**Supporting Information**

The Driving Effects of Common Atmospheric Molecules for Formation of Prenucleation Clusters: The Case of Sulfuric Acid, Formic Acid, Nitric Acid, Ammonia, and Dimethyl Amine

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Section 1: Figures of Minimum Energy Clusters

Section 2: Sequential Hydration Tables

Section 3: Energy Tables

Section 4: Optimized Geometries

Section 5: Derivation of Complete Basis Set Limit Extrapolation Formulas

Section 6: Example Calculation of Stepwise Energies

**Section 1: Figures of Minimum Energy Clusters**

The figures of the minimum energy monomers, dimers, and trimer systems consisting of a single acid with two bases and three acids are present in the word document titled “Figures of Cluster Minima”.

**Section 2: Tables**

The comparison of aug-cc-pVnZ and cc-pVnZ from prior work, the comparison of scaled and unscaled ωB97X-D energies, the energies of formation and sequential hydration for the monomers, dimers, and trimer systems consisting of a single acid with two bases and three acids, and the equilibrium concentrations of clusters using different parameters are present in the word document titled “Tables”.

**Section 3: Energetics of Structures**

The electronic energies, G correction values, and DLPNO-CCSD(T) electronic energies with the cc-pVnZ basis sets (n=D,T,Q) are present in excel files under the folder titled “Energetics of Structures”. The clusters are organized based on the number of molecules (not including water) present in the cluster, with individual sheets inside the excel files containing the clusters.

**Section 4: Optimized Geometries**

The ωB97Xd coordinate files of all structures within one kcal mol-1 of the ∆G˚ minimum for each system are presented as .xyz files within the folder titled “XYZ Files”. The .xyz files are organized based on the number of molecules in the cluster (not including water), the cluster itself, and the number of waters present.

**Section 5: Derivation of Complete Basis Set Limit Extrapolation Formulas**

The CBS extrapolation formulas are shown in the word document titled “CBS Extrapolation Formulas”.

**Section 6: Example Calculation of Stepwise Energies**

An example for how to calculate the stepwise energies from the energy tables is given in the document titled “Stepwise Energy Calculation”.