

Supporting Information

Rayleigh Light Scattering Properties of Atmospheric Molecular Clusters Consisting of Sulfuric Acid and Bases

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Stepwise formation free energies

Sulfuric acid - ammonia system

Cluster	PW91 _{red}	M06-2X _{red}	ω B97X-D _{red}	M06-2X/6-311++G(3df,3pd)
sa+a	-7.51	-6.72	-6.05	-7.43
(1sa)(1a)+sa	-11.82	-14.71	-14.51	-13.43
(1sa)(1a)+a	-3.93	-4.91	-4.63	-5.45
(2sa)(1a)+sa	-7.04	-8.47	-7.74	-10.23
(2sa)(1a)+a	-8.25	-4.73	-6.71	-6.29
(1sa)(2a)+sa	-16.14	-14.52	-16.59	-14.27
(1sa)(2a)+a	+0.78	+3.27	+1.11	+3.85
(2sa)(2a)+sa	-11.47	-15.01	-15.16	-15.50
(2sa)(2a)+a	-2.23	-4.35	-3.60	-3.62
(3sa)(2a)+sa	-6.28	-11.34	-8.34	-10.45
(3sa)(2a)+a	-11.01	-11.24	-10.28	-11.07
(2sa)(3a)+sa	-20.25	-21.91	-21.84	-22.95
(2sa)(3a)+a	-1.73	-1.06	-2.14	-1.24
(3sa)(3a)+sa	-7.42	-13.39	-10.24	-12.00
(3sa)(3a)+a	-4.23	-1.99	-3.80	-2.09
(3sa)(4a)+sa	-15.05	-19.68	-17.32	-20.07
(4sa)(3a)+a	-11.86	-8.28	-10.87	-10.16
(1sa)(1a)+(1sa)(1a)	-12.55	-12.71	-15.17	-12.29
(2sa)(2a)+(1sa)(1a)	-14.97	-19.53	-19.39	-19.14
(3sa)(3a)+(1sa)(1a)	-11.77	-14.94	-15.06	-14.73
(3sa)(1a)+sa	-3.81	-8.84	-6.02	-8.30
(3sa)(1a)+a	-12.68	-11.26	-14.13	-11.56
(1sa)(3a)+sa	-19.15	-22.13	-21.31	-21.74
(1sa)(3a)+a	-0.41	-0.69	+0.72	-1.81
(1sa)(4a)+sa	-20.47	-22.51	-24.17	-21.17
(4sa)(1a)+a	-15.15	-13.77	-16.45	-13.71
(2sa)(4a)+sa	-22.75	-22.83	-23.49	-23.81
(4sa)(2a)+a	-12.16	-13.29	-12.19	-12.63
(2sa)(1a)+(1sa)(1a)	-12.20	-13.01	-15.82	-14.36
(1sa)(2a)+(1sa)(1a)	-10.86	-12.14	-14.14	-10.46
(3sa)(1a)+(1sa)(1a)	-11.44	-15.88	-16.42	-14.57
(1sa)(3a)+(1sa)(1a)	-13.37	-16.47	-17.40	-15.55
(3sa)(2a)+(1sa)(1a)	-10.93	-17.91	-14.47	-15.64
(2sa)(3a)+(1sa)(1a)	-16.97	-17.17	-19.58	-17.61

Table 1: Stepwise gibbs free energy of $(\text{H}_2\text{SO}_4)_a(\text{NH}_3)_b$ cluster formation in kcal/mol.

Stepwise formation free energies

Sulfuric acid - dimethylamine system

Cluster	PW91 _{red}	M06-2X _{red}	ω B97X-D _{red}	M06-2X/6-311++G(3df,3pd)
sa+dma	-11.71	-10.62	-13.10	-11.42
(1sa)(1dma)+sa	-15.18	-20.15	-18.35	-19.33
(1sa)(1dma)+dma	-4.18	-4.19	-1.87	-3.01
(2sa)(1dma)+sa	-6.85	-11.86	-9.69	-12.23
(2sa)(1dma)+dma	-11.71	-10.92	-12.20	-11.31
(1sa)(2dma)+sa	-22.71	-26.88	-28.68	-27.63
(1sa)(2dma)+dma	+1.31	-2.68	-2.68	-3.23
(2sa)(2dma)+sa	-5.45	-15.79	-10.56	-15.88
(2sa)(2dma)+dma	-4.94	-6.30	-4.98	-5.78
(3sa)(2dma)+sa	-16.90	-15.98	-15.78	-15.54
(3sa)(2dma)+dma	-19.77	-15.69	-21.42	-16.43
(2sa)(3dma)+sa	-20.28	-25.18	-27.00	-26.53
(2sa)(3dma)+dma	-2.85	-3.16	-6.76	-5.16
(3sa)(3dma)+sa	-11.59	-15.05	-12.47	-14.62
(3sa)(3dma)+dma	-9.09	-9.51	-9.99	-8.56
(3sa)(4dma)+sa	-9.16	-18.14	-17.69	-18.67
(4sa)(3dma)+dma	-6.66	-12.60	-15.22	-12.60
(1sa)(1dma)+(1sa)(1dma)	-15.18	-20.45	-17.45	-19.21
(2sa)(2dma)+(1sa)(1dma)	-13.51	-20.86	-18.88	-20.89
(3sa)(3dma)+(1sa)(1dma)	-6.54	-17.04	-14.59	-15.80
(3sa)(1dma)+sa	-3.21	-7.92	-5.28	-6.10
(3sa)(1dma)+dma	-10.31	-14.84	-13.07	-14.97
(1sa)(3dma)+sa	-28.96	-30.49	-30.98	-30.18
(1sa)(3dma)+dma	-0.62	+0.71	-1.29	+1.66
(1sa)(4dma)+sa	-31.20	-34.36	-36.45	-37.00
(4sa)(1dma)+dma	-24.00	-22.90	-23.58	-24.41
(2sa)(4dma)+sa	-26.51	-31.52	-30.23	-29.93
(4sa)(2dma)+dma	-14.46	-14.76	-18.11	-15.51
(2sa)(1dma)+(1sa)(1dma)	-5.45	-16.09	-9.66	-15.77
(1sa)(2dma)+(1sa)(1dma)	-15.94	-22.56	-20.56	-21.98
(3sa)(1dma)+(1sa)(1dma)	-15.50	-20.20	-15.75	-19.08
(1sa)(3dma)+(1sa)(1dma)	-20.10	-23.04	-24.64	-23.92
(3sa)(2dma)+(1sa)(1dma)	-19.65	-20.12	-20.79	-19.63
(2sa)(3dma)+(1sa)(1dma)	-17.66	-24.07	-23.89	-23.67

Table 2: Stepwise gibbs free energy of $(\text{H}_2\text{SO}_4)_a(\text{NH}(\text{CH}_3)_2)_b$ cluster formation in kcal/mol.