Supplementary material to: Effects of counterpoise correction and basis set extrapolation on the MP2 geometries of hydrogen bonded dimers of second row element hydrides

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TABLE I: Intra- and intermolecular geometry parameters and energies of the NH_3, H_2O and HF dimers as obtained by counterpoise corrected as well as uncorrected geometry optimizations with the aug-cc-pVTZ to aug-cc-pV5Z basis set as well as basis set extrapolated results. Site names used to specify distances and angles may be inferred from figure 1 of the paper. Distances R are given in Ångstrom, angles Θ in degrees, and energies E in kJ/mol.

		not counterpoise corrected					counterpoise corrected				
		TZ	QZ	5Z	ext(TQZ)	ext(Q5Z)	TZ	QZ	5Z	ext(TQZ)	ext(Q5Z)
$(NH_3)_2$	R_{DA}	3.234	3.218	3.213	3.202	3.207	3.232	3.219	3.213	3.208	3.208
asymm.	θ_{1DA}	17.07	19.47	20.70	22.39	22.03	22.92	22.14	22.29	22.32	22.32
	θ_{3AD}	76.31	72.24	70.14	67.52	67.98	66.96	68.01	67.70	67.63	67.62
	R_{1D}	1.016	1.014	1.014	1.014	1.013	1.016	1.014	1.014	1.013	1.013
	R_{3A}	1.013	1.011	1.011	1.011	1.011	1.013	1.011	1.011	1.011	1.011
	R_{2D}	1.012	1.010	1.010	1.010	1.009	1.012	1.010	1.010	1.010	1.009
	R_{4A}	1.013	1.011	1.010	1.010	1.010	1.012	1.011	1.010	1.010	1.010
	θ_{1D2}	107.20	107.32	107.36	107.37	107.39	107.18	107.30	107.35	107.36	107.39
	θ_{3A4}	106.82	106.93	106.99	107.00	107.05	106.85	106.96	107.00	107.01	107.04
	θ_{2D2}	106.46	106.57	106.62	106.63	106.67	106.48	106.58	106.63	106.64	106.67
	θ_{4A4}	106.71	106.81	106.86	106.85	106.89	106.68	106.80	106.85	106.85	106.89
	E_{int}	−13.83	−13.56	−13.39	−13.40	−13.27	−12.66	−13.02	−13.13	−13.26	−13.26
	E_{stab}	−13.76	−13.48	−13.32	−13.32	−13.20	−12.60	−12.95	−13.06	−13.19	−13.18
$(NH_3)_2$	R_{DA}	3.168	3.164	3.164	3.161	3.163	3.190	3.175	3.169	3.165	3.164
cyclic	θ_{1DA}	42.34	42.37	42.38	42.42	42.40	42.55	42.47	42.44	42.42	42.42
	R_{1D}	1.014	1.012	1.012	1.012	1.012	1.014	1.012	1.012	1.012	1.012
	R_{2D}	1.012	1.010	1.010	1.010	1.010	1.012	1.010	1.010	1.010	1.010
	θ_{1D2}	107.09	107.19	107.23	107.23	107.27	107.06	107.18	107.22	107.23	107.26
	θ_{2D2}	106.57	106.68	106.72	106.73	106.76	106.56	106.68	106.72	106.73	106.76
	E_{int}	−13.62	−13.43	−13.29	−13.34	−13.18	−12.60	−12.94	−13.06	−13.19	−13.19
	E_{stab}	−13.56	−13.38	−13.23	−13.29	−13.12	−12.55	−12.89	−13.01	−13.14	−13.14
$(NH_3)_2$	R_{DA}	3.250	3.243	3.243	3.237	3.241	3.270	3.254	3.249	3.244	3.243
linear	θ_{1DA}	12.94	13.48	13.64	13.90	13.85	14.18	13.98	13.98	13.98	13.98
	θ_{3AD}	140.14	141.11	141.37	141.94	141.76	142.48	142.02	142.02	142.02	142.00
	R_{1D}	1.017	1.015	1.015	1.014	1.014	1.017	1.015	1.014	1.014	1.014
	R_{3A}	1.012	1.010	1.010	1.010	1.010	1.012	1.010	1.010	1.010	1.010
	R_{2D}	1.012	1.010	1.010	1.010	1.009	1.012	1.010	1.010	1.009	1.009
	R_{4A}	1.013	1.011	1.010	1.010	1.010	1.013	1.011	1.010	1.010	1.010
	θ_{1D2}	107.18	107.30	107.34	107.35	107.37	107.16	107.28	107.33	107.34	107.37
	θ_{3A4}	106.84	106.95	107.00	107.00	107.05	106.84	106.95	107.00	107.01	107.04
	θ_{2D2}	106.43	106.54	106.58	106.58	106.62	106.43	106.54	106.58	106.59	106.62
	θ_{4A4}	106.48	106.57	106.62	106.62	106.65	106.46	106.57	106.61	106.62	106.64
	E_{int}	−13.63	−13.33	−13.14	−13.14	−13.00	−12.40	−12.76	−12.87	−13.00	−12.99
	E_{stab}	−13.54	−13.23	−13.05	−13.04	−12.90	−12.32	−12.67	−12.78	−12.90	−12.90
$(H_2O)_2$	R_{DA}	2.907	2.903	2.904	2.898	2.905	2.933	2.918	2.913	2.908	2.907
	θ_{H_DDA}	5.55	5.50	5.42	5.58	5.30	5.54	5.53	5.55	5.58	5.60
	θ_{acc} [a]	123.35	124.39	124.82	124.54	125.26	124.72	125.01	124.99	124.95	124.87
	R_{H_DD}	0.969	0.966	0.966	0.966	0.966	0.968	0.966	0.966	0.965	0.966
	R_{HD}	0.960	0.958	0.957	0.957	0.957	0.960	0.958	0.957	0.957	0.957
	R_{HA}	0.962	0.960	0.959	0.959	0.959	0.962	0.960	0.959	0.959	0.959
	θ_{H_DDH}	104.48	104.64	104.69	104.74	104.75	104.44	104.61	104.69	104.71	104.76
	θ_{HAH}	104.53	104.69	104.77	104.79	104.84	104.52	104.69	104.77	104.79	104.83
	E_{int}	−21.86	−21.49	−21.24	−21.29	−21.10	−19.89	−20.50	−20.69	−20.88	−20.90
	E_{stab}	−21.69	−21.31	−21.06	−21.10	−20.93	−19.74	−20.34	−20.52	−20.71	−20.73
$(HF)_2$	R_{DA}	2.746	2.736	2.739	2.732	2.740	2.771	2.753	2.749	2.745	2.744
	θ_{H_DDA}	6.37	6.41	6.32	6.60	6.26	6.74	6.64	6.71	6.72	6.77
	θ_{HAD}	111.12	111.49	111.92	111.32	112.20	111.66	111.80	111.68	111.64	111.53
	R_{H_DD}	0.928	0.925	0.925	0.924	0.925	0.928	0.925	0.925	0.924	0.925
	R_{HA}	0.925	0.922	0.921	0.921	0.921	0.925	0.922	0.921	0.921	0.921
	E_{int}	−19.85	−19.54	−19.30	−19.35	−19.26	−17.83	−18.44	−18.62	−18.74	−18.80
	E_{stab}	−19.72	−19.39	−19.16	−19.19	−19.13	−17.71	−18.31	−18.48	−18.61	−18.66

[a] θ_{acc} is the angle between the bisection line of the HOH angle of the hydrogen bond acceptor water monomer and the OO-axis.

TABLE II: Intra- and intermolecular geometry parameters and energies of the NH_3, H_2O and HF dimers as obtained by counterpoise corrected and uncorrected geometry optimizations with the aug'-cc-pVTZ to aug'-cc-pV5Z basis set as well as basis set extrapolated results. Site names used to specify distances and angles may be inferred from figure 1 of the paper. Distances R are given in Ångstrom, angles Θ in degrees, and energies E in kJ/mol.

		not counterpoise corrected					counterpoise corrected				
		TZ	QZ	5Z	cbs(TQZ)	cbs(Q5Z)	TZ	QZ	5Z	cbs(TQZ)	cbs(Q5Z)
$(NH_3)_2$	R_{DA}	3.236	3.214	3.209	3.193	3.207	3.245	3.221	3.215	3.210	3.210
asymm.	θ_{1DA}	17.32	20.92	21.70	25.08	22.46	21.21	22.12	22.25	21.70	21.74
	θ_{3AD}	76.10	70.09	68.58	63.40	67.31	69.67	68.21	68.03	68.55	68.56
	R_{1D}	1.016	1.014	1.014	1.013	1.013	1.016	1.014	1.014	1.013	1.013
	R_{3A}	1.013	1.011	1.011	1.011	1.011	1.013	1.011	1.011	1.010	1.010
	R_{2D}	1.012	1.010	1.010	1.009	1.009	1.012	1.010	1.010	1.009	1.009
	R_{4A}	1.012	1.011	1.010	1.010	1.010	1.012	1.011	1.010	1.009	1.010
	θ_{1D2}	107.17	107.31	107.37	107.37	107.42	107.13	107.27	107.34	107.36	107.42
	θ_{3A4}	106.79	106.93	107.01	107.03	107.08	106.79	106.92	106.99	107.00	107.07
	θ_{2D2}	106.44	106.56	106.63	106.64	106.64	106.43	106.55	106.61	106.63	106.69
	θ_{4A4}	106.68	106.79	106.86	106.84	106.92	106.64	106.77	106.84	106.85	106.92
	E_{stab}	−13.20	−13.23	−13.19	−13.30	−13.16	−12.31	−12.79	−13.00	−13.14	−13.20
$(H_2O)_2$	R_{DA}	2.911	2.906	2.906	2.903	2.906	2.936	2.918	2.913	2.907	2.907
	θ_{H_DDA}	5.45	5.60	5.46	5.76	5.46	5.61	5.51	5.57	5.53	5.59
	θ_{acc} [a]	123.53	124.41	124.91	124.75	125.19	124.46	125.14	124.96	125.13	124.97
	R_{H_DD}	0.969	0.966	0.966	0.965	0.965	0.968	0.966	0.966	0.965	0.965
	R_{HD}	0.960	0.958	0.957	0.957	0.957	0.960	0.958	0.957	0.957	0.957
	R_{HA}	0.962	0.960	0.959	0.958	0.959	0.962	0.960	0.959	0.958	0.959
	θ_{H_DDH}	104.47	104.65	104.70	104.74	104.76	104.46	104.60	104.70	104.70	104.77
	θ_{HAH}	104.52	104.69	104.75	104.79	104.85	104.51	104.68	104.76	104.78	104.85
	E_{stab}	−21.07	−20.90	−20.81	−20.80	−20.75	−19.61	−20.21	−20.48	−20.63	−20.74
$(HF)_2$	R_{DA}	2.750	2.742	2.741	2.736	2.741	2.774	2.753	2.749	2.744	2.744
	θ_{H_DDA}	6.34	6.49	6.52	6.71	6.61	6.75	6.57	6.66	6.58	6.78
	θ_{HAD}	111.57	111.61	111.84	111.39	111.91	111.87	111.92	111.75	111.87	111.53
	R_{H_DD}	0.928	0.925	0.925	0.924	0.924	0.928	0.925	0.925	0.923	0.924
	R_{HA}	0.925	0.922	0.921	0.920	0.921	0.925	0.922	0.921	0.920	0.921
	E_{stab}	−19.14	−18.90	−18.80	−18.77	−18.76	−17.65	−18.20	−18.44	−18.56	−18.67

[a] θ_{acc} is the angle between the bisection line of the HOH angle of the hydrogen bond acceptor water monomer and the OO-axis.

TABLE III: Intra- and intermolecular geometry parameters of the NH_3, H_2O and HF dimers as obtained by counterpoise corrected and uncorrected geometry optimizations with the aug-cc-pVTZ to aug-cc-pV5Z basis set as well as basis set extrapolated results. For MP2, all electrons are fully correlated. Site names used to specify distances and angles may be inferred from figure 1 of the paper. Distances R are given in Ångstrom and angles Θ in degrees.

		not counterpoise corrected					counterpoise corrected				
		TZ	QZ	5Z	ext(TQZ)	ext(Q5Z)	TZ	QZ	5Z	ext(TQZ)	ext(Q5Z)
$(NH_3)_2$	R_{DA}	3.238	3.218	3.210		3.203	3.231	3.218	3.213	3.207	3.207
asymm.	θ_{1DA}	9.98	17.27	18.34		18.88	22.92	21.87	21.77	21.81	21.75
	θ_{3AD}	88.52	75.83	73.73		72.63	66.75	68.24	68.33	68.25	68.30
	R_{1D}	1.014	1.013	1.012		1.011	1.013	1.012	1.011	1.012	1.011
	R_{3A}	1.010	1.009	1.008		1.008	1.011	1.009	1.009	1.009	1.008
	R_{2D}	1.010	1.008	1.007		1.007	1.010	1.008	1.007	1.008	1.007
	R_{4A}	1.010	1.009	1.008		1.007	1.010	1.008	1.008	1.008	1.007
	θ_{1D2}	107.39	107.51	107.55		107.58	107.44	107.48	107.53	107.48	107.58
	θ_{3A4}	107.00	107.09	107.15		107.21	107.10	107.13	107.18	107.13	107.23
	θ_{2D2}	106.68	106.75	106.81		106.86	106.74	106.76	106.82	106.75	106.86
	θ_{4A4}	106.97	106.99	107.05		107.11	106.94	106.98	107.03	106.97	107.07
$(NH_3)_2$	R_{DA}	3.150	3.156	3.157	3.161	3.158	3.189	3.173	3.168	3.163	3.162
cyclic	θ_{1DA}	42.07	42.30	42.26	42.50	42.22	42.47	42.39	42.36	42.35	42.34
	R_{1D}	1.012	1.010	1.010	1.010	1.009	1.012	1.010	1.010	1.010	1.009
	R_{2D}	1.010	1.008	1.008	1.008	1.007	1.010	1.008	1.008	1.008	1.007
	θ_{1D2}	107.38	107.38	107.41	107.36	107.44	107.32	107.35	107.40	107.35	107.45
	θ_{2D2}	106.84	106.85	106.91	106.83	106.95	106.82	106.85	106.90	106.85	106.95
$(NH_3)_2$	R_{DA}	3.248	3.232	3.230	3.214	3.227	3.269	3.252	3.247	3.241	3.240
linear	θ_{1DA}	8.01	13.10	12.94	18.08	12.79	14.06	13.85	13.84	13.84	13.82
	θ_{3AD}	130.09	140.39	139.85	149.62	139.33	142.03	141.65	141.67	141.74	141.60
	R_{1D}	1.014	1.013	1.012	1.013	1.012	1.014	1.013	1.012	1.012	1.011
	R_{3A}	1.010	1.008	1.008	1.008	1.007	1.010	1.008	1.007	1.008	1.007
	R_{2D}	1.010	1.008	1.007	1.008	1.007	1.010	1.008	1.007	1.008	1.007
	R_{4A}	1.010	1.009	1.008	1.008	1.007	1.010	1.009	1.008	1.008	1.007
	θ_{1D2}	107.39	107.48	107.53	107.49	107.56	107.43	107.46	107.51	107.46	107.56
	θ_{3A4}	107.05	107.12	107.18	107.12	107.23	107.09	107.13	107.18	107.13	107.22
	θ_{2D2}	106.66	106.72	106.77	106.71	106.81	106.70	106.72	106.77	106.71	106.82
	θ_{4A4}	106.76	106.75	106.79	106.66	106.82	106.71	106.74	106.79	106.73	106.83
$(H_2O)_2$	R_{DA}	2.888	2.893	2.894	2.894	2.894	2.931	2.915	2.909	2.905	2.904
	θ_{H_DDA}	5.03	5.60	4.95	6.26	4.26	5.44	5.47	5.48	5.55	5.52
	θ_{acc} [a]	123.21	124.12	125.07	123.88	126.23	125.34	125.47	125.52	125.27	125.47
	R_{H_DD}	0.965	0.965	0.964	0.966	0.964	0.966	0.965	0.964	0.965	0.964
	R_{HD}	0.958	0.957	0.956	0.956	0.955	0.958	0.957	0.956	0.957	0.955
	R_{HA}	0.960	0.958	0.958	0.958	0.957	0.960	0.958	0.958	0.958	0.957
	θ_{H_DDH}	104.65	104.78	104.81	104.86	104.84	104.59	104.72	104.82	104.80	104.91
	θ_{HAH}	104.66	104.81	104.90	104.89	104.98	104.69	104.81	104.90	104.88	104.99
$(HF)_2$	R_{DA}	2.726	2.729	2.727	2.734	2.724	2.770	2.751	2.747	2.742	2.742
	θ_{H_DDA}	5.80	6.25	5.56	6.78	5.00	6.68	6.61	6.67	6.71	6.73
	θ_{HAD}	111.70	111.64	112.92	111.17	113.90	111.95	112.00	111.93	111.79	111.81
	R_{H_DD}	0.926	0.924	0.924	0.924	0.923	0.926	0.924	0.923	0.924	0.923
	R_{HA}	0.923	0.921	0.920	0.920	0.920	0.923	0.921	0.920	0.920	0.920

[a] θ_{acc} is the angle between the bisection line of the HOH angle of the hydrogen bond acceptor water monomer and the OO-axis.

TABLE IV: Intra- and intermolecular geometry parameters and energies of the NH_3, H_2O and HF dimers as obtained by MP2-F12 geometry optimizations. Site names used to specify distances and angles may be inferred from figure 1 of the paper. Distances R are given in Ångstrom, angles Θ in degrees, and energies E in kJ/mol.

Molecule		TZ	QZ	QZ/R12[b]
$(NH_3)_2$	R_{DA}	3.205	3.208	
asymm.	θ_{1DA}	22.28	21.84	
	θ_{3AD}	67.72	68.34	
	R_{1D}	1.014	1.014	
	R_{3A}	1.011	1.011	
	R_{2D}	1.010	1.010	
	R_{4A}	1.010	1.010	
	θ_{1D2}	107.36	107.39	
	θ_{3A4}	107.01	107.04	
	θ_{2D2}	106.62	106.66	
	θ_{4A4}	106.85	106.88	
	E_{int}	−13.25	−13.26	
$(NH_3)_2$	R_{DA}	3.163	3.163	
cyclic	θ_{1DA}	42.44	42.43	
	R_{1D}	1.012	1.012	
	R_{2D}	1.010	1.010	
	θ_{1D2}	107.23	107.26	
	θ_{2D2}	106.72	106.75	
	E_{int}	−13.19	−13.20	
$(NH_3)_2$	R_{DA}	3.241	3.243	
linear	θ_{1DA}	13.78	13.81	
	θ_{3AD}	141.67	141.63	
	R_{1D}	1.015	1.014	
	R_{3A}	1.010	1.010	
	R_{2D}	1.010	1.010	
	R_{4A}	1.010	1.010	
	θ_{1D2}	107.34	107.37	
	θ_{3A4}	107.01	107.04	
	θ_{2D2}	106.59	106.61	
	θ_{4A4}	106.61	106.65	
	E_{int}	−12.97	−12.98	
$(H_2O)_2$	R_{DA}	2.906	2.906	2.907
	θ_{H_DDA}	5.74	5.52	5.57
	θ_{acc} [a]	124.22	124.83	124.87
	R_{H_DD}	0.966	0.966	0.966
	R_{HD}	0.958	0.957	0.958
	R_{HA}	0.959	0.959	0.960
	θ_{H_DDH}	104.76	104.74	104.76
	θ_{HAH}	104.82	104.82	104.83
	E_{int}	−20.81	−20.87	
$(HF)_2$	R_{DA}	2.745	2.742	
	θ_{H_DDA}	6.72	6.62	
	θ_{HAD}	111.51	111.66	
	R_{H_DD}	0.925	0.925	
	R_{HA}	0.922	0.922	
	E_{int}	−18.76	−18.80	

[a] θ_{acc} is the angle between the bisection line of the HOH angle of the hydrogen bond acceptor water monomer and the OO-axis.
[b] A specifically designed QZ basis set, in conjunction with MP2-R12, see E. Kordel, C. Villani and W. Klopper *Mol. Phys.*, 2007.