O   | 1.869854          | -1.712373 | -0.014388 |
| H   | 4.349279          | -1.700141 | -0.757482 |
| H   | 4.698316          | -0.087285 | -0.057616 |
| H   | 4.319982          | -1.483504 | 0.990357 |
| H   | 0.881155          | -1.523843 | -0.041254 |

(MSA)₁(MA)₁(GlyA)₁

|     | (MSA)₁(MA)₁(GlyA)₁ |     |     |     |
|-----|-------------------|-----|-----|-----|
| N   | 0.335474          | 2.165995 | 0.007774 |
| H   | 0.912236          | 1.807009 | -0.776533 |
| H   | 0.855186          | 1.801867 | 0.826247 |
| C   | 0.115221          | 3.623520 | 0.005352 |
| H   | 1.077229          | 4.133908 | 0.044203 |
| H   | -0.414474         | 3.904787 | -0.904332 |
| H   | -0.483310         | 3.898720 | 0.873379 |
| S   | 1.942431          | -0.557970 | -0.000876 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| O | 0.953178 | -1.671244 | -0.073122 |
| O | 1.821887 | 0.235698 | 1.250357 |
| O | 1.920191 | 0.307981 | -1.209471 |
| H | -0.544569 | 1.615340 | -0.022892 |
| C | 3.530032 | -1.361419 | 0.036114 |
| H | 3.636449 | -1.939021 | -0.882014 |
| H | 4.297457 | -0.590094 | 0.099713 |
| H | 3.559183 | -2.012153 | 0.909971 |
| C | -3.788756 | -0.956059 | 0.019572 |
| C | -2.284178 | -0.627856 | -0.013448 |
| O | -1.577460 | -1.716648 | -0.005364 |
| O | -1.887697 | 0.525984 | -0.042288 |
| O | -4.625754 | -0.094686 | 0.015911 |
| H | -4.028954 | -2.034279 | 0.047411 |
| H | -0.562322 | -1.586325 | -0.029277 |

(MSA)₁(MA)₁(OxaA)₁

|   |   |   |   |   |
|---|---|---|---|
| C | -2.029621 | -0.359488 | -0.077176 |
| C | -3.570145 | -0.501405 | 0.040959 |
| O | -4.185530 | 0.678117 | -0.063029 |
| O | -1.397919 | -1.468410 | -0.016511 |
| H | -3.499967 | 1.354353 | -0.192477 |
| H | -0.372953 | -1.416629 | -0.124422 |
| O | -1.570243 | 0.779183 | -0.215126 |
| O | -4.135086 | -1.542727 | 0.207837 |
| N | 0.842192 | 2.170479 | 0.059739 |
| H | 1.231980 | 1.738706 | 0.914932 |
| H | -0.074556 | 1.706571 | -0.084393 |
| C | 0.755770 | 3.641962 | 0.088891 |
| H | 0.097633 | 3.950481 | 0.900879 |
| H | 1.750283 | 4.059339 | 0.243841 |
| H | 0.354773 | 3.997223 | -0.860076 |
| S | 2.184088 | -0.664715 | -0.009839 |
| O | 1.083356 | -1.619610 | -0.332454 |
| O | 1.982736 | 0.011860 | 1.297072 |
| O | 2.427034 | 0.312121 | -1.106161 |
| H | 1.474695 | 1.779601 | -0.670352 |
| C | 3.644168 | -1.671695 | 0.116891 |
| H | 3.795249 | -2.164971 | -0.843079 |
| H | 4.484026 | -1.019399 | 0.355929 |
|    | (MSA)$_1$(MA)$_1$(PyrA)$_1$ |                   |                   |                   |
|----|---------------------------|-------------------|-------------------|-------------------|
|    | C                         | -2.039879         | -0.128253         | 0.013331          |
|    | C                         | -3.594756         | -0.149546         | 0.018471          |
|    | C                         | -4.271478         | -1.484849         | -0.112197         |
|    | O                         | -4.178928         | 0.900938          | 0.123406          |
|    | O                         | -1.437686         | 0.932702          | 0.014151          |
|    | O                         | -1.523819         | -1.322260         | 0.008699          |
|    | H                         | -3.960853         | -1.972889         | -1.041037         |
|    | H                         | -5.352134         | -1.343435         | -0.099715         |
|    | H                         | -3.961729         | -2.145296         | 0.702939          |
|    | H                         | -0.504363         | -1.353111         | 0.011191          |
|    | N                         | 1.011649          | 2.191511          | -0.012881         |
|    | H                         | 1.497493          | 1.769085          | 0.798201          |
|    | H                         | 0.052943          | 1.791482          | 0.003023          |
|    | C                         | 1.032059          | 3.664380          | -0.057588         |
|    | H                         | 0.532043          | 4.058857          | 0.826476          |
|    | H                         | 2.064836          | 4.011651          | -0.082294         |
|    | H                         | 0.508814          | 4.003427          | -0.951170         |
|    | S                         | 2.149817          | -0.758273         | 0.008386          |
|    | O                         | 0.992094          | -1.696359         | 0.016915          |
|    | O                         | 2.220425          | 0.080067          | 1.233782          |
|    | O                         | 2.211587          | 0.065163          | -1.229101         |
|    | H                         | 1.489642          | 1.720358          | -0.804401         |
|    | C                         | 3.589933          | -1.805067         | 0.008555          |
|    | H                         | 3.562231          | -2.417184         | 0.910056          |
|    | H                         | 3.555591          | -2.428280         | -0.885048         |
|    | H                         | 4.472206          | -1.164891         | 0.001516          |

|    | (MSA)$_1$(MA)$_1$(MalA)$_1$ |                   |                   |                   |
|----|---------------------------|-------------------|-------------------|-------------------|
|    | C                         | -2.970744         | -1.368828         | -0.263544         |
|    | C                         | -3.949160         | -0.227602         | -0.140017         |
|    | C                         | -1.546277         | -0.915908         | 0.003575          |
|    | O                         | -4.389693         | -0.078006         | 1.120860          |
|    | O                         | -4.310334         | 0.477609          | -1.050989         |
|    | O                         | -0.699751         | -1.898538         | -0.081194         |
|    | O                         | -1.275792         | 0.253065          | 0.258422          |
|    | H                         | -3.214341         | -2.173063         | 0.434831          |
|    | H                         | -3.015803         | -1.767492         | -1.279453         |
|   |   |   |   |
|---|---|---|---|
| H | -4.986029 | 0.683801 | 1.129336 |
| H | 0.269143  | -1.645164 | 0.097120  |
| N | 0.746601  | 2.090902  | -0.016726 |
| H | -0.034449 | 1.420935  | 0.142403  |
| H | 1.203209  | 1.765959  | -0.884467 |
| C | 0.303849  | 3.496552  | -0.033007 |
| H | -0.440093 | 3.630367  | -0.818044 |
| H | -0.140267 | 3.741090  | 0.931486  |
| H | 1.159375  | 4.145503  | -0.218968 |
| S | 2.665388  | -0.395826 | 0.022741  |
| O | 2.297338  | 0.212720  | -1.282387 |
| O | 1.785008  | -1.541925 | 0.386346  |
| O | 2.752714  | 0.623808  | 1.103221  |
| H | 1.467775  | 1.863363  | 0.696918  |
| C | 4.292424  | -1.095742 | -0.156930 |
| H | 4.981105  | -0.292967 | -0.420042 |
| H | 4.570488  | -1.550193 | 0.793908  |
| H | 4.250995  | -1.845925 | -0.946509 |

(MSA)$_1$(MA)$_1$(MaleA)$_1$

|   |   |   |   |
|---|---|---|---|
| N | 0.826939 | 2.546133 | -0.478341 |
| H | 1.242735 | 3.455997 | -0.293528 |
| H | 0.221895 | 2.283963 | 0.326471  |
| C | 0.007315 | 2.545871 | -1.714960 |
| H | -0.778981| 3.295295 | -1.629736 |
| H | 0.648469 | 2.755088 | -2.570869 |
| H | -0.440945| 1.557239 | -1.815716 |
| S | 2.129851 | -0.562199| 0.081139  |
| O | 1.294486 | -1.543776| -0.639644 |
| O | 1.498094 | -0.026096| 1.324520  |
| O | 2.592906 | 0.566354 | -0.783348 |
| H | 1.596696 | 1.820804 | -0.558817 |
| C | 3.595277 | -1.430562| 0.593774  |
| H | 3.286171 | -2.255722| 1.235451  |
| H | 4.093658 | -1.803391| -0.300924 |
| H | 4.234286 | -0.734395| 1.136567  |
| C | -3.107920| 0.367122 | 0.813536  |
| C | -3.346967 | -0.535774| -0.140096 |
| C | -1.721505| 0.719902 | 1.246934  |
| C | -2.268039| -1.325904| -0.809727 |
|   |   |   |   |
|---|---|---|---|
|   | -1.059731 | -0.279882 | 1.767623 |
| O | -1.286160 | 1.859633  | 1.106437 |
| O | -1.166517 | -0.599050 | -1.031739|
| O | -2.400034 | -2.489414 | -1.106403|
| H | -3.917732 | 0.918222  | 1.281692 |
| H | -4.362262 | -0.782991 | -0.431515|
| H | -0.070682 | -0.126856 | 1.735890 |
| H | -0.352821 | -1.157090 | -1.101136|

(MSA)$_1$(MA)$_1$(SucA)$_1$

|   |   |   |   |
|---|---|---|---|
| N | 1.494872 | 2.100632 | 0.033998 |
| H | 1.990533 | 1.748692 | 0.871889 |
| H | 0.641504 | 1.507389 | -0.051655|
| C | 1.200801 | 3.544060 | 0.045673 |
| H | 0.543242 | 3.772804 | 0.884142 |
| H | 2.131673 | 4.102096 | 0.145034 |
| H | 0.706984 | 3.816969 | -0.886629|
| S | 3.209223 | -0.518273 | 0.005963 |
| O | 2.208576 | -1.600972 | -0.188092|
| O | 3.025200 | 0.210740 | 1.289764 |
| O | 3.275119 | 0.416248 | -1.151745|
| H | 2.134523 | 1.790620 | -0.724229|
| C | 4.785707 | -1.341111 | 0.092105 |
| H | 4.942216 | -1.866774 | -0.849806|
| H | 5.554557 | -0.583882 | 0.245693 |
| H | 4.756999 | -2.041537 | 0.926661 |
| C | -4.954837 | -0.138784 | 0.033940 |
| O | -5.409715 | -1.249211 | 0.181119 |
| O | -5.738268 | 0.955719  | -0.045023|
| H | -6.654845 | 0.656311  | 0.035067 |
| C | -3.495555 | 0.214835  | -0.082144|
| H | -3.350303 | 0.749708  | -1.026222|
| H | -3.256668 | 0.938362  | 0.703501 |
| C | -2.596095 | -1.007465 | 0.002723 |
| H | -2.763394 | -1.553628 | 0.936658 |
| H | -2.819354 | -1.723628 | -0.793356|
| C | -1.128263 | -0.661299 | -0.069421|
| O | -0.364183 | -1.717073 | -0.062314|
| H | 0.626570  | -1.531362 | -0.104486|
| O | -0.730037 | 0.502597  | -0.121573|
### (MSA)$_1$(MA)$_1$(GluA)$_1$

| Atom | x  | y  | z   |
|------|----|----|-----|
| C    | 1.987775 | -1.073292 | 1.309092 |
| C    | 3.004035 | -1.531008 | 0.257885 |
| C    | 2.808115 | -0.897877 | -1.135634 |
| C    | 1.354154 | -0.740581 | -1.502142 |
| H    | 3.256150 | 0.095611  | -1.169739 |
| H    | 2.287361 | -1.444426 | 2.296655  |
| H    | 1.004745 | -1.508121 | 1.106070  |
| H    | 4.019518 | -1.298248 | 0.588913  |
| O    | 0.666342 | -1.861175 | -1.489992 |
| C    | 1.858519 | 0.431567  | 1.437965  |
| O    | 2.758879 | 1.215534  | 1.234142  |
| O    | 0.652227 | 0.888992  | 1.813660  |
| H    | -0.311743 | -1.660563 | -1.492855 |
| H    | 3.294323 | -1.524121 | -1.890623 |
| H    | -0.066251 | 0.204966  | 1.721548  |
| H    | 2.921945 | -2.618567 | 0.180445  |
| O    | 0.844799 | 0.348553  | -1.747252 |
| N    | -0.238999 | 2.430624  | -0.363505 |
| H    | 0.204694 | 2.410088  | 0.561304  |
| H    | -1.148590 | 1.909112  | -0.263921 |
| C    | -0.409991 | 3.787649  | -0.915732 |
| H    | -1.043017 | 4.372720  | -0.249076 |
| H    | 0.563739  | 4.266587  | -1.016738 |
| H    | -0.885563 | 3.709446  | -1.892858 |
| S    | -2.234065 | -0.568863 | 0.148922  |
| O    | -1.905350 | -1.320825 | -1.084085 |
| O    | -2.445555 | 0.888247  | -0.079897 |
| O    | -1.265505 | -0.822881 | 1.255077  |
| H    | 0.337999  | 1.820805  | -0.970289 |
| C    | -3.799106 | -1.203606 | 0.712641  |
| H    | -4.535400 | -1.031623 | -0.072465 |
| H    | -3.677448 | -2.270048 | 0.902030  |
| H    | -4.072148 | -0.674858 | 1.625710  |

### (MSA)$_1$(MA)$_1$(AdiA)$_1$

| Atom | x  | y  | z   |
|------|----|----|-----|
| N    | -0.638022 | -1.579531 | 0.795203 |
| H    | -0.370559 | -0.599384 | 1.015831 |
| H    | -0.914074 | -1.555377 | -0.202230 |
|   |   |   |
|---|---|---|
| C | 0.416431 | -2.558542 | 1.123315 |
| H | 1.323171 | -2.315888 | 0.566979 |
| H | 0.618179 | -2.517349 | 2.193802 |
| H | 0.074018 | -3.557965 | 0.854872 |
| S | -3.381550 | -0.403244 | -0.229968 |
| O | -2.347749 | -0.835457 | -1.210784 |
| O | -3.323175 | 1.059165 | 0.046595 |
| O | -3.351162 | -1.230356 | 1.004949 |
| H | -1.550856 | -1.733047 | 1.260241 |
| C | -4.969269 | -0.679438 | -0.989395 |
| H | -5.012754 | -0.091079 | -1.905936 |
| H | -5.062177 | -1.743609 | -1.206225 |
| H | -5.738622 | -0.358590 | -0.287021 |
| C | 2.465321 | 2.242176 | 0.398265 |
| C | 2.771820 | 0.950255 | -0.360326 |
| C | 4.090615 | 0.316554 | 0.082459 |
| C | 1.141203 | 2.878824 | -0.016166 |
| C | 4.245850 | -1.101580 | -0.403458 |
| C | -0.070564 | 2.034621 | 0.318288 |
| O | 5.515782 | -1.408430 | -0.715290 |
| O | 3.351023 | -1.916628 | -0.488337 |
| O | -1.156477 | 2.438342 | -0.281866 |
| O | -0.011947 | 1.078195 | 1.089742 |
| H | 2.439017 | 2.030999 | 1.473317 |
| H | 3.269132 | 2.969689 | 0.23270 |
| H | 1.966113 | 0.231136 | -0.194499 |
| H | 2.806100 | 1.148210 | -1.438863 |
| H | 4.124260 | 0.262617 | 1.179204 |
| H | 4.956251 | 0.905656 | -0.231122 |
| H | 1.114693 | 3.092496 | -1.08998 |
| H | 1.002123 | 3.843421 | 0.486015 |
| H | 5.531443 | -2.338703 | -0.983037 |
| H | -1.963298 | 1.859518 | -0.089514 |

(MSA)_1(MA)_1(BenA)_1

|   |   |   |
|---|---|---|
| C | -2.737301 | -0.175483 | -0.040216 |
| C | -5.518865 | -0.251643 | 0.079604 |
| C | -3.398304 | -1.402730 | 0.059051 |
| C | -3.471830 | 1.012022 | -0.081161 |
| C | -4.860565 | 0.973264 | -0.022199 |
|   |     |     |     |
|---|-----|-----|-----|
| C | -4.787775 | -1.437747 | 0.119724 |
| C | -1.248412 | -0.106555 | -0.099152 |
| O | -0.663168 | -1.272520 | -0.066539 |
| H | 0.343569  | -1.251323 | -0.117337 |
| H | -2.819803 | -2.318906 | 0.089095  |
| H | -5.300023 | -2.391017 | 0.199640  |
| H | -6.603083 | -0.281898 | 0.128405  |
| H | -5.429460 | 1.896959  | -0.054761 |
| H | -2.942386 | 1.955235  | -0.160581 |
| O | -0.659595 | 0.974543  | -0.169343 |
| N | 1.805096  | 2.122724  | 0.051858  |
| H | 0.865978  | 1.677242  | -0.057673 |
| H | 2.398826  | 1.733750  | -0.705978 |
| C | 1.737484  | 3.593299  | 0.096416  |
| H | 1.304442  | 3.961216  | -0.833510 |
| H | 1.109330  | 3.899206  | 0.932893  |
| H | 2.740165  | 4.002191  | 0.220965  |
| S | 3.068905  | -0.732954 | 0.001651  |
| O | 3.009699  | -0.004974 | 1.297530  |
| O | 3.319414  | 0.191408  | -1.138224 |
| O | 1.884632  | -1.606296 | -0.219163 |
| H | 2.226369  | 1.681048  | 0.887694  |
| C | 4.462348  | -1.838664 | 0.081289  |
| H | 4.292191  | -2.538620 | 0.899368  |
| H | 4.528914  | -2.364799 | -0.870939 |
| H | 5.358262  | -1.243955 | 0.259079  |

(MSA)\(_1\)(MA)\(_1\)(PinA)\(_1\)

|   |     |     |     |
|---|-----|-----|-----|
| O | 1.786498 | 2.417461 | -0.196248 |
| O | -0.337581 | -0.984749 | -1.727560 |
| O | -0.757591 | -2.526650 | -0.152798 |
| C | 2.550771  | -1.476936 | -0.758573 |
| C | 2.676646  | -0.761986 | 0.627381  |
| C | 3.212405  | 0.492830  | -0.177496 |
| C | 2.626858  | -0.107092 | -1.464632 |
| C | 1.349413  | -0.498457 | 1.337125  |
| C | 3.671861  | -1.391646 | 1.594050  |
| C | 2.746071  | 1.840652  | 0.296299  |
| C | 3.501067  | 2.450261  | 1.449065  |
| C | 1.425228  | -2.474436 | -1.057273 |
|  |  |  |  |
|---|---|---|---|
| C | 0.018422 | -1.915863 | -1.010054 |
| H | 3.490692 | -2.014714 | -0.932928 |
| H | 4.308606 | 0.477550 | -0.170773 |
| H | 3.241641 | -0.043480 | -2.365370 |
| H | 1.638986 | 0.295421 | -1.684256 |
| H | 0.910115 | -1.433772 | 1.694026 |
| H | 1.499077 | 0.147064 | 2.209825 |
| H | 0.602946 | -0.014344 | 0.704104 |
| H | 3.836640 | -0.752146 | 2.469008 |
| H | 4.640377 | -1.568329 | 1.114355 |
| H | 3.291423 | -2.352842 | 1.957637 |
| H | 2.980425 | 3.330658 | 1.825761 |
| H | 3.625181 | 1.711826 | 2.248270 |
| H | 4.506603 | 2.731234 | 1.116579 |
| H | 1.493354 | -3.323427 | -0.372042 |
| H | 1.573279 | -2.854750 | -2.074575 |
| H | -1.666254 | -2.089719 | -0.061947 |
| N | -0.848775 | 1.676494 | -1.075077 |
| H | -0.802422 | 0.759745 | -1.547754 |
| H | 0.116358 | 1.980936 | -0.885801 |
| C | -1.623698 | 2.669993 | -1.848020 |
| H | -2.637977 | 2.286637 | -1.955445 |
| H | -1.637758 | 3.611879 | -1.299647 |
| H | -1.156691 | 2.817511 | -2.822125 |
| S | -3.272873 | -0.032308 | 0.525282 |
| O | -3.069503 | -1.495118 | 0.335564 |
| O | -3.762396 | 0.670226 | -0.673591 |
| O | -2.057775 | 0.629195 | 1.102517 |
| H | -1.313403 | 1.446686 | -0.158484 |
| C | -4.538961 | 0.100984 | 1.774993 |
| H | -4.184046 | -0.395208 | 2.678227 |
| H | -4.722085 | 1.159589 | 1.959746 |
| H | -5.437375 | -0.385278 | 1.394376 |

185 \[(MSA)_{1}(ForA)_{1}\]

|  |  |  |  |
|---|---|---|---|
| O | -2.448986 | -1.114963 | -0.089408 |
| C | -2.844299 | 0.128536 | -0.011037 |
| O | -2.129012 | 1.118969 | -0.031538 |
| H | -1.460991 | -1.173114 | -0.167857 |
| H | -3.932726 | 0.208240 | 0.081094 |
|        |   S    |        |        |        |        |        |        |        |        |        |        |        |        |        |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
|        | 1.120729 | -0.078290 | 0.141887 |        |        |        |        |        |        |        |        |        |        |        |
|        | 0.223553 | -1.138499 | -0.346948 |        |        |        |        |        |        |        |        |        |        |        |
|        | 1.512126 | -0.108908 | 1.534837 |        |        |        |        |        |        |        |        |        |        |        |
|        | 0.483250 | 1.319765 | -0.244940 |        |        |        |        |        |        |        |        |        |        |        |
|        | -0.516596 | 1.275754 | -0.157511 |        |        |        |        |        |        |        |        |        |        |        |
|        | 2.253160 | -0.048775 | -0.886128 |        |        |        |        |        |        |        |        |        |        |        |
|        | 3.171590 | 0.025663 | -1.926914 |        |        |        |        |        |        |        |        |        |        |        |
|        | 3.100346 | 0.807412 | -0.590274 |        |        |        |        |        |        |        |        |        |        |        |
| (ForA)2 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
|        | -1.504618 | 1.073962 | 0.000318 |        |        |        |        |        |        |        |        |        |        |        |
|        | -1.892188 | -0.174674 | -0.000201 |        |        |        |        |        |        |        |        |        |        |        |
|        | -1.161047 | -1.153849 | -0.000050 |        |        |        |        |        |        |        |        |        |        |        |
|        | -0.507891 | 1.133231 | 0.000551 |        |        |        |        |        |        |        |        |        |        |        |
|        | -2.983856 | -0.269172 | -0.000957 |        |        |        |        |        |        |        |        |        |        |        |
|        | 1.504743 | -1.073998 | 0.000229 |        |        |        |        |        |        |        |        |        |        |        |
|        | 1.892138 | 0.174729 | -0.000141 |        |        |        |        |        |        |        |        |        |        |        |
|        | 1.160942 | 1.153864 | -0.000185 |        |        |        |        |        |        |        |        |        |        |        |
|        | 0.508093 | -1.133529 | 0.000329 |        |        |        |        |        |        |        |        |        |        |        |
|        | 2.983792 | 0.269309 | -0.000367 |        |        |        |        |        |        |        |        |        |        |        |
| (MSA)2(ForA)1 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
|        | 2.417544 | 2.281834 | 0.392595 |        |        |        |        |        |        |        |        |        |        |        |
|        | 3.598876 | 1.939107 | -0.094857 |        |        |        |        |        |        |        |        |        |        |        |
|        | 3.970700 | 0.805600 | -0.304406 |        |        |        |        |        |        |        |        |        |        |        |
|        | 1.881667 | 1.474448 | 0.551995 |        |        |        |        |        |        |        |        |        |        |        |
|        | 4.214343 | 2.826174 | -0.290655 |        |        |        |        |        |        |        |        |        |        |        |
|        | 0.929319 | -1.180519 | -0.056028 |        |        |        |        |        |        |        |        |        |        |        |
|        | 0.806263 | 0.027431 | 0.799752 |        |        |        |        |        |        |        |        |        |        |        |
|        | 0.717687 | -0.963717 | -1.474909 |        |        |        |        |        |        |        |        |        |        |        |
|        | -0.061008 | -2.271778 | 0.512793 |        |        |        |        |        |        |        |        |        |        |        |
|        | -0.991245 | -1.908411 | 0.468199 |        |        |        |        |        |        |        |        |        |        |        |
|        | 2.477708 | -1.962130 | 0.263691 |        |        |        |        |        |        |        |        |        |        |        |
|        | 3.242057 | -1.245543 | -0.047173 |        |        |        |        |        |        |        |        |        |        |        |
|        | 2.540223 | -2.167339 | 1.332012 |        |        |        |        |        |        |        |        |        |        |        |
|        | 2.512974 | -2.878923 | -0.324626 |        |        |        |        |        |        |        |        |        |        |        |
|        | -2.669919 | 0.408188 | 0.063389 |        |        |        |        |        |        |        |        |        |        |        |
|        | -3.985475 | 0.899634 | 0.382273 |        |        |        |        |        |        |        |        |        |        |        |
|        | -2.362741 | -1.008709 | 0.309859 |        |        |        |        |        |        |        |        |        |        |        |
|      | (ForA) 1         | (MSA) 1(ForA) 2 | (ForA) 3         |
|------|-----------------|-----------------|-----------------|
| O    | -1.623882       | 2.009645        | 1.494300        |
| H    | -0.741115       | 0.851918        | 0.370404        |
| C    | -2.277379       | 0.760806        | -0.190712       |
| H    | -2.979128       | 0.191689        | 1.803269        |
| H    | -2.406286       | 1.831312        | -0.028606       |
| H    | -1.251833       | 0.441772        | 2.072314        |
| O    | -2.167278       | 2.009645        | -0.255435       |
| C    | -3.251696       | 1.311354        | 0.576732        |
| O    | -3.315268       | 0.097434        | -0.075134       |
| H    | -1.368288       | 1.426349        | 0.370404        |
| H    | -4.141703       | 1.945336        | -0.190712       |
| O    | 2.201918        | 1.995349        | 1.074187        |
| C    | 3.325364        | 1.305704        | 0.994165        |
| O    | 3.407275        | 0.129844        | 0.781166        |
| H    | 1.434672        | 1.405437        | 2.072314        |
| H    | 4.196137        | 1.941745        | -0.023057       |
| S    | -0.023057       | -1.038931       | -0.255435       |
| O    | 0.251829        | -1.237600       | -0.075134       |
| O    | -0.007138       | 0.368787        | 0.370404        |
| O    | -1.411959       | -1.655654       | -0.190712       |
| H    | -2.161710       | -1.005299       | 1.803269        |
| C    | 1.074187        | -1.993573       | 0.190712        |
| H    | 0.994165        | -3.032543       | 0.994165        |
| H    | 0.781166        | -1.870608       | -0.007138       |
| H    | 2.072314        | -1.587082       | -1.411959       |

31
|     |           |           |           |
|-----|-----------|-----------|-----------|
| C   | 2.003502  | -1.528732 | -0.267494 |
| O   | 2.369625  | -0.506795 | 0.286601  |
| H   | 0.089389  | -1.376505 | 0.000946  |
| H   | 2.719069  | -2.233041 | -0.708078 |

(MA)₁(ForA)₁

|     |           |           |           |
|-----|-----------|-----------|-----------|
| O   | -1.041581 | 1.072200  | -0.260310 |
| C   | -1.720066 | -0.047383 | -0.104249 |
| O   | -1.269971 | -1.098545 | 0.303906  |
| H   | -0.078507 | 0.924644  | 0.031216  |
| H   | -2.773729 | 0.079923  | -0.393205 |
| C   | 1.960328  | -0.489186 | -0.470096 |
| H   | 1.198805  | -1.261636 | -0.597434 |
| H   | 2.103094  | 0.013754  | -1.429476 |
| H   | 2.904487  | -0.963482 | -0.178060 |
| N   | 1.464421  | 0.483663  | 0.512910  |
| H   | 1.305642  | 0.024882  | 1.405397  |
| H   | 2.140108  | 1.225058  | 0.668498  |

(MSA)₁(MA)₁(ForA)₁

|     |           |           |           |
|-----|-----------|-----------|-----------|
| N   | 1.139107  | 1.719249  | 0.000203  |
| H   | 0.486508  | 1.629418  | -0.800794 |
| H   | 1.706188  | 0.845109  | -0.000211 |
| C   | 1.959672  | 2.943036  | -0.000008 |
| H   | 2.588597  | 2.954246  | -0.889954 |
| H   | 1.307824  | 3.816561  | 0.000728  |
| H   | 2.589943  | 2.953705  | 0.888990  |
| S   | -1.463822 | -0.040312 | -0.000059 |
| O   | -0.980346 | -1.447880 | -0.001385 |
| O   | -1.076705 | 0.700946  | -1.230781 |
| O   | -1.075784 | 0.698949  | 1.231565  |
| H   | 0.487372  | 1.629115  | 0.801811  |
| C   | -3.240262 | -0.158332 | 0.000462  |
| H   | -3.542310 | -0.697548 | -0.897325 |
| H   | -3.541669 | -0.699047 | 0.897565  |
| H   | -3.647806 | 0.852585  | 0.001463  |
| C   | 2.444384  | -1.853859 | 0.000114  |
| O   | 2.567125  | -0.634695 | -0.000331 |
| O   | 1.342657  | -2.537361 | 0.000139  |
| H   | 0.488288  | -1.990810 | -0.000355 |
|     |         |         |         |         |
|-----|---------|---------|---------|---------|
| H   | 3.326128| -2.507817| 0.000549|

(MA)\(_{2}\)\(\text{ForA}\)_2

|     |         |         |         |
|-----|---------|---------|---------|
| O   | 2.344383| -0.409782| -0.577745|
| C   | 1.792691| -1.460996| -0.061939|
| O   | 0.661091| -1.536071| 0.406872|
| H   | 1.691821| 0.446013 | -0.550236|
| H   | 2.455644| -2.337978| -0.066013|
| C   | 0.667152| 1.959870 | 1.000051 |
| H   | 0.374316| 1.058503 | 1.543716 |
| H   | 1.633105| 2.292291 | 1.387360 |
| H   | -0.079805| 2.738792 | 1.183687 |
| N   | 0.795622| 1.620014 | -0.424299|
| H   | -0.121113| 1.333174 | -0.777254|
| H   | 1.097722| 2.426103 | -0.963008|
| O   | -1.977248| -1.202386| 0.467315 |
| C   | -2.539979| -0.195840| -0.160643|
| O   | -1.967930| 0.688830 | -0.767087|
| H   | -0.989060| -1.199166| 0.385133 |
| H   | -3.633533| -0.240756| -0.072942|

(MSA)\(_{2}\)(MA)\(_{1}\)(ForA)\(_{1}\)

|     |         |         |         |         |
|-----|---------|---------|---------|---------|
| N   | -0.766017| -1.566752| 1.395612|
| H   | 0.205458 | -1.422704| 1.064663|
| H   | -1.344665| -1.842814| 0.580712|
| C   | -0.828417| -2.567973| 2.478924|
| H   | -0.230547| -2.221514| 3.321418|
| H   | -1.864935| -2.698669| 2.788711|
| H   | -0.431771| -3.514810| 2.113648|
| S   | -0.915813| 1.705066 | 0.453357 |
| O   | -0.736495| 0.650229 | -0.635900|
| O   | 0.340726 | 2.407927 | 0.708258 |
| O   | -1.569173| 1.088762 | 1.630080|
| H   | -1.111631| -0.630683| 1.686295|
| C   | -2.075651| 2.873470 | -0.226874|
| H   | -2.247658| 3.642425 | 0.526707 |
| H   | -1.632470| 3.305659 | -1.124106|
| H   | -3.003289| 2.350752 | -0.461470|
| S   | 2.634304 | -0.433375| -0.400034|
| O   | 3.691847 | -1.186866| -1.034516|
|   |        |        |        |
|---|--------|--------|--------|
| O | 1.870324 | -1.071560 | 0.683126 |
| O | 1.629629 | 0.017961 | -1.535746 |
| H | 0.741670 | 0.311774 | -1.166490 |
| C | 3.270444 | 1.100929 | 0.227433 |
| H | 3.970579 | 0.853286 | 1.026090 |
| H | 3.781888 | 1.605808 | -0.592194 |
| H | 2.428936 | 1.691072 | 0.597420 |
| O | -2.693975 | -0.469040 | -1.969969 |
| C | -3.004545 | -1.683834 | -1.598431 |
| O | -2.510086 | -2.307198 | -0.673343 |
| H | -1.954862 | -0.075547 | -1.417360 |
| H | -3.793791 | -2.111115 | -2.228720 |

(MSA)₁(MA)₁(ForA)₂

|   |        |        |        |
|---|--------|--------|--------|
| O | -1.937706 | -2.095459 | -0.485490 |
| C | -2.828882 | -1.580784 | -1.144684 |
| O | -3.145612 | -0.318979 | -1.188827 |
| H | -0.437131 | -1.739822 | 0.350879 |
| H | -3.479483 | -2.182684 | -1.792085 |
| C | 0.604343 | -2.815486 | 1.809567 |
| H | -0.228228 | -2.849005 | 2.511819 |
| H | 0.622835 | -3.731607 | 1.219890 |
| H | 1.543265 | -2.710197 | 2.352620 |
| N | 0.433975 | -1.659283 | 0.908265 |
| H | 0.373456 | -0.755268 | 1.419034 |
| H | 1.236090 | -1.560767 | 0.257883 |
| O | 2.817039 | -1.394421 | -0.531744 |
| C | 3.354724 | -0.436035 | -1.065912 |
| O | 2.807620 | 0.718481 | 1.328823 |
| H | -2.577258 | 0.261921 | -0.597558 |
| H | 4.403924 | -0.471486 | -1.385669 |
| S | -0.383733 | 1.504220 | 0.438873 |
| O | 0.182069 | 0.986943 | 1.708331 |
| O | -1.855876 | 1.359165 | 0.343182 |
| O | 0.292107 | 0.900478 | -0.750571 |
| H | 1.836369 | 0.763290 | -1.059383 |
| C | -0.048538 | 3.252136 | 0.403923 |
| H | 1.030479 | 3.395204 | 0.466910 |
| H | -0.441971 | 3.653120 | -0.530192 |
| H | -0.547451 | 3.706104 | 1.260206 |
### (MA)$_1$(ForA)$_3$

|   |        |        |        |
|---|--------|--------|--------|
| O | 2.772514 | 1.159237 | -0.704914 |
| C | 3.572652 | 0.244271 | -0.596538 |
| O | 3.330212 | -0.957811 | -0.142699 |
| H | 0.829259 | 1.578080 | -0.511463 |
| H | 4.626666 | 0.360077 | -0.883268 |
| C | 0.117331 | 2.108354 | 1.365425 |
| H | 1.102425 | 2.002805 | 1.819706 |
| H | -0.076070 | 3.157002 | 1.139378 |
| H | -0.643890 | 1.735921 | 2.050746 |
| N | 0.075648 | 1.307651 | 0.126922 |
| H | 0.282716 | 0.283089 | 0.333546 |
| H | -0.857550 | 1.351651 | -0.316645 |
| O | 0.837081 | -1.189749 | 0.504283 |
| C | -0.004306 | -2.132836 | 0.340378 |
| O | -1.230758 | -2.003902 | 0.216216 |
| H | 2.362165 | -1.089682 | 0.121301 |
| H | 0.413838 | -3.154252 | 0.311782 |
| O | -3.431300 | -0.745869 | -0.191452 |
| C | -3.515008 | 0.507239 | -0.529041 |
| O | -2.595537 | 1.305881 | -0.642627 |
| H | -2.495716 | -1.087947 | -0.031548 |
| H | -4.555099 | 0.805231 | -0.713791 |

### (MSA)$_1$(MA)$_2$(ForA)$_1$

|   |        |        |        |
|---|--------|--------|--------|
| N | 0.519734 | -2.417492 | -0.193626 |
| H | 0.704203 | -3.252702 | -0.744707 |
| H | -0.350176 | -1.960159 | -0.559539 |
| C | 0.336804 | -2.741442 | 1.239389 |
| H | -0.442371 | -3.496285 | 1.349125 |
| H | 1.279882 | -3.103437 | 1.649001 |
| H | 0.024342 | -1.826759 | 1.743079 |
| N | 0.856499 | 1.873940 | 0.183974 |
| H | 1.372188 | -1.785249 | -0.310495 |
| H | 0.314145 | 1.293969 | 0.843009 |
| C | 1.087409 | 3.236232 | 0.697957 |
| H | 1.643905 | 3.807396 | -0.044907 |
| H | 0.132990 | 3.722843 | 0.902287 |
| H | 1.677069 | 3.175627 | 1.612587 |
| S | -1.934423 | 0.108252 | -0.219600 |
|     | 36   | 36   | 36   |
|-----|------|------|------|
|     | 0.749677 | 1.172968 | 0.638352 |
|     | 0.016239 | 2.187268 | 0.345592 |
|     | -1.193319 | 2.156605 | 0.105924 |
|     | 0.030051 | -0.221604 | 0.413850 |
|     | 0.545838 | 3.158563 | 0.317561 |
|     | -0.525136 | -2.090318 | 1.234002 |
|     | 0.420364 | -2.234119 | 1.757578 |
|     | -1.250865 | -1.645300 | 1.915527 |
|     | -0.898814 | -3.053251 | 0.882924 |
|     | -0.316652 | -1.180986 | 0.095181 |
|     | 0.442851 | -1.507081 | -0.510835 |
|     | -1.208281 | -0.995194 | -0.437886 |
|     | 3.168812 | 0.678429 | -0.007132 |
|     | 3.291903 | -0.505702 | -0.541103 |
|     | 2.405147 | -1.324499 | -0.730944 |
|     | 2.209024 | 0.909915 | 0.258635 |
|     | 4.334790 | -0.714158 | -0.819106 |
|     | -3.904560 | -0.421375 | -0.202752 |
|     | -4.708245 | 0.305984 | -0.372748 |
|     | -4.285387 | -1.419638 | -0.436868 |
|     | -3.656086 | -0.396137 | 0.861955 |
|     | -2.693142 | -0.150221 | -0.980941 |
|     | -2.907260 | -0.123613 | -1.972479 |
|     | -2.312640 | 0.766808 | -0.721829 |
|    |       |       |       |
|----|-------|-------|-------|
| N  | 0.120939 | 2.264367 | -0.332194 |
| H  | -0.795890 | 1.882291 | -0.662722 |
| H  | 0.883974  | 1.742386 | -0.809971 |
| C  | 0.214150  | 3.714348 | -0.592016 |
| H  | -0.598983 | 4.222593 | -0.074105 |
| H  | 1.172336  | 4.086653 | -0.229810 |
| H  | 0.130956  | 3.889371 | -1.664283 |
| N  | -0.295226 | -2.301939 | -0.044039 |
| H  | -0.522313 | -1.698812 | 0.757229 |
| H  | 0.654582  | -2.026781 | -0.382454 |
| C  | -0.342230 | -3.731111 | 0.318771 |
| H  | -1.339720 | -3.977024 | 0.682649 |
| H  | -0.113477 | -4.328775 | -0.563130 |
| H  | 0.396798  | -3.927946 | 1.095143 |
| S  | -2.684454 | -0.041064 | -0.577925 |
| O  | -2.304215 | 1.272738  | -1.160322 |
| O  | -2.124226 | -0.240182 | 0.783796 |
| O  | -2.374457 | -1.192619 | -1.468730 |
| H  | -1.011537 | -2.044601 | -0.757985 |
| C  | -4.459522 | 0.001469  | -0.416729 |
| H  | -4.720878 | 0.830000  | 0.241759 |
| H  | -4.886291 | 0.147679  | -1.409104 |
| H  | -4.787485 | -0.947519 | 0.007730 |
| S  | 2.719871  | -0.199176 | -0.516669 |
| O  | 2.255091  | -1.591071 | -0.749872 |
| O  | 2.490960  | 0.244564  | 0.890023 |
| O  | 2.176439  | 0.775954  | -1.492063 |
| H  | 0.187900  | 2.064105  | 0.680086 |
| C  | 4.484781  | -0.226429 | -0.746216 |
| H  | 4.684142  | -0.533255 | -1.772982 |
| H  | 4.866836  | 0.777407  | -0.561133 |
| H  | 4.907417  | -0.939098 | -0.038106 |
| O  | 0.468593  | -0.511568 | 2.353959 |
| C  | -0.298516 | 0.497711  | 2.721560 |
| O  | -0.109110 | 1.664501  | 2.435144 |
| H  | 1.258742  | -0.191305 | 1.820520 |
| H  | -1.138343 | 0.164997  | 3.340124 |
\[(\text{MSA})_1(\text{MA})_2(\text{ForA})_2\]

|   |   |   |
|---|---|---|
| O | 2.147051 | 1.112107 | -0.039581 |
| C | 2.029713 | 2.375363 | -0.121190 |
| O | 0.971141 | 3.024824 | -0.059839 |
| H | 1.130973 | -0.320090 | 0.169522 |
| H | 2.968676 | 2.942151 | -0.259357 |
| C | 0.876120 | -1.608120 | 1.782720 |
| H | 1.721980 | -1.162701 | 2.306680 |
| H | -0.064468 | -1.173913 | 2.121436 |
| H | 0.865095 | -2.685613 | 1.945778 |
| N | 1.014038 | -1.339189 | 0.334676 |
| H | 1.887534 | -1.750291 | -0.030396 |
| H | 0.172492 | -1.682915 | -0.175432 |
| O | 4.505196 | 0.178499 | -0.377790 |
| C | 4.606199 | -1.120798 | -0.412470 |
| O | 3.699131 | -1.929699 | -0.282552 |
| H | 3.547401 | 0.515979 | -0.237249 |
| H | 5.642716 | -1.444473 | -0.576374 |
| C | -2.321654 | 3.372246 | 0.393561 |
| H | -2.191018 | 4.104843 | -0.402533 |
| H | -3.376339 | 3.113468 | 0.490280 |
| H | -1.954840 | 3.794158 | 1.329037 |
| N | -1.539421 | 2.163784 | 0.072390 |
| H | -1.868326 | 1.700048 | -0.788611 |
| H | -0.505536 | 2.397734 | -0.004050 |
| S | -2.413524 | -1.010283 | -0.296298 |
| O | -1.442717 | -2.065127 | -0.683404 |
| O | -2.627551 | 0.020248 | -1.340632 |
| O | -2.063684 | -0.394198 | 1.022219 |
| H | -1.669785 | 1.409224 | 0.768038 |
| C | -3.974509 | -1.841414 | -0.072242 |
| H | -3.851783 | -2.598106 | 0.702713 |
| H | -4.717532 | -1.100905 | 0.223596 |
| H | -4.246933 | -2.303148 | -1.021415 |

\[(\text{MA})_2(\text{ForA})_3\]

|   |   |   |
|---|---|---|
| O | -3.206279 | -1.457326 | -0.515162 |
| C | -4.047340 | -0.573055 | -0.476657 |
| O | -3.840161 | 0.693542 | -0.235246 |
| H | -1.319501 | -1.617293 | -0.323028 |
|   | (MSA)$_2$(MA)$_3$(ForA)$_1$ |   |
|---|-----------------------------|---|
| H | -5.111496 | -0.781869 | -0.650815 |
| C | -0.298370 | -1.837030 | 1.473635 |
| H | -1.166516 | -1.557038 | 2.070586 |
| H | -0.223787 | -2.922887 | 1.414150 |
| H | 0.615106  | -1.437451 | 1.914313 |
| N | -0.447190 | -1.286040 | 0.109482 |
| H | -0.577369 | -0.250916 | 0.143321 |
| H | 0.402009  | -1.525847 | -0.467839 |
| O | -1.362638 | 1.267044  | 0.143111 |
| C | -0.916968 | 2.429164  | 0.407733 |
| O | 0.283063  | 2.746458  | 0.478797 |
| H | -2.859315 | 0.918615  | -0.077624 |
| H | -1.672321 | 3.215305  | 0.585129 |
| O | 2.957129  | -1.156818 | 0.728543 |
| C | 2.784006  | -2.001752 | -0.191316 |
| O | 1.885139  | -1.958623 | -1.072509 |
| H | 1.391760  | 1.664542  | -0.022052 |
| H | 3.488926  | -2.853542 | -0.227518 |
| C | 3.405477  | 1.959805  | -0.505794 |
| H | 3.205961  | 2.807525  | -1.161591 |
| H | 3.643640  | 2.325462  | 0.492346 |
| H | 4.242201  | 1.374010  | -0.886867 |
| N | 2.204195  | 1.104588  | -0.412254 |
| H | 1.935954  | 0.739026  | -1.325627 |
| H | 2.414873  | 0.235531  | 0.176642 |

|   | (MSA)$_2$(MA)$_3$(ForA)$_1$ |   |
|---|-----------------------------|---|
| C | -1.705930 | -0.947300 | -3.145942 |
| H | -1.872921 | -2.005318 | -3.347344 |
| H | -2.569719 | -0.375069 | -3.483211 |
| H | -0.809655 | -0.605317 | -3.664215 |
| N | -1.545104 | -0.754006 | -1.691345 |
| H | -0.736403 | -1.284736 | -1.332709 |
| H | -1.402988 | 0.249202  | -1.473808 |
| N | 2.669559  | 1.426285  | -0.017017 |
| H | 2.328146  | 2.276854  | -0.495307 |
| H | 2.613898  | 0.611823  | -0.667079 |
| C | 4.009846  | 1.541259  | 0.585961 |
| H | 4.019648  | 2.368507  | 1.295511 |
| H | 4.229482  | 0.605482  | 1.099485 |
|        |        |        |
|--------|--------|--------|
| H      | 4.745358 | 1.719125 | -0.198298 |
| N      | -1.003316 | -0.810358 | 1.679645 |
| H      | -0.715583 | 0.136002 | 1.376391 |
| H      | -0.520527 | -1.473307 | 1.056025 |
| C      | -0.603995 | -1.040894 | 3.081763 |
| H      | -1.071672 | -0.284790 | 3.712383 |
| H      | -0.949336 | -2.027514 | 3.391495 |
| H      | 0.482152  | -0.983720 | 3.159033 |
| S      | -0.390270 | 2.639381  | -0.195529 |
| O      | 0.792243  | 3.299147  | -0.798305 |
| O      | 0.021461  | 1.700359  | 0.902788 |
| O      | -1.286801 | 1.986572  | -1.173227 |
| H      | -2.070893 | -0.920109 | 1.559320 |
| C      | -1.350341 | 3.920740  | 0.586783 |
| H      | -0.724958 | 4.409784  | 1.333612 |
| H      | -1.655635 | 4.627985  | -0.184503 |
| H      | -2.221989 | 3.457640  | 1.049790 |
| S      | 1.899220  | -1.846300 | -0.186720 |
| O      | 0.466484  | -2.246326 | -0.330065 |
| O      | 2.181165  | -1.248780 | 1.136813 |
| O      | 2.356123  | -0.984989 | -1.312468 |
| H      | 1.938884  | 1.244292  | 0.686976 |
| C      | 2.830655  | -3.361373 | -0.301488 |
| H      | 2.641795  | -3.805606 | -1.278750 |
| H      | 3.887511  | -3.120682 | -0.185326 |
| H      | 2.496828  | -4.026449 | 0.495039 |
| O      | -3.799826 | -1.591279 | -0.631925 |
| C      | -4.239760 | -1.468041 | 0.538547 |
| O      | -3.600411 | -1.114425 | 1.562795 |
| H      | -2.426913 | -1.088545 | -1.175950 |
| H      | -5.312031 | -1.696852 | 0.687454 |

\[(\text{MSA})_1(\text{MA})_3(\text{ForA})_2\]

|        |        |        |
|--------|--------|--------|
| C      | -1.340115 | -0.035807 | 3.115523 |
| H      | -0.283710 | -0.047605 | 3.386641 |
| H      | -1.820614 | 0.856521  | 3.516790 |
| H      | -1.834033 | -0.919385 | 3.519664 |
| N      | -1.471662 | -0.038181 | 1.646897 |
| H      | -0.986411 | -0.849588 | 1.233364 |
| H      | -2.505955 | -0.064597 | 1.339259 |
$$\text{(MA)}_3(\text{ForA})_3$$

|    |    |    |
|----|----|----|
| O  | -0.371058 | 1.575967 | 1.372149 |
| C  | -1.459085 | 1.840500 | 1.951935 |
| O  | -2.569302 | 1.307469 | 1.706833 |
| H  | -0.147919 | -0.160922 | 1.082007 |
| H  | -1.432998 | 2.604870 | 2.750012 |
|   |   |   |   |
|---|---|---|---|
| C | -0.484378 | -1.882535 | 2.190487 |
| H | -0.004922 | -1.507651 | 3.094780 |
| H | -1.559801 | -1.708187 | 2.252414 |
| H | -0.282801 | -2.948920 | 2.091021 |
| N | 0.074170  | -1.173648 | 1.023535 |
| H | 1.142776  | -1.276222 | 1.009123 |
| H | -0.303735 | -1.549325 | 0.131334 |
| O | 3.531956  | 0.061144  | -0.165653 |
| C | 3.611559  | -0.956076 | 0.573088 |
| O | 2.674017  | -1.552563 | 1.155486 |
| H | 2.257261  | 0.841874  | -0.446326 |
| H | 4.626599  | -1.369380 | 0.723225 |
| C | -3.596654 | -0.809545 | -0.839261 |
| H | -3.789267 | -1.067624 | -1.880767 |
| H | -3.032149 | -1.622111 | -0.384940 |
| H | -4.535191 | -0.651757 | -0.307185 |
| N | -2.778000 | 0.420838  | -0.771564 |
| H | -3.239774 | 1.191114  | -1.250399 |
| H | -2.634227 | 0.729005  | 0.247725 |
| O | -0.478539 | 0.028293  | -2.139604 |
| C | -0.348677 | -1.232329 | -2.293340 |
| O | -0.753956 | -2.099039 | -1.496972 |
| H | -1.835359 | 0.277728  | -1.239779 |
| H | 0.165638  | -1.563162 | -3.214118 |
| C | 2.055528  | 2.712800  | -1.379352 |
| H | 2.730361  | 3.194882  | -0.672079 |
| H | 2.624136  | 2.400263  | -2.255078 |
| H | 1.272563  | 3.411077  | -1.678346 |
| N | 1.463499  | 1.521798  | -0.742837 |
| H | 0.903250  | 1.764306  | 0.087327 |
| H | 0.823180  | 1.020170  | -1.383149 |
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