**Table S1.** Comparison of aug-cc-pVnZ and cc-pVnZ basis sets on the (SA)(Gly)(Ser)(A) system from table 7 of reference 70.

Bready, C. J.; Vanovac, S.; Odbadrakh, T. T.; Shields, G. C. Amino Acids Compete with Ammonia in Sulfuric Acid-Based Atmospheric Aerosol Prenucleation: The Case of Glycine and Serine. *J. Phys. Chem. A.* **2022**, *126* (31), 5195-1206. DOI: 10.1021/acs.jpca.2c03539

DLPNO-CCSD(T) ∆G˚ values in kcal mol-1 at 298.15 K for formation of dry clusters using the non-augmented and augmented DZ, TZ, QZ basis sets, along with CBS extrapolation, using ωB97X-D/6-31++G\*\* geometries and a scaling factor of 0.971.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Cluster Reaction | DZa | TZb | QZc | CBSd |
| SA + Gly → (SA)(Gly) | -7.31  -5.80 | -6.21  -6.51 | -5.99  -6.13 | -5.90  -5.48 |
| SA + Ser → (SA)(Ser) | -7.99  -10.20 | -8.18  -9.60 | -8.66  -9.25 | -9.28  -8.88 |
| SA + A → (SA)(A) | -8.93  -6.46 | -7.43  -6.72 | -6.88  -6.60 | -6.41  -6.40 |
| Gly + Ser → (Gly)(Ser) | -5.05  -3.62 | -3.72  -3.86 | -3.35  -3.52 | -3.09  -3.00 |
| Gly + A → (Gly)(A) | -4.27  -1.50 | -2.31  -1.38 | -1.59  -1.27 | -0.98  -1.14 |
| Ser + A → (Ser)(A) | -4.83  -1.96 | -2.63  -1.69 | -1.95  -1.63 | -1.44  -1.58 |
| SA + Gly + Ser → (SA)(Gly)(Ser) | -14.67  -14.71 | -11.96  -13.27 | -11.32  -11.84 | -10.96  -10.16 |
| SA + Gly + A → (SA)(Gly)(A) | -16.54  -12.42 | -13.65  -13.13 | -12.76  -12.57 | -12.07  -11.67 |
| SA + Ser + A → (SA)(Ser)(A) | -13.82  -12.47 | -11.18  -12.22 | -11.23  -11.72 | -11.78  -11.08 |
| Gly + Ser + A → (Gly)(Ser)(A) | -5.90  -2.83 | -2.91  -2.49 | -1.99  -1.84 | -1.30  -1.00 |
| SA + Gly + Ser + A → (SA)(Gly)(Ser)(A) | -18.69  -18.55 | -15.91  -17.03 | -15.21  -15.61 | -14.77  -13.96 |

acc-pVDZ values are listed on top with the aug-cc-pVDZ values below

bcc-pVTZ values are listed on top with the aug-cc-pVTZ values below

ccc-pVQZ values are listed on top with the aug-cc-pVQZ values below

dCBS values are listed on top with the aug-CBS values below

**Table S2.** Comparison of scaled versus unscaled Gibbs free energy values (kcal mol-1) associated with the formation of (SA)3 clusters from table 4 of reference 59.

Kurfman, L. A.; Odbadrakh, T. T.; Shields, G. C., Calculating Reliable Gibbs Free Energies for Formation of Gas-Phase Clusters that Are Critical for Atmospheric Chemistry: (H2SO4)3. J Phys Chem A 2021, 125 (15), 3169-3176.

Changes in the thermodynamic corrections (kcal mol-1) associated with the formation of (H2SO4)3 structure T2 from infinitely separated monomers computed using unscaled (1.000) and scaled (0.973) harmonic frequencies at the M08-HX/MG3S level of theory. The difference between the scaled and unscaled values are listed in the last row (∆).

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Scaling Factor | 0 K | 216.65 K | | 273.15 K | | 298.15 K | |
| ZPE | Hcorr | Gcorr | Hcorr | Gcorr | Hcorr | Gcorr |
| 1.000 | 2.320 | -0.472 | 19.948 | -0.338 | 24.654 | -0.261 | 26.727 |
| 0.973 | 2.259 | -0.448 | 19.805 | -0.305 | 24.481 | -0.229 | 26.541 |
| ∆ | -0.061 | 0.024 | -0.143 | 0.033 | -0.173 | 0.032 | -0.186 |

**Table S3.** DLPNO-CCSD(T)/CBS//ωB97X-D/6-31++G\*\* Gibbs free energy changes associated with the sequential hydration of sulfuric acid, formic acid, and nitric acid monomers at atmospherically relevant temperatures and 1 atm pressure.

|  |  |  |  |
| --- | --- | --- | --- |
| Cluster | 216.65 K | 273.15 K | 298.15 K |
| SA + W ⇌ (SA)(W) | -4.42 | -2.79 | -2.06 |
| (SA)(W) + W ⇌ (SA)(W)2 | -3.64 | -1.86 | -1.08 |
| (SA)(W)2 + W ⇌ (SA)(W)3 | -2.85 | -1.05 | -0.28 |
| (SA)(W)3 + W ⇌ (SA)(W)4 | -3.15 | -1.38 | -0.57 |
| (SA)(W)4 + W ⇌ (SA)(W)5 | -0.67 | 1.04 | 1.79 |
| FA + W ⇌ (FA)(W) | -1.50 | 0.24 | 1.01 |
| (FA)(W) + W ⇌ (FA)(W)2 | -2.26 | -0.46 | 0.34 |
| (FA)(W)2 + W ⇌ (FA)(W)3 | -0.75 | 0.79 | 1.47 |
| (FA)(W)3 + W ⇌ (FA)(W)4 | 0.31 | 2.32 | 3.21 |
| (FA)(W)4 + W ⇌ (FA)(W)5 | 0.57 | 2.37 | 3.16 |
| NA + W ⇌ (NA)(W) | -2.03 | -0.39 | 0.33 |
| (NA)(W) + W ⇌ (NA)(W)2 | -1.50 | 0.12 | 0.83 |
| (NA)(W)2 + W ⇌ (NA)(W)3 | -0.54 | 1.20 | 1.97 |
| (NA)(W)3 + W ⇌ (NA)(W)4 | -0.41 | 1.39 | 2.19 |
| (NA)(W)4 + W ⇌ (NA)(W)5 | -0.64 | 0.91 | 1.57 |

**Table S4.** DLPNO-CCSD(T)/CBS//ωB97X-D/6-31++G\*\* Gibbs free energy changes associated with the sequential hydration of ammonia and dimethyl amine monomers at atmospherically relevant temperatures and 1 atm pressure.

|  |  |  |  |
| --- | --- | --- | --- |
| Cluster | 216.65 K | 273.15 K | 298.15 K |
| A + W ⇌ (A)(W) | -0.05 | 1.14 | 1.66 |
| (A)(W) + W ⇌ (A)(W)2 | 0.53 | 2.45 | 3.30 |
| (A)(W)2 + W ⇌ (A)(W)3 | -1.05 | 0.75 | 1.55 |
| (A)(W)3 + W ⇌ (A)(W)4 | -0.47 | 1.08 | 1.74 |
| (A)(W)4 + W ⇌ (A)(W)5 | -0.31 | 1.20 | 1.90 |
| DMA + W ⇌ (DMA)(W) | -0.51 | 0.88 | 1.49 |
| (DMA)(W) + W ⇌ (DMA)(W)2 | -0.28 | 1.45 | 2.21 |
| (DMA)(W)2 + W ⇌ (DMA)(W)3 | -0.90 | 0.99 | 1.81 |
| (DMA)(W)3 + W ⇌ (DMA)(W)4 | -0.53 | 1.09 | 1.82 |
| (DMA)(W)4 + W ⇌ (DMA)(W)5 | -0.21 | 1.62 | 2.44 |

**Table S5.** DLPNO-CCSD(T)/CBS//ωB97X-D/6-31++G\*\* Gibbs free energy changes associated with the formation and sequential hydration of sulfuric acid-formic acid, sulfuric acid-nitric acid, and formic acid-nitric acid dimers at atmospherically relevant temperatures and 1 atm pressure.

|  |  |  |  |
| --- | --- | --- | --- |
| Cluster | 216.65 K | 273.15 K | 298.15 K |
| SA + FA ⇌ (SA)(FA) | -8.28 | -6.26 | -5.37 |
| (SA)(FA) + W ⇌ (SA)(FA)(W) | -3.97 | -2.23 | -1.46 |
| (SA)(FA)(W) + W ⇌ (SA)(FA)(W)2 | -3.11 | -1.30 | -0.49 |
| (SA)(FA)(W)2 + W ⇌ (SA)(FA)(W)3 | -1.17 | 0.45 | 1.17 |
| (SA)(FA)(W)3 + W ⇌ (SA)(FA)(W)4 | -0.63 | 1.08 | 1.83 |
| (SA)(FA)(W)4 + W ⇌ (SA)(FA)(W)5 | -0.83 | 1.46 | 2.48 |
| SA + NA ⇌ (SA)(NA) | -4.84 | -2.96 | -2.13 |
| (SA)(NA) + W ⇌ (SA)(NA)(W) | -4.53 | -2.81 | -2.06 |
| (SA)(NA)(W) + W ⇌ (SA)(NA)(W)2 | -3.18 | -1.33 | -0.51 |
| (SA)(NA)(W)2 + W ⇌ (SA)(NA)(W)3 | -2.52 | -0.87 | -0.14 |
| (SA)(NA)(W)3 + W ⇌ (SA)(NA)(W)4 | -1.32 | 0.33 | 1.06 |
| (SA)(NA)(W)4 + W ⇌ (SA)(NA)(W)5 | 0.00 | 2.15 | 3.10 |
| FA + NA ⇌ (FA)(NA) | -4.73 | -2.73 | -1.85 |
| (FA)(NA) + W ⇌ (FA)(NA)(W) | -0.83 | 0.70 | 1.38 |
| (FA)(NA)(W) + W ⇌ (FA)(NA)(W)2 | -1.53 | 0.20 | 0.91 |
| (FA)(NA)(W)2 + W ⇌ (FA)(NA)(W)3 | -0.09 | 1.59 | 2.31 |
| (FA)(NA)(W)3 + W ⇌ (FA)(NA)(W)4 | -0.72 | 0.96 | 1.77 |
| (FA)(NA)(W)4 + W ⇌ (FA)(NA)(W)5 | -1.31 | 0.59 | 1.44 |

**Table S6.** DLPNO-CCSD(T)/CBS//ωB97X-D/6-31++G\*\* Gibbs free energy changes associated with the formation and sequential hydration of sulfuric acid-ammonia, formic acid-ammonia, and nitric acid-ammonia dimers at atmospherically relevant temperatures and 1 atm pressure.

|  |  |  |  |
| --- | --- | --- | --- |
| Cluster | 216.65 K | 273.15 K | 298.15 K |
| SA + A ⇌ (SA)(A) | -8.66 | -7.10 | -6.41 |
| (SA)(A) + W ⇌ (SA)(A)(W) | -3.35 | -1.48 | -0.65 |
| (SA)(A)(W) + W ⇌ (SA)(A)(W)2 | -6.61 | -4.73 | -3.91 |
| (SA)(A)(W)2 + W ⇌ (SA)(A)(W)3 | -1.15 | 0.41 | 1.10 |
| (SA)(A)(W)3 + W ⇌ (SA)(A)(W)4 | -3.11 | -1.09 | -0.20 |
| (SA)(A)(W)4 + W ⇌ (SA)(A)(W)5 | -0.65 | 1.56 | 2.54 |
| FA + A ⇌ (FA)(A) | 0.38 | 1.77 | 2.38 |
| (FA)(A) + W ⇌ (FA)(A)(W) | -5.22 | -3.21 | -2.32 |
| (FA)(A)(W) + W ⇌ (FA)(A)(W)2 | -0.29 | 1.17 | 1.81 |
| (FA)(A)(W)2 + W ⇌ (FA)(A)(W)3 | 0.12 | 1.60 | 2.26 |
| (FA)(A)(W)3 + W ⇌ (FA)(A)(W)4 | 0.31 | 2.56 | 3.56 |
| (FA)(A)(W)4 + W ⇌ (FA)(A)(W)5 | -0.14 | 1.37 | 2.04 |
| NA + A ⇌ (NA)(A) | -5.62 | -4.03 | -3.33 |
| (NA)(A) + W ⇌ (NA)(A)(W) | -0.08 | 1.61 | 2.35 |
| (NA)(A)(W) + W ⇌ (NA)(A)(W)2 | -0.14 | 1.47 | 2.18 |
| (NA)(A)(W)2 + W ⇌ (NA)(A)(W)3 | -0.75 | 1.52 | 2.52 |
| (NA)(A)(W)3 + W ⇌ (NA)(A)(W)4 | -2.83 | -0.66 | 0.31 |
| (NA)(A)(W)4 + W ⇌ (NA)(A)(W)5 | -2.44 | -0.48 | 0.38 |

**Table S7.** DLPNO-CCSD(T)/CBS//ωB97X-D/6-31++G\*\* Gibbs free energy changes associated with the formation and sequential hydration of sulfuric acid-dimethyl amine, formic acid-dimethyl amine, and nitric acid-dimethyl amine dimers at atmospherically relevant temperatures and 1 atm pressure.

|  |  |  |  |
| --- | --- | --- | --- |
| Cluster | 216.65 K | 273.15 K | 298.15 K |
| SA + DMA ⇌ (SA)(DMA) | -16.03 | -14.36 | -13.62 |
| (SA)(DMA) + W ⇌ (SA)(DMA)(W) | -4.47 | -2.48 | -1.61 |
| (SA)(DMA)(W) + W ⇌ (SA)(DMA)(W)2 | -3.00 | -1.13 | -0.35 |
| (SA)(DMA)(W)2 + W ⇌ (SA)(DMA)(W)3 | -3.54 | -1.74 | -0.89 |
| (SA)(DMA)(W)3 + W ⇌ (SA)(DMA)(W)4 | -0.53 | 1.54 | 2.46 |
| (SA)(DMA)(W)4 + W ⇌ (SA)(DMA)(W)5 | -3.16 | -1.24 | -0.38 |
| FA + DMA ⇌ (FA)(DMA) | -4.68 | -2.85 | -2.04 |
| (FA)(DMA) + W ⇌ (FA)(DMA)(W) | -2.28 | -0.56 | 0.20 |
| (FA)(DMA)(W) + W ⇌ (FA)(DMA)(W)2 | 0.92 | 2.50 | 3.16 |
| (FA)(DMA)(W)2 + W ⇌ (FA)(DMA)(W)3 | -3.50 | -1.31 | -0.31 |
| (FA)(DMA)(W)3 + W ⇌ (FA)(DMA)(W)4 | -0.39 | 1.43 | 2.23 |
| (FA)(DMA)(W)4 + W ⇌ (FA)(DMA)(W)5 | 0.40 | 2.45 | 3.36 |
| NA + DMA ⇌ (NA)(DMA) | -7.46 | -5.56 | -4.72 |
| (NA)(DMA) + W ⇌ (NA)(DMA)(W) | -3.06 | -1.23 | -0.42 |
| (NA)(DMA)(W) + W ⇌ (NA)(DMA)(W)2 | -2.82 | -1.02 | -0.23 |
| (NA)(DMA)(W)2 + W ⇌ (NA)(DMA)(W)3 | -2.47 | -0.97 | -0.30 |
| (NA)(DMA)(W)3 + W ⇌ (NA)(DMA)(W)4 | -0.68 | 1.59 | 2.59 |
| (NA)(DMA)(W)4 + W ⇌ (NA)(DMA)(W)5 | 3.32 | 5.37 | 6.27 |

**Table S8.** DLPNO-CCSD(T)/CBS//ωB97X-D/6-31++G\*\* Gibbs free energy changes associated with the formation and sequential hydration of ammonia-dimethyl amine dimer at atmospherically relevant temperatures and 1 atm pressure.

|  |  |  |  |
| --- | --- | --- | --- |
| Cluster | 216.65 K | 273.15 K | 298.15 K |
| A + DMA ⇌ (A)(DMA) | 1.72 | 2.78 | 3.24 |
| (A)(DMA) + W ⇌ (A)(DMA)(W) | -1.37 | 0.62 | 1.50 |
| (A)(DMA)(W) + W ⇌ (A)(DMA)(W)2 | -1.22 | 0.56 | 1.35 |
| (A)(DMA)(W)2 + W ⇌ (A)(DMA)(W)3 | -0.15 | 1.37 | 2.03 |
| (A)(DMA)(W)3 + W ⇌ (A)(DMA)(W)4 | 0.01 | 2.07 | 3.00 |
| (A)(DMA)(W)4 + W ⇌ (A)(DMA)(W)5 | -0.31 | 1.39 | 2.14 |

**Table S9.** DLPNO-CCSD(T)/CBS//ωB97X-D/6-31++G\*\* Gibbs free energy changes associated with the formation and sequential hydration of sulfuric acid-ammonia-dimethyl amine, formic acid-ammonia-dimethyl amine, and nitric acid-ammonia-dimethyl amine trimers at atmospherically relevant temperatures and 1 atm pressure.

|  |  |  |  |
| --- | --- | --- | --- |
| Cluster | 216.65 K | 273.15 K | 298.15 K |
| SA + A + DMA ⇌ (SA)(A)(DMA) | -20.22 | -16.64 | -15.06 |
| (SA)(A)(DMA) + W ⇌ (SA)(A)(DMA)(W) | -4.34 | -2.55 | -1.76 |
| (SA)(A)(DMA)(W) + W ⇌ (SA)(A)(DMA)(W)2 | -2.96 | -1.00 | -0.13 |
| (SA)(A)(DMA)(W)2 + W ⇌ (SA)(A)(DMA)(W)3 | -1.88 | 0.14 | 0.91 |
| (SA)(A)(DMA)(W)3 + W ⇌ (SA)(A)(DMA)(W)4 | -3.83 | -2.08 | -1.17 |
| (SA)(A)(DMA)(W)4 + W ⇌ (SA)(A)(DMA)(W)5 | -1.59 | 0.68 | 1.70 |
| FA + A + DMA ⇌ (FA)(A)(DMA) | -4.96 | -1.46 | -0.06 |
| (FA)(A)(DMA) + W ⇌ (FA)(A)(DMA)(W) | -1.19 | 0.52 | 1.41 |
| (FA)(A)(DMA)(W) + W ⇌ (FA)(A)(DMA)(W)2 | 0.01 | 1.14 | 1.58 |
| (FA)(A)(DMA)(W)2 + W ⇌ (FA)(A)(DMA)(W)3 | -1.75 | 1.19 | 2.56 |
| (FA)(A)(DMA)(W)3 + W ⇌ (FA)(A)(DMA)(W)4 | -1.77 | -0.40 | 0.21 |
| (FA)(A)(DMA)(W)4 + W ⇌ (FA)(A)(DMA)(W)5 | 1.03 | 3.09 | 3.96 |
| NA + A + DMA ⇌ (NA)(A)(DMA) | -10.30 | -6.61 | -4.99 |
| (NA)(A)(DMA) + W ⇌ (NA)(A)(DMA)(W) | -3.01 | -1.44 | -0.75 |
| (NA)(A)(DMA)(W) + W ⇌ (NA)(A)(DMA)(W)2 | -1.59 | 0.39 | 1.26 |
| (NA)(A)(DMA)(W)2 + W ⇌ (NA)(A)(DMA)(W)3 | -1.43 | 0.52 | 1.38 |
| (NA)(A)(DMA)(W)3 + W ⇌ (NA)(A)(DMA)(W)4 | -2.49 | -0.55 | 0.30 |
| (NA)(A)(DMA)(W)4 + W ⇌ (NA)(A)(DMA)(W)5 | 1.70 | 3.56 | 4.39 |

**Table S10.** DLPNO-CCSD(T)/CBS//ωB97X-D/6-31++G\*\* Gibbs free energy changes associated with the formation and sequential hydration of sulfuric acid-formic acid-nitric acid trimer at atmospherically relevant temperatures and 1 atm pressure.

|  |  |  |  |
| --- | --- | --- | --- |
| Cluster | 216.65 K | 273.15 K | 298.15 K |
| SA + FA + NA ⇌ (SA)(FA)(NA) | -13.45 | -9.50 | -7.76 |
| (SA)(FA)(NA) + W ⇌ (SA)(FA)(NA)(W) | -2.82 | -1.21 | -0.50 |
| (SA)(FA)(NA)(W) + W ⇌ (SA)(FA)(NA)(W)2 | -1.42 | 0.30 | 1.06 |
| (SA)(FA)(NA)(W)2 + W ⇌ (SA)(FA)(NA)(W)3 | -2.01 | 0.15 | 1.11 |
| (SA)(FA)(NA)(W)3 + W ⇌ (SA)(FA)(NA)(W)4 | -2.93 | -1.29 | -0.57 |
| (SA)(FA)(NA)(W)4 + W ⇌ (SA)(FA)(NA)(W)5 | -0.18 | 1.91 | 2.84 |

**Table S11.** Equilibrium concentrations of clusters that form at more than 1 cm-3 at 298 K. Initial concentrations of the monomers were: SA = 5.00E7, FA = 2.00E11, NA = 9.80E10, A = 2.00E11, DMA = 1.00E6.

|  |  |
| --- | --- |
| Cluster | 298.15 K |
| SA | 2.24E+07 |
| FA | 1.99E+11 |
| NA | 9.63E+10 |
| A | 2.00E+11 |
| DMA | 9.84E+05 |
| SA-FA | 1.58E+03 |
| SA-NA | 3.21E+00 |
| SA-A | 9.05E+03 |
| SA-DMA | 8.70E+03 |
| FA-NA | 1.76E+04 |
| FA-A | 2.90E+01 |
| NA-A | 2.14E+05 |
| NA-DMA | 1.12E+01 |
| SA-FA-DMA | 7.40E+00 |
| SA-W1 | 2.29E+07 |
| SA-W2 | 4.41E+06 |
| SA-W3 | 2.23E+05 |
| SA-W4 | 1.83E+04 |
| SA-W5 | 2.77E+01 |
| FA-W1 | 1.13E+09 |
| FA-W2 | 1.98E+07 |
| FA-W3 | 5.21E+04 |
| FA-W4 | 7.23E+00 |
| NA-W1 | 1.74E+09 |
| NA-W2 | 1.33E+07 |
| NA-W3 | 1.50E+04 |
| NA-W4 | 1.17E+01 |
| A-W1 | 3.80E+08 |
| A-W2 | 4.53E+04 |
| A-W3 | 1.03E+02 |
| DMA-W1 | 2.48E+03 |
| DMA-W2 | 1.87E+00 |
| SA-FA-W1 | 5.84E+02 |
| SA-FA-W2 | 4.20E+01 |
| SA-NA-W1 | 3.23E+00 |
| SA-A-W1 | 8.44E+02 |
| SA-A-W2 | 1.93E+04 |
| SA-A-W3 | 9.45E+01 |
| SA-A-W4 | 4.16E+00 |

|  |  |
| --- | --- |
| SA-DMA-W1 | 4.09E+03 |
| SA-DMA-W2 | 2.31E+02 |
| SA-DMA-W3 | 3.24E+01 |
| FA-NA-W1 | 5.39E+01 |
| FA-A-W1 | 4.56E+01 |
| NA-A-W1 | 1.26E+02 |

**Table S12.** Equilibrium concentrations of clusters that form at more than 1 cm-3 at 298 K. Initial concentrations of the monomers were: SA = 5.00E7, FA = 2.00E11, NA = 9.80E10, A = 2.00E11, DMA = 1.00E4.

|  |  |
| --- | --- |
| Cluster | 298.15 K |
| SA | 2.24E+07 |
| FA | 1.99E+11 |
| NA | 9.63E+10 |
| A | 2.00E+11 |
| DMA | 9.84E+03 |
| SA-FA | 1.58E+03 |
| SA-NA | 3.21E+00 |
| SA-A | 9.05E+03 |
| SA-DMA | 8.70E+01 |
| FA-NA | 1.76E+04 |
| FA-A | 2.90E+01 |
| NA-A | 2.14E+05 |
| SA-W1 | 2.29E+07 |
| SA-W2 | 4.41E+06 |
| SA-W3 | 2.23E+05 |
| SA-W4 | 1.83E+04 |
| SA-W5 | 2.77E+01 |
| FA-W1 | 1.13E+09 |
| FA-W2 | 1.98E+07 |
| FA-W3 | 5.21E+04 |
| FA-W4 | 7.23E+00 |
| NA-W1 | 1.74E+09 |
| NA-W2 | 1.33E+07 |
| NA-W3 | 1.50E+04 |
| NA-W4 | 1.17E+01 |
| A-W1 | 3.80E+08 |
| A-W2 | 4.53E+04 |
| A-W3 | 1.03E+02 |
| DMA-W1 | 2.48E+01 |
| SA-FA-W1 | 5.84E+02 |
| SA-FA-W2 | 4.20E+01 |
| SA-NA-W1 | 3.23E+00 |
| SA-A-W1 | 8.44E+02 |
| SA-A-W2 | 1.93E+04 |
| SA-A-W3 | 9.46E+01 |
| SA-A-W4 | 4.16E+00 |
| SA-DMA-W1 | 4.09E+01 |
| SA-DMA-W2 | 2.31E+00 |
| FA-NA-W1 | 5.39E+01 |
| FA-A-W1 | 4.56E+01 |

|  |  |
| --- | --- |
| NA-A-W1 | 1.26E+02 |

**Table S13.** Equilibrium concentrations of clusters that form at more than 1 cm-3 at 298 K. Initial concentrations of the monomers were: SA = 5.00E7, FA = 2.00E11, NA = 9.80E10, A = 2.00E11, DMA = 1.00E2.

|  |  |
| --- | --- |
| Cluster | 298.15 K |
| SA | 2.24E+07 |
| FA | 1.99E+11 |
| NA | 9.63E+10 |
| A | 2.00E+11 |
| DMA | 9.84E+01 |
| SA-FA | 1.58E+03 |
| SA-NA | 3.21E+00 |
| SA-A | 9.05E+03 |
| FA-NA | 1.76E+04 |
| FA-A | 2.90E+01 |
| NA-A | 2.14E+05 |
| SA-W1 | 2.29E+07 |
| SA-W2 | 4.41E+06 |
| SA-W3 | 2.23E+05 |
| SA-W4 | 1.83E+04 |
| SA-W5 | 2.77E+01 |
| FA-W1 | 7.61E+08 |
| FA-W2 | 1.05E+07 |
| FA-W3 | 1.46E+04 |
| FA-W4 | 1.21E+00 |
| NA-W1 | 1.74E+09 |
| NA-W2 | 1.33E+07 |
| NA-W3 | 1.50E+04 |
| NA-W4 | 1.17E+01 |
| A-W1 | 3.80E+08 |
| A-W2 | 4.53E+04 |
| A-W3 | 1.03E+02 |
| SA-FA-W1 | 1.58E+03 |
| SA-FA-W2 | 4.20E+01 |
| SA-NA-W1 | 3.23E+00 |
| SA-A-W1 | 8.44E+02 |
| SA-A-W2 | 1.93E+04 |
| SA-A-W3 | 9.46E+01 |
| SA-A-W4 | 4.16E+00 |
| FA-NA-W1 | 5.39E+01 |
| FA-A-W1 | 4.56E+01 |
| NA-A-W1 | 1.26E+02 |