**ACID MONOMERS**

**Table T1.** DLPNO-CCSD(T)/CBS//ωB97X-D/6-31++G\*\* Gibbs free energy changes (kcal mol-1) associated with the sequential hydration of one 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 |
| 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 |
| 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 |
| HCl + W ⇌ (HCl)(W) | 0.37 | 1.68 | 2.25 |
| (HCl)(W) + W ⇌ (HCl)(W)2 | -0.02 | 1.71 | 2.47 |
| (HCl)(W)2 + W ⇌ (HCl)(W)3 | -1.82 | -0.11 | 0.64 |

**BASE MONOMERS**

**Table T2.** DLPNO-CCSD(T)/CBS//ωB97X-D/6-31++G\*\* Gibbs free energy changes (kcal mol-1) associated with the sequential hydration of one base 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 |
| 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 |

**ACID-AMMONIA DIMERS**

**Table T3.** DLPNO-CCSD(T)/CBS//ωB97X-D/6-31++G\*\* Gibbs free energy changes (kcal mol-1) associated with the formation and sequential hydration of one acid and 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 |
| 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 |
| 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 |
| HCl + A ⇌ (HCl)(A) | -1.57 | -0.16 | 0.46 |
| (HCl)(A) + W ⇌ (HCl)(A)(W) | -0.12 | 1.59 | 2.35 |
| (HCl)(A)(W) + W ⇌ (HCl)(A)(W)2 | -3.66 | -1.83 | -1.03 |
| (HCl)(A)(W)2 + W ⇌ (HCl)(A)(W)3 | -4.37 | -2.63 | -1.86 |

**ACID-DMA DIMERS**

**Table T4.** DLPNO-CCSD(T)/CBS//ωB97X-D/6-31++G\*\* Gibbs free energy changes (kcal mol-1) associated with the formation and sequential hydration of one acid and dimethylamine 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 |
| 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 |
| 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 |
| HCl + DMA ⇌ (HCl)(DMA) | -4.84 | -3.12 | -2.35 |
| (HCl)(DMA) + W ⇌ (HCl)(DMA)(W) | -5.24 | -3.68 | -2.99 |
| (HCl)(DMA)(W) + W ⇌ (HCl)(DMA)(W)2 | -3.88 | -2.07 | -1.28 |
| (HCl)(DMA)(W)2 + W ⇌ (HCl)(DMA)(W)3 | -3.61 | -1.58 | -0.68 |
|  |  |  |  |
|  |  |  |  |
|  |  |  |  |

**ACID-BASE-BASE TRIMERS**

**Table T5.** DLPNO-CCSD(T)/CBS//ωB97X-D/6-31++G\*\* Gibbs free energy changes (kcal mol-1) associated with the formation and sequential hydration of one acid and ammonia and dimethylamine 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 |
| 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 |
| 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 |
| HCl + A + DMA ⇌ (HCl)(A)(DMA) | -8.93 | -5.59 | -4.11 |
| (HCl)(A)(DMA) + W ⇌ (HCl)(A)(DMA)(W) | -4.12 | -2.39 | -1.63 |
| (HCl)(A)(DMA)(W) + W ⇌ (HCl)(A)(DMA)(W)2 | -3.12 | -1.42 | -0.68 |
| (HCl)(A)(DMA)(W)2 + W ⇌ (HCl)(A)(DMA)(W)3 | -2.90 | -1.01 | -0.18 |

**ACID-ACID-ACID TRIMERS**

**Table T6.** DLPNO-CCSD(T)/CBS//ωB97X-D/6-31++G\*\* Gibbs free energy changes (kcal mol-1) associated with the formation and sequential hydration of three acid trimers 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 + HCl ⇌ (SA)(FA)(HCl) | -8.18 | -4.60 | -3.02 |
| (SA)(FA)(HCl) + W ⇌ (SA)(FA)(HCl)(W) | -4.22 | -2.49 | -1.72 |
| (SA)(FA)(HCl)(W) + W ⇌ (SA)(FA)(HCl)(W)2 | -1.30 | 0.37 | 1.08 |
| (SA)(FA)(HCl)(W)2 + W ⇌ (SA)(FA)(HCl)(W)3 | -1.54 | 0.34 | 1.13 |
| SA + NA + HCl ⇌ (SA)(NA)(HCl) | -4.51 | -1.07 | 0.44 |
| (SA)(NA)(HCl) + W ⇌ (SA)(NA)(HCl)(W) | -4.75 | -3.24 | -2.58 |
| (SA)(NA)(HCl)(W) + W ⇌ (SA)(NA)(HCl)(W)2 | -2.95 | -1.10 | -0.29 |
| (SA)(NA)(HCl)(W)2 + W ⇌ (SA)(NA)(HCl)(W)3 | -1.64 | 0.41 | 1.28 |

**ALL DRY TRIMERS, TETRAMERS, AND PENTAMERS**

**Table T7.** DLPNO-CCSD(T)/CBS//ωB97X-D/6-31++G\*\* Gibbs free energy changes (kcal mol-1) associated with the formation of all dry trimers, tetramers, and pentamer in the systems (SA)(FA)(NA)(A)(DMA)a, (SA)(FA)(HCl)(A)(DMA)b, and (SA)(NA)(HCl)(A)(DMA) at atmospherically relevant temperatures and 1 atm pressure. a – Reference 1. b – Reference 2.

|  |  |  |  |
| --- | --- | --- | --- |
| Cluster | 216.65 K | 273.15 K | 298.15 K |
| SA + FA + NA ⇌ (SA)(FA)(NA)a | -13.45 | -9.50 | -7.76 |
| SA + FA + HCl ⇌ (SA)(FA)(HCl)b | -8.18 | -4.60 | -3.02 |
| SA + NA + HCl ⇌ (SA)(NA)(HCl) | -4.51 | -1.07 | 0.44 |
| SA + FA + A ⇌ (SA)(FA)(A)a | -17.13 | -13.39 | -11.74 |
| SA + NA + A ⇌ (SA)(NA)(A)a | -15.74 | -11.99 | -10.40 |
| SA + HCl + A ⇌ (SA)(HCl)(A)b | -13.15 | -9.52 | -7.90 |
| FA + NA + A ⇌ (FA)(NA)(A)a | -8.42 | -5.25 | -3.87 |
| FA + HCl + A ⇌ (FA)(HCl)(A)b | -6.65 | -3.04 | -1.45 |
| NA + HCl + A ⇌ (NA)(HCl)(A) | -4.73 | -1.99 | -0.78 |
| SA + FA + DMA ⇌ (SA)(FA)(DMA)a | -26.08 | -22.19 | -20.48 |
| SA + NA + DMA ⇌ (SA)(NA)(DMA)a | -25.19 | -21.37 | -19.69 |
| SA + HCl + DMA ⇌ (SA)(HCl)(DMA)b | -23.69 | -20.10 | -18.50 |
| FA + NA + DMA ⇌ (FA)(NA)(DMA)a | -15.58 | -11.46 | -9.65 |
| FA + HCl + DMA ⇌ (FA)(HCl)(DMA)b | -15.73 | -12.09 | -10.48 |
| NA + HCl + DMA ⇌ (NA)(HCl)(DMA) | -14.50 | -10.92 | -9.34 |
| SA + FA + NA + A ⇌ (SA)(FA)(NA)(A)a | -24.77 | -18.82 | -16.28 |
| SA + FA + HCl + A ⇌ (SA)(FA)(HCl)(A)b | -20.20 | -14.83 | -12.47 |
| SA + NA + HCl + A ⇌ (SA)(NA)(HCl)(A) | -18.76 | -13.41 | -11.05 |
| SA + FA + NA + DMA ⇌ (SA)(FA)(NA)(DMA)a | -33.41 | -27.50 | -24.90 |
| SA + FA + HCl + DMA ⇌ (SA)(FA)(HCl)(DMA)b | -28.92 | -23.10 | -20.59 |
| SA + NA + HCl + DMA ⇌ (SA)(NA)(HCl)(DMA) | -29.60 | -24.16 | -21.76 |
| SA + FA + A + DMA ⇌ (SA)(FA)(A)(DMA)a | -30.63 | -24.98 | -22.49 |
| SA + NA + A + DMA ⇌ (SA)(NA)(A)(DMA)a | -33.31 | -27.23 | -24.55 |
| SA + HCl + A + DMA ⇌ (SA)(HCl)(A)(DMA)b | -36.33 | -30.87 | -28.45 |
| FA + NA + A + DMA ⇌ (FA)(NA)(A)(DMA)a | -19.35 | -13.94 | -11.57 |
| FA + HCl + A + DMA ⇌ (FA)(HCl)(A)(DMA)b | -17.85 | -12.63 | -10.32 |
| NA + HCl + A + DMA ⇌ (NA)(HCl)(A)(DMA) | -24.37 | -18.73 | -16.25 |
| SA + FA + NA + A + DMA ⇌ (SA)(FA)(NA)(A)(DMA)a | -39.56 | -31.53 | -28.00 |
| SA + FA + HCl + A + DMA ⇌ (SA)(FA)(HCl)(A)(DMA)b | -43.08 | -35.34 | -32.02 |
| SA + NA + HCl + A + DMA ⇌ (SA)(NA)(HCl)(A)(DMA) | -42.74 | -35.29 | -32.00 |

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2. O. M. Longsworth, C. J. Bready and G. C. Shields, The Driving Effects of Common Atmospheric Molecules for Formation of Clusters: The Case of Sulfuric Acid, Formic Acid, Hydrochloric Acid, Ammonia, and Dimethyl Amine, *Environmental Science: Atmospheres*, 2023, **submitted**.