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Supporting Information

Basis Set Convergence of the Binding Energies of Strongly Hydrogen-Bonded Atmospheric Clusters

Jonas Elm[a,*] **and Kasper Kristensen**[b]

[a] *Division of Atmospheric Sciences, Department of Physics, Helsinki University, Finland.*
[b] *qLEAP Center for Theoretical Chemistry, Department of Chemistry, Aarhus University, Denmark.*

E-mail: jonas.elm@helsinki.fi

Cluster Structures

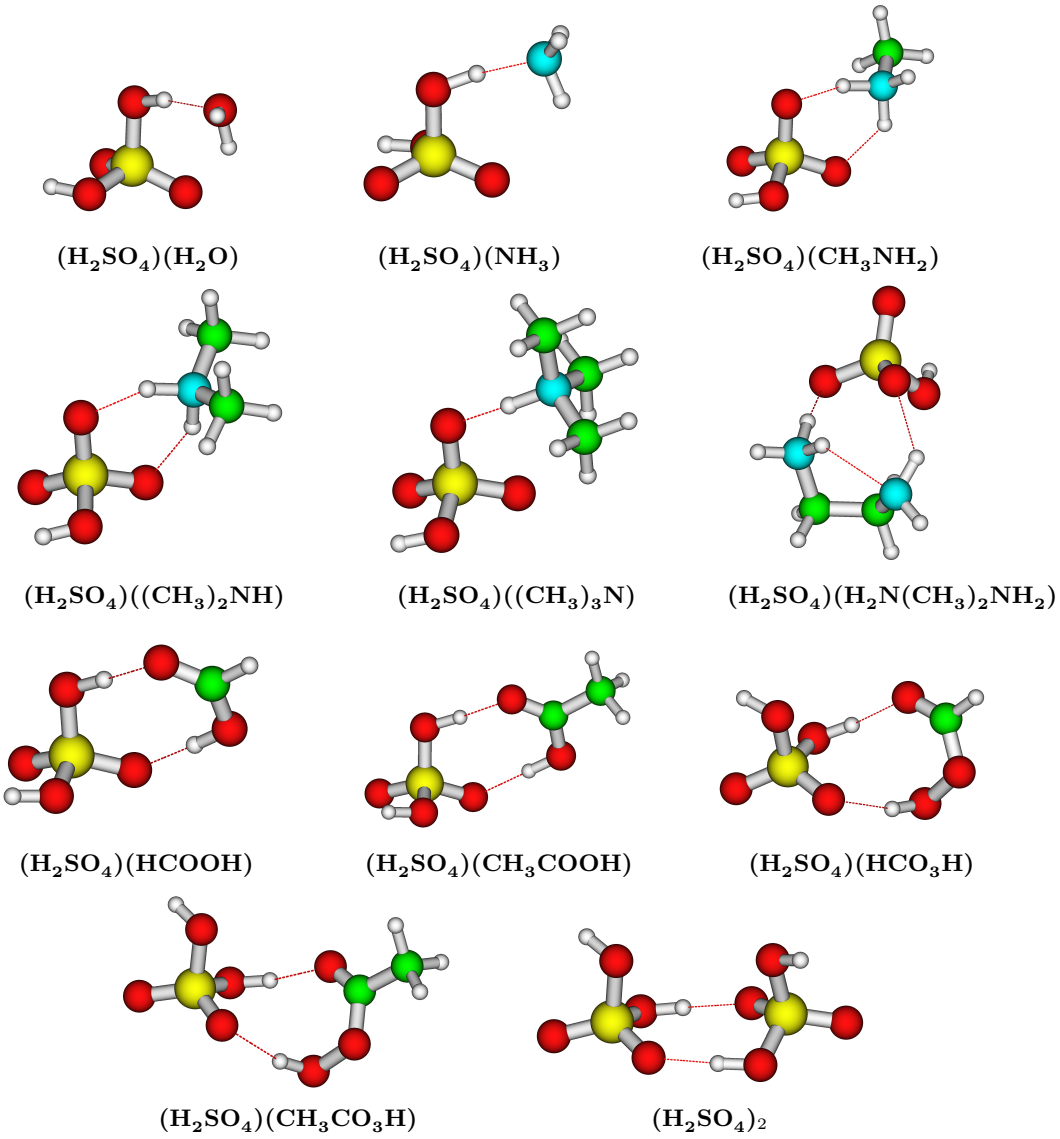

Figure S1: Minimum structures of the studied clusters optimized at the MP2/aug-cc-pVTZ level of theory. Color coding: yellow = sulfur, green = carbon, blue = nitrogen and white = hydrogen.

Model	Basis	UC	UC-F12	CP	CP-F12	SNOOP	SNOOP-F12	EXTR
MP2/int	DZ	-14.14	-13.91	-11.91	-13.58	-12.67	-13.64	—
MP2/int	TZ	-14.22	-13.92	-13.09	-13.78	-13.35	-13.81	-13.23
MP2/int	QZ	-14.13	-13.88	-13.53	-13.81	-13.61	-13.81	-13.69
MP2/rel	DZ	1.43	1.23	—	—	—	—	—
MP2/rel	TZ	1.25	1.25	—	—	—	—	1.25
MP2/rel	QZ	1.28	1.25	—	—	—	—	1.28
MP2/bind	DZ	-12.71	-12.67	-10.48	-12.35	-11.24	-12.41	—
MP2/bind	TZ	-12.97	-12.67	-11.84	-12.54	-12.10	-12.56	-11.98
MP2/bind	QZ	-12.84	-12.63	-12.24	-12.55	-12.33	-12.56	-12.41
$\Delta^{\mathrm{int,CCSD(T)}}$	DZ	-0.03	—	0.14	—	0.06	—	—
$\Delta^{\mathrm{int,CCSD(T)}}$	TZ	-0.02	—	-0.03	—	-0.03	—	-0.05
$\Delta^{\mathrm{rel,CCSD(T)}}$	DZ	0.01	—	—	—	—	—	—
$\Delta^{\mathrm{rel,CCSD(T)}}$	TZ	0.01	—	—	—	—	—	0.01
$\Delta^{\mathrm{bind,CCSD(T)}}$	DZ	-0.02	—	0.15	—	0.07	—	—
$\Delta^{\mathrm{bind,CCSD(T)}}$	TZ	-0.01	—	-0.01	—	-0.02	—	-0.04

Table S1: Interaction, relaxation, and binding energies for MP2 and the corresponding $\Delta^{(\mathrm{T})}$ contributions for the $(H_2SO_4)(H_2O)$ cluster. All values are in kcal/mol.

Model	Basis	UC	UC-F12	CP	CP-F12	SNOOP	SNOOP-F12	EXTR
MP2/int	DZ	-20.87	-20.77	-18.23	-20.37	-19.23	-20.46	—
MP2/int	TZ	-20.90	-20.73	-19.72	-20.58	-19.98	-20.60	-19.89
MP2/int	QZ	-20.86	-20.70	-20.24	-20.62	-20.31	-20.63	-20.45
MP2/rel	DZ	3.92	3.83	—	—	—	—	—
MP2/rel	TZ	3.85	3.90	—	—	—	—	3.86
MP2/rel	QZ	3.94	3.92	—	—	—	—	3.96
MP2/bind	DZ	-16.95	-16.95	-14.31	-16.54	-15.31	-16.63	—
MP2/bind	TZ	-17.05	-16.83	-15.87	-16.69	-16.13	-16.71	-16.03
MP2/bind	QZ	-16.92	-16.78	-16.29	-16.70	-16.36	-16.71	-16.49
$\Delta^{\mathrm{int,CCSD(T)}}$	DZ	0.53	—	0.66	—	0.60	—	—
$\Delta^{\mathrm{int,CCSD(T)}}$	TZ	0.45	—	0.41	—	0.41	—	0.37
$\Delta^{\mathrm{rel,CCSD(T)}}$	DZ	0.04	—	—	—	—	—	—
$\Delta^{\mathrm{rel,CCSD(T)}}$	TZ	0.06	—	—	—	—	—	0.06
$\Delta^{\mathrm{bind,CCSD(T)}}$	DZ	0.57	—	0.70	—	0.64	—	—
$\Delta^{\mathrm{bind,CCSD(T)}}$	TZ	0.51	—	0.47	—	0.47	—	0.44

Table S2: Interaction, relaxation, and binding energies for MP2 and the corresponding $\Delta^{(\mathrm{T})}$ contributions for the $(H_2SO_4)(NH_3)$ cluster. All values are in kcal/mol.

Model	Basis	UC	UC-F12	CP	CP-F12	SNOOP	SNOOP-F12	EXTR
MP2/int	DZ	-94.96	-95.88	-89.90	-95.11	-91.05	-95.25	—
MP2/int	TZ	-96.08	-96.16	-93.61	-95.89	-93.98	-95.93	-93.99
MP2/int	QZ	-96.28	-96.20	-95.02	-96.08	-95.14	-96.09	-95.52
MP2/rel	DZ	73.16	74.10	—	—	—	—	—
MP2/rel	TZ	74.20	74.32	—	—	—	—	74.26
MP2/rel	QZ	74.48	74.42	—	—	—	—	74.50
MP2/bind	DZ	-21.80	-21.78	-16.74	-21.02	-17.89	-21.15	—
MP2/bind	TZ	-21.88	-21.85	-19.41	-21.57	-19.78	-21.61	-19.73
MP2/bind	QZ	-21.80	-21.79	-20.54	-21.66	-20.66	-21.67	-21.02
$\Delta^{\mathrm{int,CCSD(T)}}$	DZ	1.98	—	2.19	—	2.10	—	—
$\Delta^{\mathrm{int,CCSD(T)}}$	TZ	1.52	—	1.37	—	1.38	—	1.26
$\Delta^{\mathrm{rel,CCSD(T)}}$	DZ	-0.78	—	—	—	—	—	—
$\Delta^{\mathrm{rel,CCSD(T)}}$	TZ	-0.39	—	—	—	—	—	-0.34
$\Delta^{\mathrm{bind,CCSD(T)}}$	DZ	1.20	—	1.41	—	1.33	—	—
$\Delta^{\mathrm{bind,CCSD(T)}}$	TZ	1.13	—	0.98	—	0.99	—	0.92

Table S3: Interaction, relaxation, and binding energies for MP2 and the corresponding $\Delta^{(\mathrm{T})}$ contributions for the $(H_2SO_4)((CH_3)NH_2)$ cluster. All values are in kcal/mol.

Model	Basis	UC	UC-F12	CP	CP-F12	SNOOP	SNOOP-F12	EXTR
MP2/int	DZ	-110.76	-111.22	-104.90	-110.33	-106.27	-110.50	—
MP2/int	TZ	-111.70	-111.44	-108.72	-111.12	-109.20	-111.17	-109.13
MP2/int	QZ	-111.68	-111.46	-110.20	-111.31	-110.34	-111.33	-110.72
MP2/rel	DZ	84.29	85.52	—	—	—	—	—
MP2/rel	TZ	85.58	85.77	—	—	—	—	85.65
MP2/rel	QZ	85.91	85.88	—	—	—	—	85.96
MP2/bind	DZ	-26.47	-25.70	-20.61	-24.81	-21.98	-24.98	—
MP2/bind	TZ	-26.12	-25.68	-23.13	-25.35	-23.61	-25.40	-23.48
MP2/bind	QZ	-25.77	-25.58	-24.29	-25.44	-24.43	-25.45	-24.77
$\Delta^{\mathrm{int,CCSD(T)}}$	DZ	2.46	—	2.70	—	2.61	—	—
$\Delta^{\mathrm{int,CCSD(T)}}$	TZ	1.89	—	1.74	—	1.75	—	1.60
$\Delta^{\mathrm{rel,CCSD(T)}}$	DZ	-1.36	—	—	—	—	—	—
$\Delta^{\mathrm{rel,CCSD(T)}}$	TZ	-0.86	—	—	—	—	—	-0.79
$\Delta^{\mathrm{bind,CCSD(T)}}$	DZ	1.10	—	1.34	—	1.25	—	—
$\Delta^{\mathrm{bind,CCSD(T)}}$	TZ	1.03	—	0.88	—	0.89	—	0.81

Table S4: Interaction, relaxation, and binding energies for MP2 and the corresponding $\Delta^{(\mathrm{T})}$ contributions for the $(H_2SO_4)((CH_3)_2NH)$ cluster. All values are in kcal/mol.

Model	Basis	UC	UC-F12	CP	CP-F12	SNOOP	SNOOP-F12	EXTR
MP2/int	DZ	-90.06	-89.03	-83.26	-88.00	-85.29	-88.20	—
MP2/int	TZ	-89.86	-89.04	-86.54	-88.68	-87.18	-88.74	-86.92
MP2/int	QZ	-89.47	-89.01	-87.85	-88.84	-88.06	-88.86	-88.32
MP2/rel	DZ	61.50	62.25	—	—	—	—	—
MP2/rel	TZ	62.31	62.51	—	—	—	—	62.37
MP2/rel	QZ	62.63	62.60	—	—	—	—	62.67
MP2/bind	DZ	-28.56	-26.78	-21.76	-25.75	-23.79	-25.95	—
MP2/bind	TZ	-27.55	-26.53	-24.22	-26.16	-24.86	-26.23	-24.55
MP2/bind	QZ	-26.84	-26.41	-25.22	-26.24	-25.43	-26.26	-25.64
$\Delta^{\mathrm{int,CCSD(T)}}$	DZ	1.68	—	1.96	—	1.82	—	—
$\Delta^{\mathrm{int,CCSD(T)}}$	TZ	1.33	—	1.19	—	1.20	—	1.08
$\Delta^{\mathrm{rel,CCSD(T)}}$	DZ	-0.61	—	—	—	—	—	—
$\Delta^{\mathrm{rel,CCSD(T)}}$	TZ	-0.32	—	—	—	—	—	-0.28
$\Delta^{\mathrm{bind,CCSD(T)}}$	DZ	1.07	—	1.36	—	1.22	—	—
$\Delta^{\mathrm{bind,CCSD(T)}}$	TZ	1.01	—	0.87	—	0.88	—	0.80

Table S5: Interaction, relaxation, and binding energies for MP2 and the corresponding $\Delta^{(\mathrm{T})}$ contributions for the $(H_2SO_4)((CH_3)_3N)$ cluster. All values are in kcal/mol.

Model	Basis	UC	UC-F12	CP	CP-F12	SNOOP	SNOOP-F12	EXTR
MP2/int	DZ	-94.42	-93.86	-87.86	-92.94	-89.73	-93.12	—
MP2/int	TZ	-94.56	-94.01	-91.45	-93.67	-92.01	-93.73	-91.82
MP2/int	QZ	-94.34	-94.00	-92.80	-93.84	-92.98	-93.86	-93.29
MP2/rel	DZ	66.55	67.11	—	—	—	—	—
MP2/rel	TZ	67.25	67.32	—	—	—	—	67.29
MP2/rel	QZ	67.50	67.42	—	—	—	—	67.53
MP2/bind	DZ	-27.87	-26.75	-21.31	-25.84	-23.19	-26.01	—
MP2/bind	TZ	-27.31	-26.69	-24.20	-26.35	-24.77	-26.41	-24.53
MP2/bind	QZ	-26.84	-26.58	-25.30	-26.42	-25.48	-26.44	-25.76
$\Delta^{\mathrm{int,CCSD(T)}}$	DZ	1.69	—	2.00	—	1.86	—	—
$\Delta^{\mathrm{int,CCSD(T)}}$	TZ	1.36	—	1.23	—	1.23	—	1.12
$\Delta^{\mathrm{rel,CCSD(T)}}$	DZ	-0.49	—	—	—	—	—	—
$\Delta^{\mathrm{rel,CCSD(T)}}$	TZ	-0.17	—	—	—	—	—	-0.13
$\Delta^{\mathrm{bind,CCSD(T)}}$	DZ	1.20	—	1.51	—	1.37	—	—
$\Delta^{\mathrm{bind,CCSD(T)}}$	TZ	1.19	—	1.06	—	1.06	—	0.99

Table S6: Interaction, relaxation, and binding energies for MP2 and the corresponding $\Delta^{(\mathrm{T})}$ contributions for the $(H_2SO_4)(H_2N(CH_3)_2NH_2)$ cluster. All values are in kcal/mol.

Model	Basis	UC	UC-F12	CP	CP-F12	SNOOP	SNOOP-F12	EXTR
MP2/int	DZ	-22.10	-21.63	-18.60	-21.12	-19.92	-21.22	—
MP2/int	TZ	-22.43	-21.64	-20.47	-21.41	-21.00	-21.46	-20.65
MP2/int	QZ	-22.12	-21.56	-21.07	-21.43	-21.23	-21.45	-21.28
MP2/rel	DZ	4.52	3.90	—	—	—	—	—
MP2/rel	TZ	4.00	3.88	—	—	—	—	3.99
MP2/rel	QZ	3.97	3.88	—	—	—	—	3.97
MP2/bind	DZ	-17.58	-17.73	-14.09	-17.22	-15.40	-17.31	—
MP2/bind	TZ	-18.44	-17.76	-16.47	-17.53	-17.00	-17.58	-16.65
MP2/bind	QZ	-18.15	-17.68	-17.10	-17.56	-17.26	-17.57	-17.32
$\Delta^{\mathrm{int,CCSD(T)}}$	DZ	-0.30	—	-0.04	—	-0.18	—	—
$\Delta^{\mathrm{int,CCSD(T)}}$	TZ	-0.25	—	-0.26	—	-0.28	—	-0.30
$\Delta^{\mathrm{rel,CCSD(T)}}$	DZ	0.13	—	—	—	—	—	—
$\Delta^{\mathrm{rel,CCSD(T)}}$	TZ	0.11	—	—	—	—	—	0.11
$\Delta^{\mathrm{bind,CCSD(T)}}$	DZ	-0.18	—	0.09	—	-0.05	—	—
$\Delta^{\mathrm{bind,CCSD(T)}}$	TZ	-0.14	—	-0.15	—	-0.17	—	-0.19

Table S7: Interaction, relaxation, and binding energies for MP2 and the corresponding $\Delta^{(\mathrm{T})}$ contributions for the (H_2SO_4)(HCOOH) cluster. All values are in kcal/mol.

Model	Basis	UC	UC-F12	CP	CP-F12	SNOOP	SNOOP-F12	EXTR
MP2/int	DZ	-23.69	-23.06	-19.93	-22.54	-21.37	-22.64	—
MP2/int	TZ	-23.95	-23.07	-21.85	-22.83	-22.40	-22.88	-22.03
MP2/int	QZ	-23.58	-22.99	-22.47	-22.85	-22.65	-22.87	-22.69
MP2/rel	DZ	5.22	4.60	—	—	—	—	—
MP2/rel	TZ	4.70	4.59	—	—	—	—	4.70
MP2/rel	QZ	4.69	4.59	—	—	—	—	4.68
MP2/bind	DZ	-18.47	-18.46	-14.71	-17.94	-16.15	-18.03	—
MP2/bind	TZ	-19.25	-18.48	-17.14	-18.24	-17.70	-18.29	-17.33
MP2/bind	QZ	-18.89	-18.40	-17.78	-18.26	-17.96	-18.28	-18.01
$\Delta^{\mathrm{int,CCSD(T)}}$	DZ	-0.34	—	-0.07	—	-0.21	—	—
$\Delta^{\mathrm{int,CCSD(T)}}$	TZ	-0.28	—	-0.31	—	-0.32	—	-0.34
$\Delta^{\mathrm{rel,CCSD(T)}}$	DZ	0.12	—	—	—	—	—	—
$\Delta^{\mathrm{rel,CCSD(T)}}$	TZ	0.11	—	—	—	—	—	0.11
$\Delta^{\mathrm{bind,CCSD(T)}}$	DZ	-0.22	—	0.05	—	-0.09	—	—
$\Delta^{\mathrm{bind,CCSD(T)}}$	TZ	-0.17	—	-0.20	—	-0.21	—	-0.23

Table S8: Interaction, relaxation, and binding energies for MP2 and the corresponding $\Delta^{(\mathrm{T})}$ contributions for the $(H_2SO_4)(CH_3COOH)$ cluster. All values are in kcal/mol.

Model	Basis	UC	UC-F12	CP	CP-F12	SNOOP	SNOOP-F12	EXTR
MP2/int	DZ	-20.12	-18.81	-16.23	-18.36	-17.65	-18.44	—
MP2/int	TZ	-19.78	-18.87	-17.81	-18.66	-18.34	-18.70	-17.98
MP2/int	QZ	-19.36	-18.80	-18.35	-18.67	-18.52	-18.69	-18.54
MP2/rel	DZ	5.51	5.72	—	—	—	—	—
MP2/rel	TZ	5.55	5.71	—	—	—	—	5.59
MP2/rel	QZ	5.67	5.69	—	—	—	—	5.72
MP2/bind	DZ	-14.62	-13.09	-10.72	-12.64	-12.15	-12.71	—
MP2/bind	TZ	-14.23	-13.17	-12.26	-12.95	-12.78	-13.00	-12.39
MP2/bind	QZ	-13.69	-13.11	-12.67	-12.98	-12.85	-13.00	-12.82
$\Delta^{\mathrm{int,CCSD(T)}}$	DZ	-0.63	—	-0.29	—	-0.44	—	—
$\Delta^{\mathrm{int,CCSD(T)}}$	TZ	-0.48	—	-0.48	—	-0.49	—	-0.50
$\Delta^{\mathrm{rel,CCSD(T)}}$	DZ	0.15	—	—	—	—	—	—
$\Delta^{\mathrm{rel,CCSD(T)}}$	TZ	0.15	—	—	—	—	—	0.14
$\Delta^{\mathrm{bind,CCSD(T)}}$	DZ	-0.47	—	-0.14	—	-0.29	—	—
$\Delta^{\mathrm{bind,CCSD(T)}}$	TZ	-0.33	—	-0.33	—	-0.35	—	-0.36

Table S9: Interaction, relaxation, and binding energies for MP2 and the corresponding $\Delta^{(\mathrm{T})}$ contributions for the $(H_2SO_4)(HCO_3H)$ cluster. All values are in kcal/mol.

Model	Basis	UC	UC-F12	CP	CP-F12	SNOOP	SNOOP-F12	EXTR
MP2/int	DZ	-21.83	-20.39	-17.69	-19.91	-19.19	-19.99	—
MP2/int	TZ	-21.45	-20.45	-19.33	-20.21	-19.88	-20.26	-19.51
MP2/int	QZ	-20.96	-20.36	-19.89	-20.23	-20.08	-20.25	-20.09
MP2/rel	DZ	7.02	7.08	—	—	—	—	—
MP2/rel	TZ	6.99	7.07	—	—	—	—	7.02
MP2/rel	QZ	7.05	7.05	—	—	—	—	7.09
MP2/bind	DZ	-14.82	-13.31	-10.68	-12.83	-12.17	-12.91	—
MP2/bind	TZ	-14.47	-13.37	-12.34	-13.14	-12.90	-13.19	-12.49
MP2/bind	QZ	-13.91	-13.31	-12.83	-13.18	-13.03	-13.20	-13.00
$\Delta^{\mathrm{int,CCSD(T)}}$	DZ	-0.65	—	-0.31	—	-0.46	—	—
$\Delta^{\mathrm{int,CCSD(T)}}$	TZ	-0.49	—	-0.50	—	-0.51	—	-0.53
$\Delta^{\mathrm{rel,CCSD(T)}}$	DZ	0.14	—	—	—	—	—	—
$\Delta^{\mathrm{rel,CCSD(T)}}$	TZ	0.12	—	—	—	—	—	0.11
$\Delta^{\mathrm{bind,CCSD(T)}}$	DZ	-0.51	—	-0.17	—	-0.32	—	—
$\Delta^{\mathrm{bind,CCSD(T)}}$	TZ	-0.38	—	-0.38	—	-0.40	—	-0.41

Table S10: Interaction, relaxation, and binding energies for MP2 and the corresponding $\Delta^{(\mathrm{T})}$ contributions for the $(H_2SO_4)(CH_3CO_3H)$ cluster. All values are in kcal/mol.

Model	Basis	UC	UC-F12	CP	CP-F12	SNOOP	SNOOP-F12	EXTR
MP2/int	DZ	-22.41	-21.10	-18.15	-20.52	-19.71	-20.62	—
MP2/int	TZ	-22.41	-21.10	-20.06	-20.83	-20.72	-20.89	-20.23
MP2/int	QZ	-21.83	-20.99	-20.59	-20.84	-20.82	-20.85	-20.78
MP2/rel	DZ	4.85	3.47	—	—	—	—	—
MP2/rel	TZ	3.64	3.31	—	—	—	—	3.62
MP2/rel	QZ	3.45	3.27	—	—	—	—	3.42
MP2/bind	DZ	-17.57	-17.64	-13.30	-17.05	-14.87	-17.15	—
MP2/bind	TZ	-18.77	-17.79	-16.42	-17.53	-17.08	-17.58	-16.61
MP2/bind	QZ	-18.39	-17.72	-17.14	-17.56	-17.37	-17.58	-17.36
$\Delta^{\mathrm{int,CCSD(T)}}$	DZ	-0.51	—	-0.14	—	-0.32	—	—
$\Delta^{\mathrm{int,CCSD(T)}}$	TZ	-0.35	—	-0.33	—	-0.35	—	-0.35
$\Delta^{\mathrm{rel,CCSD(T)}}$	DZ	0.07	—	—	—	—	—	—
$\Delta^{\mathrm{rel,CCSD(T)}}$	TZ	0.04	—	—	—	—	—	0.04
$\Delta^{\mathrm{bind,CCSD(T)}}$	DZ	-0.45	—	-0.08	—	-0.25	—	—
$\Delta^{\mathrm{bind,CCSD(T)}}$	TZ	-0.30	—	-0.28	—	-0.30	—	-0.31

Table S11: Interaction, relaxation, and binding energies for MP2 and the corresponding $\Delta^{(\mathrm{T})}$ contributions for the $(H_2SO_4)_2$ cluster. All values are in kcal/mol.