Supplementary material

1 Calculating the binding energy, free energy of formation and evaporation rate of the sulfuric acid dimer from first principles

For single, covalently-bound, closed-shell molecules, established multistep methods such as the Gn series are able to provide formation and reaction energies accurate to within 1 kcal/mol. Unfortunately, the suitability of these methods for more weakly bound clusters is questionable. For example, geometry optimizations are typically carried out using basis sets without any diffuse functions, which may lead to significant errors. The recently developed Wn series of methods would undoubtedly provide sufficient accuracy also for cluster formation energies, but their applicability is unfortunately limited to very small systems (*e.g.* water dimers). Thus, evaluating the binding and formation free energy of the sulfuric acid dimer as accurately as possible (given the limitations of current computer hardware) requires some "manual" combining of different methods. In this paper, we have used a variety of advanced quantum chemical methods to calculate the binding energy and formation free energy of the sulfuric acid dimer. Ideally, we would have liked to perform calculations such as those recently done for HSO_3 and $HOSO$ (Klopper *et al.*, 2008; Wheeler and Schaefer, 2009) systems, with high-level correlation treatment for the binding energies combined with large basis sets and coupled-cluster – level geometry optimizations. The size of our system (10 heavy atoms) renders coupled-cluster geometry and vibrational frequency calculations impossible. Thus, we are forced to use MP2 and DFT methods for these steps, and use advanced wavefunction – based methods for energy corrections only. Nevertheless, the values presented here are significantly more reliable than any earlier results, and also serve as a useful benchmark for studies on even larger clusters.

Computational details

RI-MP2 calculations were performed using the Turbomole 6.0 program (Ahlrichs *et al.*, 1989). CCSD(T) and CCSD calculations were performed using the Molpro 2006.1 program (Werner *et al.*, 2006). Douglas-Kroll-Hess calculations (at the HF and MP2 levels) and PW91 calculations (including anharmonic frequency calculations), were performed using the Gaussian 03 program suite (Frisch *et al.*, 2004). Basis sets used were the 6-311++G(2d,2p) and 6-311++G(3df,3pd) Pople-style basis sets and the correlation-consistent basis sets aug-cc-pVXZ, aug-cc-pV(X+d)Z, aug-cc-pwCVXZ, cc-pVXZ and cc-pVXZ-DK, where X=T, Q, 5 (not all combinations were used). Default convergence criteria for the programs in question were used except for the anharmonic frequency calculations, where tight convergence criteria and the ultrafine integration grid were used. Unless otherwise noted, all correlated wavefunction-based calculations use the frozen core approximation.

Results

First, the sulfuric acid monomer and the three dimer configurations/isomers (with c1, c2 and ci symmetry; see Figure S1 for the structures) were optimized at the RI-MP2/aug-cc-pV(T+d)Z level. Next, four different energy corrections were computed, corresponding to higher-order correlation, basis-set effects, core-valence correlation and scalar relativistic effects. (We have omitted Born-Oppenheimer corrections as their contribution is likely smaller.) To estimate the thermal contributions to the enthalpy and entropy, we further performed a new geometry optimization followed by an anharmonic frequency calculation at the PW91/6-311++G(3df,3pd)

level using density fitting, based on the results by Nadykto *et al.* (2007) showing that this method results in reasonably reliable vibrational spectra for sulfuric acid hydrates.
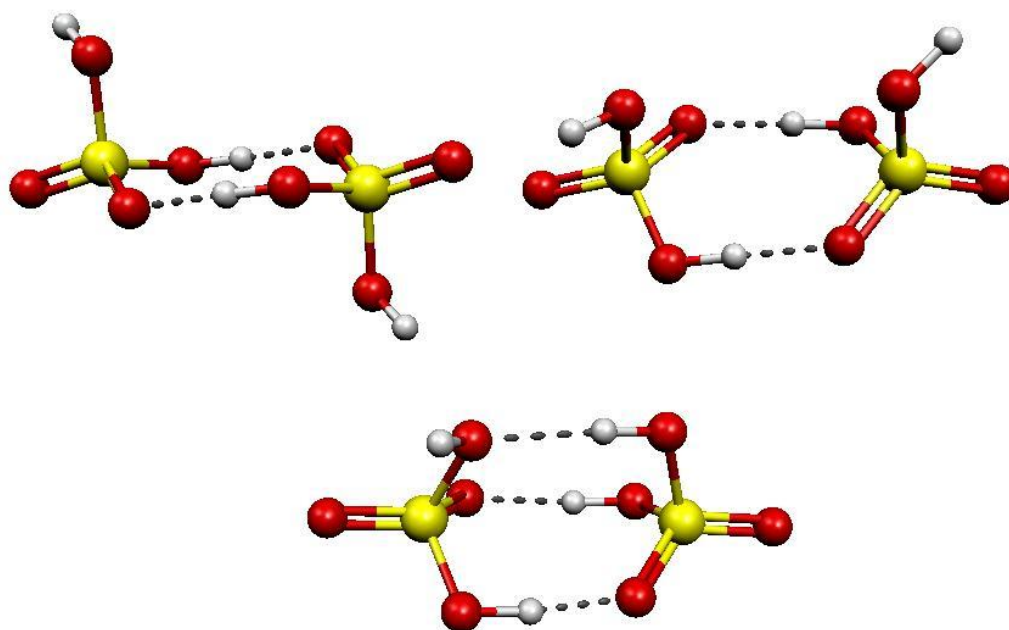

Figure S1.1. Structure of the $(H_2SO_4)_2$ clusters with ci symmetry (top left), c2 symmetry (top right) and c1 symmetry (bottom). Hydrogen bonds are indicated by dashed lines. Color coding: yellow = sulfur, red = oxygen and white = hydrogen.

Higher-order correlation

The effect of higher-order correlation was estimated by performing a CCSD(T) energy calculation using the largest basis set feasible on our computer hardware. For the c1 and ci configurations, this proved to be 6-311++G(2d,2p). For the c2 configuration, in which symmetry could be used to reduce the number of configuration state functions that need to be evaluated, the largest Pople-style basis set 6-311++G(3pd,3df) basis set could also be used. The CCSD(T) results were then compared to MP2 values with the same basis sets. The results are shown in Table S2. For comparison, also CCSD values (obtained as a intermediate step of the CCSD(T) calculations) are given. For the 6-311++G(2d,2p) basis set, the difference between CCSD(T) and MP2 binding energies are about 0.35 kcal/mol for all three isomers, with CCSD(T) predicting somewhat stronger binding energies. However, the CCSD(T) – CCSD differences are considerably larger, and also more variable, ranging from 1.4 kcal/mol for the c1 isomer to 0.85 for the c2 and ci isomers. The difference between CCSD(T) results obtained with the 6-311++G(3df,3pd) and 6-311++G(2d,2p) basis sets for the c2 dimer are slightly surprising: the larger basis set results in a binding energy that is over 2 kcal/mol higher, indicating that basis-set superposition (which would tend to decrease the binding energies as the basis set size increases) is not the main error source in the 6-311++G(2d,2p) calculations. The MP2-CCSD(T) difference, however, changed only by 0.05 kcal/mol, to about 0.3 kcal/mol. This indicates that while multiple polarization functions (and probably also polarization functions corresponding to higher angular momentum quantum numbers) are required for accurate absolute binding energies, the basis-set convergence of MP2 and CCSD(T) for this system are probably similar enough that the approach employed here (where the basis-set limit is extrapolated

at the MP2 level, while higher-order correlation is evaluated using a medium-sized basis set) is valid.

	$(H_2SO_4)_2$, c1 symmetry	$(H_2SO_4)_2$, c2 symmetry	$(H_2SO_4)_2$, ci symmetry
MP2/6-311++G(2d,2p)	-17.88	-17.48	-17.61
CCSD/6-311++G(2d,2p)	-16.82	-16.99	-17.10
CCSD(T)/6-311++G(2d,2p)	-18.23	-17.84	-17.96
MP2/6-311++G(3df,3pd)	-	-19.71	-
CCSD/6-311++G(3df,3pd)	-	-19.15	-
CCSD(T)/6-311++G(3df,3pd)	-	-20.00	-

Table S1.1. Electronic energies (ΔE_{elec}) for the formation of sulfuric acid dimers (three different isomers) from monomers, at various levels of theory including higher-level correlation.

Basis-set effects

Basis set – effects beyond the aug-cc-pV(T+d)Z level were evaluated by performing single-point calculations using the RI-MP2 method together the larger basis sets aug-cc-pV(Q+d)Z and aug-cc-pV(5+d)Z. The results are presented in Table S3. Counterpoise corrections computed at the MP2/aug-cc-pV(T+d)Z level, as well as Hartree-Fock level binding energies, are also shown for reference. It can be seen from Table S3 that, contrary to our previous study on sulfuric acid – water complexes, increasing the size of the basis set beyond aug-cc-pV(T+d)Z has a fairly large, and systematic, effect on the binding energy of all three configurations of the sulfuric acid dimer. The aug-cc-pV(5+d)Z binding energy is about 1 kcal/mol lower than the aug-cc-pV(T+d)Z one for the c1 isomer, and about 0.8 kcal/mol lower for the ci and c2 isomers. This is very likely due to basis-set superposition error (BSSE). It should be noted that the counterpoise correction is still more than twice as large as the difference between aug-cc-pV(T+d)Z and aug-cc-pV(5+d)Z results. This indicates that while BSSE at the aug-cc-pV(T+d)Z level is non-negligible, it is still significantly overestimated by the counterpoise method, as previously found for the water dimer when large basis sets with multiple diffuse functions are used (Feller, 1992). It should further be noted that if basis sets even smaller than aug-cc-pV(T+d)Z are used, the counterpoise corrections lead to wildly inaccurate binding energies. For example, application of counterpoise corrections to the MP2/6-311++G(2d,2p) results given in Table S.1.1 lead to binding energies around 13 kcal/mol for all three isomers, which are likely (given the higher-level results presented here) to be at least 4-5 kcal/mol too small.

Table S1.2 also shows that correlation plays a much larger role in the binding energy of the c1 dimer than the c2 and ci isomers. The MP2-HF difference is over 7 kcal/mol for the c1 dimer (and all basis sets used), compared to around 4-4.5 kcal/mol for the c2 and ci dimers. This is likely to explain the larger CCSD(T) – CCSD differences observed in Table S2 for this isomer. We then attempted to extrapolate the basis-set limit HF and correlation energies (defined as the MP2-HF difference) using an exponential formula for the former and a polynomial formula for the latter (as recommended *e.g.* by Jensen, 2007). However, the exponential extrapolation of the HF energies led to unphysical results; when applied to the absolute HF energies the resulting "HF/aug-cc-pV(∞+d)Z" ΔE_{elec} was around +120 kcal/mol for all three dimer configurations. The reason for this might be the fact that the geometry was kept fixed at the RI-MP2/aug-cc-pV(T+d)Z level; as the basis set size for the HF calculation increases, the "optimal" HF geometry may drift further and further from the one used here, leading to a significant (and articifial) destabilization of the dimer structures with respect to the fairly rigid monomer. We thus estimated the "basis-set limit" binding

energy by combining the HF/aug-cc-pV(5+d)Z binding energy with the basis-set limit ("aug-cc-pV(∞+d)Z") correlation energy computed from the RI-MP2/aug-cc-pV(Q+d)Z and RI-MP2/aug-cc-pV(5+d)Z energies using the two-point formula given by Jensen (2007).

	$(H_2SO_4)_2$, c1 symmetry	$(H_2SO_4)_2$, c2 symmetry	$(H_2SO_4)_2$, ci symmetry
HF/aug-cc-pV(T+d)Z	-11.23	-14.15	-14.34
HF/aug-cc-pV(Q+d)Z	-11.07	-14.00	-14.18
HF/aug-cc-pV(5+d)Z	-10.89	-13.85	-14.03
RI-MP2/aug-cc-pV(T+d)Z	-19.27 (+2.68)	-18.86 (+2.26)	-19.03 (+2.27)
RI-MP2/aug-cc-pV(Q+d)Z	-18.69	-18.40	-18.57
RI-MP2/aug-cc-pV(5+d)Z	-18.23	-18.02	-18.19
Extrapolated	-17.94	-17.78	-17.94

Table S1.2. Electronic energies (ΔE_{elec}) for the formation of sulfuric acid dimers (three different isomers) from monomers, at the HF and RI-MP2 level, using three different basis sets. Extrapolated values correspond to HF/aug-cc-pV(5+d)Z with the correlation energy extrapolated from RI-MP2/aug-cc-pV(Q+d)Z and RI-MP2/aug-cc-pV(5+d)Z energies using a two-point polynomial formula, see text for details. The values in brackets correspond to the counterpoise correction.

Core-valence correlation

The effect of including the core electrons in the correlation treatment was tested by computing the binding energies of the sulfuric acid dimer using the RI-MP2 method together with the aug-cc-pwCVTZ basis set. These were then compared to the corresponding aug-cc-pVTZ values (Unfortunately, core-valence-polarized basis sets with extra d – basis functions for sulfur are not available.) The results, shown in Table S4, indicate that the effect of core correlation is moderately small, but surprisingly variable: for the c1 isomer, including core correlation decreases the binding energy by almost 0.2 kcal/mol, while the effect on the c2 isomer is only 0.005 kcal/mol. This is qualitatively in line with the observation above that correlation plays a larger role in the binding of the c1 dimer compared to the two others.

	$(H_2SO_4)_2$, c1 symmetry	$(H_2SO_4)_2$, c2 symmetry	$(H_2SO_4)_2$, ci symmetry
RI-MP2(FC)/aug-cc-pVTZ	-19.29	-18.79	-18.99
RI-MP2(full)/aug-cc-pw(CVTZ)	-19.10	-18.78	-18.94

Table S1.3. Electronic energies (ΔE_{elec}) for the formation of sulfuric acid dimers (three different isomers) at the RI-MP2 level using a triple-Z basis set, with and without core correlation.

Scalar relativistic effects

Scalar relativistic effects were estimated by performing a MP2 calculation with the Douglas-Kroll-Hess (DKH) one-electron Hamiltonian and the cc-pVTZ-DK basis set. (The basis corresponds to cc-pVTZ, but has been recontracted to match the relativistic atomic orbitals). These were then compared to normal MP2/cc-pVTZ results. (Unfortunately, neither diffuse functions nor additional d- basis functions for sulfur are available for the relativistically recontracted basis sets).

The results, shown in Table S1.4, indicate that relativistic effects are small, and uniform: the binding energy of all three configurations of the sulfuric acid dimer decrease by about 0.1 kcal/mol when DKH scalar relativistic corrections are applied. It can also be seen from Table S5 that the scalar relativistic effects are well captured already at the HF level, as discussed by de Jong *et al.* (2001).

	$(H_2SO_4)_2$, c1 symmetry	$(H_2SO_4)_2$, c2 symmetry	$(H_2SO_4)_2$, ci symmetry
HF/cc-pVTZ	-11.80	-14.58	-14.78
MP2/cc-pVTZ	-19.11	-18.60	-18.78
HF(DKH)/cc-pVTZ-DK	-11.70	-14.47	-14.67
MP2(DKH)/cc-pVTZ-DK	-19.00	-18.47	-18.65

Table S1.4. Electronic energies (ΔE_{elec}) for the formation of sulfuric acid dimers (three different isomers) at the HF and MP2 level using a triple-Z basis set, with and without scalar relativistic corrections.

Thermal contributions and anharmonic effects

PW91/6-311++G(3df,3pd) − level harmonic and anharmonic thermal contribution to the formation enthalpies, entropies and Gibbs free energies of the sulfuric acid dimer configurations are shown in Table S6. The anharmonic values given here have been computed by using the anharmonic fundamental vibrational frequencies in the harmonic partition functions. We attempted to compute thermochemical parameters also using the "full" anharmonic partition functions, as described in our recent paper on sulfuric acid hydrates (Kurtén *et al.*, 2007). However, this led to unphysical results, especially for the c2 isomer, where *e.g.* the absolute entropy values became negative. Even for the c1 and ci isomers, the "full" anharmonic free energies of dimer formation were predicted to be less negative than those obtained using the "fundamental frequencies" approach, which is somewhat counterintuitive given the fact that clusters are generally known to be more anharmonic than isolated monomers. The reason for these strange results (and also the difference to published MP2/aug-cc-pV(D+d)Z anharmonic results on sulfuric acid hydrates) is probably related to the fact that PW91 harmonic vibrational frequencies are already fairly close to the real fundamental frequencies, meaning that the "intra-mode" anharmonicities (and corresponding anharmonic constants) are fairly small. The perturbative anharmonic treatment used here will then mainly yield contributions from couplings between the different modes, and these can, in principle, either increase or decrease the vibrational frequencies (whereas intra-mode anharmonicity will always decrease the frequency). Especially for the c2 isomer, some anharmonic fundamental vibrational frequencies were many times larger than the corresponding harmonic frequencies, which led to spurious results when the anharmonic partition functions were computed. Given these results, it is indeed questionable whether the inclusion of anharmonic effects at the PW91/6-311++G(3df,3pd) level makes the computed thermochemical parameters at all more reliable. The anharmonic effects reported here should be considered as qualitative" estimates rather than quantitatively reliable values, and especially the values for the c2 cluster should be treated with some caution. Fortunately, this cluster proved not to be the minimum-energy (or minimum free energy) isomer, so its thermochemical parameters are not particularly relevant for determining the evaporation rate.

	$(H_2SO_4)_2$, c1 symmetry	$(H_2SO_4)_2$, c2 symmetry	$(H_2SO_4)_2$, ci symmetry
ΔH_{therm}, harmonic	+0.94 kcal/mol	+0.85 kcal/mol	+0.84 kcal/mol

ΔS_{therm}, harmonic	-39.17 cal/Kmol	-34.28 cal/Kmol	-34.56 cal/Kmol
ΔG_{therm}, harmonic	+12.62 kcal/mol	+11.07 kcal/mol	+11.14 kcal/mol
ΔH_{therm}, anharmonic	+0.68 kcal/mol	+0.43 kcal/mol	+0.61 kcal/mol
ΔS_{therm}, anharmonic	-39.98 cal/Kmol	-40.49 cal/Kmol	-32.25 cal/Kmol
ΔG_{therm}, anharmonic	+12.60 kcal/mol	+12.51 kcal/mol	+10.22 kcal/mol

Table S1.5. Thermal contributions to the enthalpy (ΔH_{therm}), entropy (ΔS_{therm}) and Gibbs free energy (ΔG_{therm}) of formation of sulfuric acid dimers (three different isomers) from monomers, at the PW91/6-311++G(3df,3pd) level with density fitting, using harmonic or anharmonic fundamental vibrational frequencies. All values correspond to 298.15 K and 1 atm.

Summary of correction terms

	$(H_2SO_4)_2$, c1 symmetry	$(H_2SO_4)_2$, c2 symmetry	$(H_2SO_4)_2$, ci symmetry
RI-MP2/aug-cc-pV(T+d)Z ΔE_{elec}	-19.27	-18.86	-19.03
Higher-order correlation correction	-0.35	-0.36	-0.36
Basis set correction	+1.32	+1.08	+1.09
Core correlation	+0.20	+0.00	+0.05
Scalar relativistic effects	+0.11	+0.13	+0.12
Corrected ΔE_{elec}	-17.99	-18.01	-18.13
Harmonic ΔG	-5.37	-6.94	-6.98
Anharmonic ΔG	-5.39	-5.50	-7.91

Table S1.6. A summary of the computed corrections to the electronic energies (ΔE_{elec}) for the formation of sulfuric acid dimers (three different isomers), and the corresponding harmonic and anharmonic Gibbs free energies of formation (at 298.15 K and 1 atm reference pressure).

Combining the MP2/aug-cc-pV(T+d)Z energy with the four different corrections computed here results in binding energies of -17.99, -18.01 and -18.14 kcal/mol for the configurations with c1, c2 and ci symmetry, respectively. See Table S7 for a summary of all energy corrections. These value are remarkably close to each other, and also fairly close to lower-level values previously published in the literature, and in this paper. Comparing the values here with those computed for the sulfuric acid hydrates (Kurtén et al., 2007) shows that the claim by Rozenberg and Loewenschuss (2009) that the sulfuric acid dimer is more weakly bound than sulfuric acid monohydrate is almost certainly incorrect.

2. RICC2B3 and CBS-QB3 data for larger clusters

We have extended the calculations for these two methods to larger clusters. The limit for CBS-QB3 calculations given our computer resources was found to be a cluster with three sulfuric acid molecules and one ammonia molecule. Table S-2.1 compares the formation free Gibbs energies from monomers for the two methods:

	RICC2B3	CBS-QB3	Difference
$(H_2SO_4)_2$	-7.89	-8.66	0.78

$(H_2SO_4)_3$	-14.30	-15.85	1.55
$H_2SO_4 \cdot (CH_3)_2NH$	-15.40	-14.37	-1.03
$(H_2SO_4)_2 \cdot (CH_3)_2NH$	-34.88	-35.08	0.21
$H_2SO_4 \cdot NH_3$	-7.61	-7.34	-0.27
$(H_2SO_4)_2 \cdot NH_3$	-23.82	-24.47	0.65
$(H_2SO_4)_3 \cdot NH_3$	-33.94	-35.58	1.64
$H_2SO_4 \cdot (NH_3)_2$	-12.43	-12.00	-0.42
$(H_2SO_4)_2 \cdot (NH_3)_2$	-33.32	-33.33	0.01
$H_2SO_4 \cdot ((CH_3)_2NH)_2$	-20.29	-18.47	-1.82
$(NH_3)_2$	4.20	4.27	-0.08
$((CH_3)_2NH)_2$	3.54	3.94	-0.40

As can be seen, the largest difference found is -1.82 kcal/mol, and the average difference is 0.74 kcal/mol. If we compare the cpu time consumed by both methods (Figure S-2.1) we can see how RICC2B3 method is several orders of magnitude faster than CBS-QB3 method.
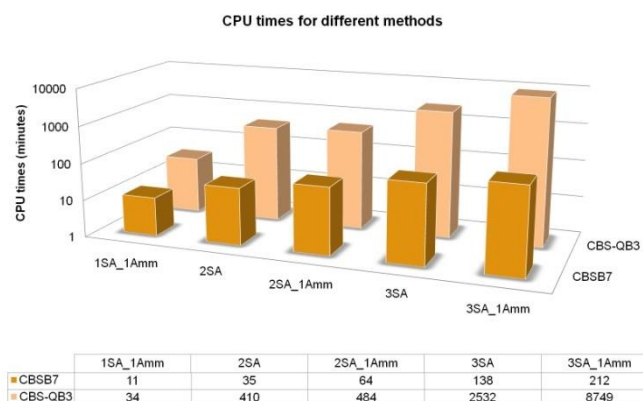

	1SA_1Amm	2SA	2SA_1Amm	3SA	3SA_1Amm
CBSB7	11	35	64	138	212
CBS-QB3	34	410	484	2532	8749

Figure S-2.1, CPU times for CBS-QB3 and RICC2B3 methods in minutes.

3. Gibbs free energies of formation, enthalpies and entropies from monomers

The following table shows Gibbs free energies of formation, enthalpies and entropies from monomers at 298.16K for all the clusters studied in this work.

Table S-3.1

		(m) ammonia			
Sulfuric acid (n)	0	1	2	3	4
0	--	--	4.20	8.70	12.01
1	--	-7.61	-12.43	-13.00	-15.05
2	-7.89	-23.82	-33.32	-38.25	-41.16
3	-14.30	-33.94	-49.40	-63.53	-69.43
4	-22.78	-42.31	-60.47	-77.68	-89.51

	(m) DMA			
Sulfuric acid (n)	1	2	3	4
0	--	3.54	5.59	5.39
1	-15.40	-20.29	-25.08	-28.46
2	-34.88	-56.17	-62.70	-68.72
3	-47.80	-67.26	-89.94	-105.71

4	-55.42	-82.79	-105.09	-124.05

Formation free Gibbs energies from monomers at 298.15K in kcal/mol

	(m) ammonia				
Sulfuric acid (n)	0	1	2	3	4
0	--	--	-1.62	-7.45	-12.30
1	--	-16.00	-29.70	-40.45	-51.30
2	-17.85	-45.00	-64.46	-79.53	-91.64
3	-35.82	-66.06	-92.09	-117.57	-132.80
4	-52.60	-87.40	-115.13	-143.63	-164.35

	(m) DMA			
Sulfuric acid (n)	1	2	3	4
0	--	-3.17	-12.68	-21.30
1	-24.65	-40.08	-56.99	-72.24
2	-57.06	-87.52	-108.24	-125.73
3	-81.46	-113.58	-146.59	-177.69
4	-101.00	-140.76	-173.65	-204.29

Enthalpies from monomers in kcal/mol

	(m) ammonia				
Sulfuric acid (n)	0	1	2	3	4
0	--	--	-19.52	-55.15	-81.56
1	--	-28.14	-57.92	-92.07	-121.57
2	-33.42	-71.02	-104.45	-138.44	-169.30
3	-72.19	-107.72	-143.17	-184.21	-212.56
4	-100.03	-151.24	-183.34	-221.20	-251.02

	(m) DMA			
Sulfuric acid (n)	1	2	3	4
0	--	-22.52	-61.30	-89.52
1	-31.01	-66.37	-107.02	-146.83
2	-74.40	-105.16	-152.75	-191.22
3	-112.90	-155.37	-190.01	-231.38
4	-152.88	-194.43	-229.95	-269.13

Entropies from monomers in cal/K·mol

4. Evaporation rates

Table S-4.1 contains all the evaporation rates for pure sulfuric acid, ammonia and DMA clusters.

Cluster	Evaporation rate (1/s)
$(H_2SO_4)_2$	$1.40 \cdot 10^4$
$(H_2SO_4)_3$	$1.88 \cdot 10^5$
$(H_2SO_4)_4$	$6.30 \cdot 10^3$
$(NH_3)_2$	$1.45 \cdot 10^{13}$
$(NH_3)_3$	$2.66 \cdot 10^{13}$
$(NH_3)_4$	$3.93 \cdot 10^{12}$
$((CH_3)_2NH)_2$	$5.69 \cdot 10^{12}$
$((CH_3)_2NH)_3$	$5.09 \cdot 10^{11}$
$((CH_3)_2NH)_4$	$1.26 \cdot 10^{10}$

Table S-4.2 non-monomer evaporations

$(H_2SO_4)_n (NH_3)_m$		Evaporation rate (1/s)		
n	m	$(H_2SO_4)_1 \cdot (NH_3)_1$	$(H_2SO_4)_2 \cdot (NH_3)_1$	$(H_2SO_4)_2 \cdot (NH_3)_2$
2	1	$1.22 \cdot 10^{-2}$		
3	1	$3.05 \cdot 10^{-4}$	$3.83 \cdot 10^{2}$	
4	1	$1.21 \cdot 10^{-5}$	$1.71 \cdot 10^{2}$	
1	2	$4.11 \cdot 10^{6}$		
2	2	$5.45 \cdot 10^{-4}$	$1.83 \cdot 10^{3}$	
3	2	$7.15 \cdot 10^{-4}$	$7.15 \cdot 10^{-4}$	$1.73 \cdot 10^{-2}$
4	2	$1.54 \cdot 10^{-4}$	4.14	$7.98 \cdot 10^{-5}$
1	3	$1.20 \cdot 10^{3}$		
2	3	$4.81 \cdot 10^{-4}$	$3.27 \cdot 10^{-4}$	$4.40 \cdot 10^{6}$
3	3	$3.03 \cdot 10^{-7}$	$1.12 \cdot 10^{-10}$	$3.03 \cdot 10^{-7}$
4	3	$8.36 \cdot 10^{-6}$	$9.61 \cdot 10^{-6}$	$9.61 \cdot 10^{-6}$
1	4	$1.86 \cdot 10^{-2}$		
2	4	$9.72 \cdot 10^{-6}$	$1.15 \cdot 10^{-9}$	23.53
3	4	$6.16 \cdot 10^{-8}$	$1.43 \cdot 10^{-14}$	$5.09 \cdot 10^{-8}$
4	4	$4.21 \cdot 10^{-4}$	$8.70 \cdot 10^{-11}$	$1.95 \cdot 10^{-7}$
$(H_2SO_4)_n((CH_3)_2NH)_m$		Evaporation rate (1/s)		
n	m	$(H_2SO_4)_1((CH_3)_2NH)_1$	$(H_2SO_4)_2((CH_3)_2NH)_1$	$(H_2SO_4)_2((CH_3)_2NH)_2$
2	1	$5.47 \cdot 10^{-5}$		
3	1	$1.17 \cdot 10^{-8}$	3.71	
4	1	$1.61 \cdot 10^{-9}$	5.74	
1	2	$3.76 \cdot 10^{6}$		
2	2	$3.05 \cdot 10^{-9}$	$3.91 \cdot 10^{-6}$	
3	2	$4.37 \cdot 10^{-3}$	$4.37 \cdot 10^{-3}$	90.80
4	2	$5.56 \cdot 10^{-5}$	3.34	$2.18 \cdot 10^{-4}$
1	3	2.89		
2	3	$2.09 \cdot 10^{-10}$	$1.52 \cdot 10^{-13}$	$2.89 \cdot 10^{5}$
3	3	$4.56 \cdot 10^{-4}$	$4.24 \cdot 10^{-16}$	$4.56 \cdot 10^{-4}$
4	3	$4.98 \cdot 10^{-7}$	0.65	0.65
1	4	$3.11 \cdot 10^{-4}$		
2	4	$2.81 \cdot 10^{-11}$	$1.84 \cdot 10^{-19}$	$2.60 \cdot 10^{-2}$
3	4	$5.38 \cdot 10^{-8}$	$2.59 \cdot 10^{-21}$	$3.31 \cdot 10^{-9}$
4	4	$2.83 \cdot 10^{-4}$	$5.32 \cdot 10^{-10}$	35.29

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