Supporting Informations to

"Overtones of the Si-H stretching-bending polyad in $SiHD_3$: internal coordinate force field, *ab initio* dipole moment surfaces, and band intensities"

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TABLE I. Matrix elements for the dipole moment operators of M_x and M_y[a].

$$\langle v+1, l+1 | \theta_+ + \theta_- | v, l \rangle = \tfrac{1}{2} a_\theta^{-\frac{1}{2}} [2(v+l+2)]^{\frac{1}{2}}$$

$$\langle v+1, l-1 | \theta_+ + \theta_- | v, l \rangle = \tfrac{1}{2} a_\theta^{-\frac{1}{2}} [2(v-l+2)]^{\frac{1}{2}}$$

$$\langle v+1, l+1 | \theta_+ - \theta_- | v, l \rangle = \tfrac{1}{2} a_\theta^{-\frac{1}{2}} [2(v+l+2)]^{\frac{1}{2}}$$

$$\langle v+1, l-1 | \theta_+ - \theta_- | v, l \rangle = -\tfrac{1}{2} a_\theta^{-\frac{1}{2}} [2(v-l+2)]^{\frac{1}{2}}$$

$$\langle v+2, l+2 | \theta_+^2 + \theta_-^2 | v, l \rangle = \tfrac{1}{2} a_\theta^{-1} [(v+l+4)(v+l+2)]^{\frac{1}{2}}$$

$$\langle v+2, l-2 | \theta_+^2 + \theta_-^2 | v, l \rangle = \tfrac{1}{2} a_\theta^{-1} [(v-l+4)(v-l+2)]^{\frac{1}{2}}$$

$$\langle v, l+2 | \theta_+^2 + \theta_-^2 | v, l \rangle = a_\theta^{-1} [(v+l+2)(v-l)]^{\frac{1}{2}}$$

$$\langle v+2, l+2 | \theta_+^2 - \theta_-^2 | v, l \rangle = \tfrac{1}{2} a_\theta^{-1} [(v+l+4)(v+l+2)]^{\frac{1}{2}}$$

$$\langle v+2, l-2 | \theta_+^2 - \theta_-^2 | v, l \rangle = -\tfrac{1}{2} a_\theta^{-1} [(v-l+4)(v-l+2)]^{\frac{1}{2}}$$

$$\langle v, l+2 | \theta_+^2 - \theta_-^2 | v, l \rangle = a_\theta^{-1} [(v+l+2)(v-l)]^{\frac{1}{2}}$$

$$\langle v+3, l+1 | \theta^2 (\theta_+ + \theta_-) | v, l \rangle = \tfrac{1}{4} a_\theta^{-\frac{3}{2}} [2(v+l+4)(v+l+2)(v-l+2)]^{\frac{1}{2}}$$

$$\langle v+3, l-1 | \theta^2 (\theta_+ + \theta_-) | v, l \rangle = \tfrac{1}{4} a_\theta^{-\frac{3}{2}} [2(v-l+4)(v-l+2)(v+l+2)]^{\frac{1}{2}}$$

$$\langle v+1, l+1 | \theta^2 (\theta_+ + \theta_-) | v, l \rangle = \tfrac{1}{4} a_\theta^{-\frac{3}{2}} (3v-l+4) [2(v+l+2)]^{\frac{1}{2}}$$

$$\langle v+1, l-1 | \theta^2 (\theta_+ + \theta_-) | v, l \rangle = \tfrac{1}{4} a_\theta^{-\frac{3}{2}} (3v+l+4) [2(v-l+2)]^{\frac{1}{2}}$$

$$\langle v+3, l+1 | \theta^2 (\theta_+ - \theta_-) | v, l \rangle = \tfrac{1}{4} a_\theta^{-\frac{3}{2}} [2(v+l+4)(v+l+2)(v-l+2)]^{\frac{1}{2}}$$

$$\langle v+3, l-1 | \theta^2 (\theta_+ - \theta_-) | v, l \rangle = -\tfrac{1}{4} a_\theta^{-\frac{3}{2}} [2(v-l+4)(v-l+2)(v+l+2)]^{\frac{1}{2}}$$

$$\langle v+1, l+1 | \theta^2 (\theta_+ - \theta_-) | v, l \rangle = \tfrac{1}{4} a_\theta^{-\frac{3}{2}} (3v-l+4) [2(v+l+2)]^{\frac{1}{2}}$$

$$\langle v+1, l-1 | \theta^2 (\theta_+ - \theta_-) | v, l \rangle = -\tfrac{1}{4} a_\theta^{-\frac{3}{2}} (3v+l+4) [2(v-l+2)]^{\frac{1}{2}}$$

$$^{b}\ \langle v_1, l_1 | A^+ + A^- | v_2, l_2 \rangle = \langle v_2, l_2 | A^+ + A^- | v_1, l_1 \rangle$$

$$^{b}\ \langle v_1, l_1 | A^+ - A^- | v_2, l_2 \rangle = -\langle v_2, l_2 | A^+ - A^- | v_1, l_1 \rangle$$

[a] $a_\theta = (F_{\theta\theta}/g_{\theta\theta}^0)^{\frac{1}{2}}/\hbar$, $|v, l\rangle$ is the eigenstate of a two-dimensional isotropic harmonic oscillator, with the vibrational quantum number v and vibrational angular momentum quantum number l.

[b] $A^\pm = \theta_\pm$, $\theta_\pm^2$, and $\theta^2 \theta_\pm$.

TABLE II. One-dimensional dipole moment surface data points of SiHD$_3$ calculated at the CCSD(T)/cc-pVQZ level.

r (Å)	M_z (D)	r (Å)	M_z (D)
-0.60	0.51390	-0.55	0.50246
-0.50	0.48247	-0.45	0.45530
-0.40	0.42194	-0.35	0.38312
-0.30	0.33944	-0.25	0.29143
-0.20	0.23952	-0.15	0.18408
-0.10	0.12544	-0.05	0.06388
0.00	0.00000	0.05	-0.06679
0.10	-0.13525	0.15	-0.20531
0.20	-0.27656	0.25	-0.34858
0.30	-0.42089	0.35	-0.49299
0.40	-0.56435	0.45	-0.63441
0.50	-0.70258	0.55	-0.76825
0.60	-0.83080	0.65	-0.88960
0.70	-0.94402	0.75	-0.99341
0.80	-1.03723	0.85	-1.07490

TABLE III. The M_x and M_z components of three-dimensional dipole moment surface of SiHD$_3$ calculated at the CCSD(T)/cc-pVQZ level[a].

R (Å)	ϕ_1 (deg)	ϕ_2 (deg)	ϕ_3 (deg)	M_x (D)	M_z (D)
1.0798	101.4712	101.4712	124.5866	...[b]	0.46921
1.0798	103.4712	101.4712	122.7613	-0.15086	0.45880
1.0798	105.4712	101.4712	120.9027	-0.10053	0.45013
1.0798	107.4712	101.4712	119.0116	-0.04938	0.44329
1.0798	109.4712	101.4712	117.0886	0.00244	0.43838
1.0798	111.4712	101.4712	115.1340	0.05476	0.43545
1.0798	113.4712	101.4712	113.1474	0.10743	0.43458
1.0798	115.4712	101.4712	111.1284	0.16031	0.43581
1.0798	117.4712	101.4712	109.0759	0.21325	0.43920
1.0798	103.4712	103.4712	120.9388	...[b]	0.44917
1.0798	105.4712	103.4712	119.0798	-0.10204	0.44133
1.0798	107.4712	103.4712	117.1851	-0.05068	0.43535
1.0798	109.4712	103.4712	115.2549	0.00134	0.43133
1.0798	111.4712	103.4712	113.2893	0.05386	0.42933
1.0798	113.4712	103.4712	111.2876	0.10673	0.42943
1.0798	115.4712	103.4712	109.2489	0.15980	0.43168
1.0798	117.4712	103.4712	107.1716	0.21291	0.43612
1.0798	105.4712	105.4712	117.2173	...[b]	0.43434
1.0798	107.4712	105.4712	115.3154	-0.05171	0.42926
1.0798	109.4712	105.4712	113.3744	0.00052	0.42617
1.0798	111.4712	105.4712	111.3937	0.05324	0.42515
1.0798	113.4712	105.4712	109.3724	0.10629	0.42627
1.0798	115.4712	105.4712	107.3089	0.15953	0.42960
1.0798	117.4712	105.4712	105.2010	0.21280	0.43517

1.0798	107.4712	107.4712	113.4028	...[b]	0.42511
1.0798	109.4712	107.4712	111.4468	0.00000	0.42301
1.0798	111.4712	107.4712	109.4465	0.05291	0.42302
1.0798	113.4712	107.4712	107.4004	0.10614	0.42523
1.0798	115.4712	107.4712	105.3063	0.15954	0.42969
1.0798	117.4712	107.4712	103.1610	0.21295	0.43646
1.0798	109.4712	109.4712	109.4712	0.00000	0.42193
1.0798	111.4712	109.4712	107.4462	0.05291	0.42303
1.0798	113.4712	109.4712	105.3695	0.10631	0.42638
1.0798	115.4712	109.4712	103.2380	0.15984	0.43206
1.0798	117.4712	109.4712	101.0473	0.21336	0.44011
1.0798	111.4712	111.4712	105.3905	...[b]	0.42528
1.0798	113.4712	111.4712	103.2764	0.10679	0.42985
1.0798	115.4712	111.4712	101.0995	0.16044	0.43680
1.0798	117.4712	111.4712	98.8540	0.21401	0.44620
1.0798	113.4712	113.4712	101.1169	...[b]	0.43569
1.0798	115.4712	113.4712	98.8850	0.16130	0.44400
1.0798	117.4712	113.4712	96.5730	0.21488	0.45484
1.0798	115.4712	115.4712	96.5866	...[b]	0.45375
1.0798	117.4712	115.4712	94.1935	0.21589	0.46610
1.0798	117.4712	117.4712	91.7008	...[b]	0.48006
1.1798	101.4712	101.4712	124.5866	...[b]	0.38658
1.1798	103.4712	101.4712	122.7613	-0.15028	0.37621
1.1798	105.4712	101.4712	120.9027	-0.10009	0.36759
1.1798	107.4712	101.4712	119.0116	-0.04909	0.36080
1.1798	109.4712	101.4712	117.0886	0.00257	0.35591
1.1798	111.4712	101.4712	115.1340	0.05472	0.35301

1.1798	113.4712	101.4712	113.1474	0.10721	0.35214
1.1798	115.4712	101.4712	111.1284	0.15990	0.35336
1.1798	117.4712	101.4712	109.0759	0.21263	0.35673
1.1798	103.4712	103.4712	120.9388	...[b]	0.36662
1.1798	105.4712	103.4712	119.0798	-0.10168	0.35881
1.1798	107.4712	103.4712	117.1851	-0.05046	0.35285
1.1798	109.4712	103.4712	115.2549	0.00141	0.34885
1.1798	111.4712	103.4712	113.2893	0.05377	0.34686
1.1798	113.4712	103.4712	111.2876	0.10647	0.34696
1.1798	115.4712	103.4712	109.2489	0.15935	0.34920
1.1798	117.4712	103.4712	107.1716	0.21227	0.35362
1.1798	105.4712	105.4712	117.2173	...[b]	0.35183
1.1798	107.4712	105.4712	115.3154	-0.05155	0.34676
1.1798	109.4712	105.4712	113.3744	0.00054	0.34368
1.1798	111.4712	105.4712	111.3937	0.05311	0.34267
1.1798	113.4712	105.4712	109.3724	0.10600	0.34379
1.1798	115.4712	105.4712	107.3089	0.15907	0.34710
1.1798	117.4712	105.4712	105.2010	0.21215	0.35266
1.1798	107.4712	107.4712	113.4028	...[b]	0.34262
1.1798	109.4712	107.4712	111.4468	0.00000	0.34051
1.1798	111.4712	107.4712	109.4465	0.05277	0.34053
1.1798	113.4712	107.4712	107.4004	0.10585	0.34273
1.1798	115.4712	107.4712	105.3063	0.15908	0.34719
1.1798	117.4712	107.4712	103.1610	0.21231	0.35397
1.1798	109.4712	109.4712	109.4712	0.00000	0.33944
1.1798	111.4712	109.4712	107.4462	0.05277	0.34054
1.1798	113.4712	109.4712	105.3695	0.10602	0.34390

1.1798	115.4712	109.4712	103.2380	0.15940	0.34958
1.1798	117.4712	109.4712	101.0473	0.21274	0.35765
1.1798	111.4712	111.4712	105.3905	...[b]	0.34280
1.1798	113.4712	111.4712	103.2764	0.10653	0.34738
1.1798	115.4712	111.4712	101.0995	0.16003	0.35436
1.1798	117.4712	111.4712	98.8540	0.21344	0.36380
1.1798	113.4712	113.4712	101.1169	...[b]	0.35326
1.1798	115.4712	113.4712	98.8850	0.16094	0.36162
1.1798	117.4712	113.4712	96.5730	0.21437	0.37254
1.1798	115.4712	115.4712	96.5866	...[b]	0.37145
1.1798	117.4712	115.4712	94.1935	0.21545	0.38393
1.1798	117.4712	117.4712	91.7008	...[b]	0.39807
1.2798	101.4712	101.4712	124.5866	...[b]	0.28681
1.2798	103.4712	101.4712	122.7613	-0.15018	0.27644
1.2798	105.4712	101.4712	120.9027	-0.09996	0.26781
1.2798	107.4712	101.4712	119.0116	-0.04893	0.26102
1.2798	109.4712	101.4712	117.0886	0.00274	0.25614
1.2798	111.4712	101.4712	115.1340	0.05489	0.25324
1.2798	113.4712	101.4712	113.1474	0.10736	0.25237
1.2798	115.4712	101.4712	111.1284	0.16002	0.25359
1.2798	117.4712	101.4712	109.0759	0.21272	0.25695
1.2798	103.4712	103.4712	120.9388	...[b]	0.26681
1.2798	105.4712	103.4712	119.0798	-0.10165	0.25898
1.2798	107.4712	103.4712	117.1851	-0.05039	0.25302
1.2798	109.4712	103.4712	115.2549	0.00150	0.24901
1.2798	111.4712	103.4712	113.2893	0.05387	0.24702
1.2798	113.4712	103.4712	111.2876	0.10657	0.24712

1.2798	115.4712	103.4712	109.2489	0.15944	0.24935
1.2798	117.4712	103.4712	107.1716	0.21233	0.25379
1.2798	105.4712	105.4712	117.2173	...[b]	0.25197
1.2798	107.4712	105.4712	115.3154	-0.05154	0.24688
1.2798	109.4712	105.4712	113.3744	0.00058	0.24379
1.2798	111.4712	105.4712	111.3937	0.05317	0.24277
1.2798	113.4712	105.4712	109.3724	0.10607	0.24390
1.2798	115.4712	105.4712	107.3089	0.15914	0.24722
1.2798	117.4712	105.4712	105.2010	0.21220	0.25281
1.2798	107.4712	107.4712	113.4028	...[b]	0.24272
1.2798	109.4712	107.4712	111.4468	0.00000	0.24060
1.2798	111.4712	107.4712	109.4465	0.05280	0.24061
1.2798	113.4712	107.4712	107.4004	0.10590	0.24283
1.2798	115.4712	107.4712	105.3063	0.15915	0.24732
1.2798	117.4712	107.4712	103.1610	0.21237	0.25414
1.2798	109.4712	109.4712	109.4712	0.00000	0.23951
1.2798	111.4712	109.4712	107.4462	0.05281	0.24063
1.2798	113.4712	109.4712	105.3695	0.10609	0.24401
1.2798	115.4712	109.4712	103.2380	0.15949	0.24974
1.2798	117.4712	109.4712	101.0473	0.21284	0.25789
1.2798	111.4712	111.4712	105.3905	...[b]	0.24291
1.2798	113.4712	111.4712	103.2764	0.10663	0.24754
1.2798	115.4712	111.4712	101.0995	0.16016	0.25461
1.2798	117.4712	111.4712	98.8540	0.21359	0.26418
1.2798	113.4712	113.4712	101.1169	...[b]	0.25351
1.2798	115.4712	113.4712	98.8850	0.16115	0.26200
1.2798	117.4712	113.4712	96.5730	0.21460	0.27311

1.2798	115.4712	115.4712	96.5866	...[b]	0.27203
1.2798	117.4712	115.4712	94.1935	0.21579	0.28479
1.2798	117.4712	117.4712	91.7008	...[b]	0.29931
1.3798	101.4712	101.4712	124.5866	...[b]	0.17317
1.3798	103.4712	101.4712	122.7613	-0.15071	0.16272
1.3798	105.4712	101.4712	120.9027	-0.10023	0.15405
1.3798	107.4712	101.4712	119.0116	-0.04895	0.14723
1.3798	109.4712	101.4712	117.0886	0.00295	0.14233
1.3798	111.4712	101.4712	115.1340	0.05532	0.13941
1.3798	113.4712	101.4712	113.1474	0.10801	0.13854
1.3798	115.4712	101.4712	111.1284	0.16087	0.13977
1.3798	117.4712	101.4712	109.0759	0.21375	0.14314
1.3798	103.4712	103.4712	120.9388	...[b]	0.15301
1.3798	105.4712	103.4712	119.0798	-0.10204	0.14512
1.3798	107.4712	103.4712	117.1851	-0.05053	0.13911
1.3798	109.4712	103.4712	115.2549	0.00161	0.13507
1.3798	111.4712	103.4712	113.2893	0.05423	0.13307
1.3798	113.4712	103.4712	111.2876	0.10714	0.13317
1.3798	115.4712	103.4712	109.2489	0.16023	0.13542
1.3798	117.4712	103.4712	107.1716	0.21332	0.13989
1.3798	105.4712	105.4712	117.2173	...[b]	0.13804
1.3798	107.4712	105.4712	115.3154	-0.05176	0.13290
1.3798	109.4712	105.4712	113.3744	0.00062	0.12978
1.3798	111.4712	105.4712	111.3937	0.05346	0.12875
1.3798	113.4712	105.4712	109.3724	0.10661	0.12988
1.3798	115.4712	105.4712	107.3089	0.15990	0.13324
1.3798	117.4712	105.4712	105.2010	0.21319	0.13888

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1.3798	107.4712	107.4712	113.4028	...[b]	0.12868
1.3798	109.4712	107.4712	111.4468	0.00000	0.12653
1.3798	111.4712	107.4712	109.4465	0.05307	0.12655
1.3798	113.4712	107.4712	107.4004	0.10643	0.12879
1.3798	115.4712	107.4712	105.3063	0.15992	0.13333
1.3798	117.4712	107.4712	103.1610	0.21337	0.14025
1.3798	109.4712	109.4712	109.4712	0.00000	0.12543
1.3798	111.4712	109.4712	107.4462	0.05308	0.12656
1.3798	113.4712	109.4712	105.3695	0.10663	0.13000
1.3798	115.4712	109.4712	103.2380	0.16029	0.13582
1.3798	117.4712	109.4712	101.0473	0.21388	0.14411
1.3798	111.4712	111.4712	105.3905	...[b]	0.12888
1.3798	113.4712	111.4712	103.2764	0.10721	0.13360
1.3798	115.4712	111.4712	101.0995	0.16102	0.14081
1.3798	117.4712	111.4712	98.8540	0.21471	0.15058
1.3798	113.4712	113.4712	101.1169	...[b]	0.13970
1.3798	115.4712	113.4712	98.8850	0.16209	0.14840
1.3798	117.4712	113.4712	96.5730	0.21582	0.15979
1.3798	115.4712	115.4712	96.5866	...[b]	0.15872
1.3798	117.4712	115.4712	94.1935	0.21717	0.17187
1.3798	117.4712	117.4712	91.7008	...[b]	0.18693
1.4798	101.4712	101.4712	124.5866	...[b]	0.04821
1.4798	103.4712	101.4712	122.7613	-0.15200	0.03762
1.4798	105.4712	101.4712	120.9027	-0.10098	0.02884
1.4798	107.4712	101.4712	119.0116	-0.04920	0.02193
1.4798	109.4712	101.4712	117.0886	0.00319	0.01698
1.4798	111.4712	101.4712	115.1340	0.05605	0.01403

1.4798	113.4712	101.4712	113.1474	0.10921	0.01316
1.4798	115.4712	101.4712	111.1284	0.16254	0.01439
1.4798	117.4712	101.4712	109.0759	0.21588	0.01780
1.4798	103.4712	103.4712	120.9388	...[b]	0.02775
1.4798	105.4712	103.4712	119.0798	-0.10295	0.01973
1.4798	107.4712	103.4712	117.1851	-0.05091	0.01364
1.4798	109.4712	103.4712	115.2549	0.00175	0.00955
1.4798	111.4712	103.4712	113.2893	0.05486	0.00752
1.4798	113.4712	103.4712	111.2876	0.10828	0.00762
1.4798	115.4712	103.4712	109.2489	0.16184	0.00991
1.4798	117.4712	103.4712	107.1716	0.21540	0.01443
1.4798	105.4712	105.4712	117.2173	...[b]	0.01253
1.4798	107.4712	105.4712	115.3154	-0.05223	0.00731
1.4798	109.4712	105.4712	113.3744	0.00068	0.00414
1.4798	111.4712	105.4712	111.3937	0.05404	0.00309
1.4798	113.4712	105.4712	109.3724	0.10769	0.00424
1.4798	115.4712	105.4712	107.3089	0.16148	0.00765
1.4798	117.4712	105.4712	105.2010	0.21525	0.01339
1.4798	107.4712	107.4712	113.4028	...[b]	0.00300
1.4798	109.4712	107.4712	111.4468	0.00002	0.00082
1.4798	111.4712	107.4712	109.4465	0.05362	0.00083
1.4798	113.4712	107.4712	107.4004	0.10750	0.00312
1.4798	115.4712	107.4712	105.3063	0.16150	0.00775
1.4798	117.4712	107.4712	103.1610	0.21546	0.01480
1.4798	109.4712	109.4712	109.4712	0.00000	-0.00029
1.4798	111.4712	109.4712	107.4462	0.05362	0.00085
1.4798	113.4712	109.4712	105.3695	0.10771	0.00436

1.4798	115.4712	109.4712	103.2380	0.16190	0.01032
1.4798	117.4712	109.4712	101.0473	0.21602	0.01880
1.4798	111.4712	111.4712	105.3905	...[b]	0.00323
1.4798	113.4712	111.4712	103.2764	0.10835	0.00807
1.4798	115.4712	111.4712	101.0995	0.16271	0.01547
1.4798	117.4712	111.4712	98.8540	0.21694	0.02552
1.4798	113.4712	113.4712	101.1169	...[b]	0.01435
1.4798	115.4712	113.4712	98.8850	0.16389	0.02332
1.4798	117.4712	113.4712	96.5730	0.21818	0.03509
1.4798	115.4712	115.4712	96.5866	...[b]	0.03401
1.4798	117.4712	115.4712	94.1935	0.21970	0.04767
1.4798	117.4712	117.4712	91.7008	...[b]	0.06342
1.5798	101.4712	101.4712	124.5866	...[b]	-0.08553
1.5798	103.4712	101.4712	122.7613	-0.15404	-0.09636
1.5798	105.4712	101.4712	120.9027	-0.10225	-0.10533
1.5798	107.4712	101.4712	119.0116	-0.04969	-0.11237
1.5798	109.4712	101.4712	117.0886	0.00348	-0.11742
1.5798	111.4712	101.4712	115.1340	0.05709	-0.12042
1.5798	113.4712	101.4712	113.1474	0.11100	-0.12132
1.5798	115.4712	101.4712	111.1284	0.16506	-0.12006
1.5798	117.4712	101.4712	109.0759	0.21912	-0.11658
1.5798	103.4712	103.4712	120.9388	...[b]	-0.10647
1.5798	105.4712	103.4712	119.0798	-0.10437	-0.11467
1.5798	107.4712	103.4712	117.1851	-0.05154	-0.12090
1.5798	109.4712	103.4712	115.2549	0.00191	-0.12509
1.5798	111.4712	103.4712	113.2893	0.05579	-0.12716
1.5798	113.4712	103.4712	111.2876	0.10997	-0.12706

1.5798	115.4712	103.4712	109.2489	0.16429	-0.12472
1.5798	117.4712	103.4712	107.1716	0.21859	-0.12010
1.5798	105.4712	105.4712	117.2173	...[b]	-0.12206
1.5798	107.4712	105.4712	115.3154	-0.05297	-0.12742
1.5798	109.4712	105.4712	113.3744	0.00074	-0.13067
1.5798	111.4712	105.4712	111.3937	0.05490	-0.13174
1.5798	113.4712	105.4712	109.3724	0.10933	-0.13056
1.5798	115.4712	105.4712	107.3089	0.16390	-0.12706
1.5798	117.4712	105.4712	105.2010	0.21842	-0.12118
1.5798	107.4712	107.4712	113.4028	...[b]	-0.13184
1.5798	109.4712	107.4712	111.4468	0.00003	-0.13408
1.5798	111.4712	107.4712	109.4465	0.05444	-0.13407
1.5798	113.4712	107.4712	107.4004	0.10912	-0.13172
1.5798	115.4712	107.4712	105.3063	0.16391	-0.12696
1.5798	117.4712	107.4712	103.1610	0.21865	-0.11971
1.5798	109.4712	109.4712	109.4712	0.00000	-0.13524
1.5798	111.4712	109.4712	107.4462	0.05444	-0.13405
1.5798	113.4712	109.4712	105.3695	0.10936	-0.13044
1.5798	115.4712	109.4712	103.2380	0.16436	-0.12430
1.5798	117.4712	109.4712	101.0473	0.21927	-0.11554
1.5798	111.4712	111.4712	105.3905	...[b]	-0.13160
1.5798	113.4712	111.4712	103.2764	0.11005	-0.12659
1.5798	115.4712	111.4712	101.0995	0.16524	-0.11894
1.5798	117.4712	111.4712	98.8540	0.22029	-0.10853
1.5798	113.4712	113.4712	101.1169	...[b]	-0.12008
1.5798	115.4712	113.4712	98.8850	0.16655	-0.11077
1.5798	117.4712	113.4712	96.5730	0.22169	-0.09852

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1.5798	115.4712	115.4712	96.5866	...[b]	-0.09962
1.5798	117.4712	115.4712	94.1935	0.22341	-0.08534
1.5798	117.4712	117.4712	91.7008	...[b]	-0.06878
1.6798	101.4712	101.4712	124.5866	...[b]	-0.22517
1.6798	103.4712	101.4712	122.7613	-0.15676	-0.23634
1.6798	105.4712	101.4712	120.9027	-0.10395	-0.24558
1.6798	107.4712	101.4712	119.0116	-0.05038	-0.25284
1.6798	109.4712	101.4712	117.0886	0.00378	-0.25804
1.6798	111.4712	101.4712	115.1340	0.05839	-0.26113
1.6798	113.4712	101.4712	113.1474	0.11328	-0.26205
1.6798	115.4712	101.4712	111.1284	0.16831	-0.26075
1.6798	117.4712	101.4712	109.0759	0.22333	-0.25718
1.6798	103.4712	103.4712	120.9388	...[b]	-0.24679
1.6798	105.4712	103.4712	119.0798	-0.10625	-0.25526
1.6798	107.4712	103.4712	117.1851	-0.05239	-0.26169
1.6798	109.4712	103.4712	115.2549	0.00208	-0.26601
1.6798	111.4712	103.4712	113.2893	0.05698	-0.26814
1.6798	113.4712	103.4712	111.2876	0.11216	-0.26804
1.6798	115.4712	103.4712	109.2489	0.16747	-0.26563
1.6798	117.4712	103.4712	107.1716	0.22275	-0.26086
1.6798	105.4712	105.4712	117.2173	...[b]	-0.26291
1.6798	107.4712	105.4712	115.3154	-0.05394	-0.26845
1.6798	109.4712	105.4712	113.3744	0.00082	-0.27181
1.6798	111.4712	105.4712	111.3937	0.05601	-0.27292
1.6798	113.4712	105.4712	109.3724	0.11146	-0.27170
1.6798	115.4712	105.4712	107.3089	0.16704	-0.26808
1.6798	117.4712	105.4712	105.2010	0.22256	-0.26200

1.6798	107.4712	107.4712	113.4028	...[b]	-0.27303
1.6798	109.4712	107.4712	111.4468	0.00004	-0.27536
1.6798	111.4712	107.4712	109.4465	0.05551	-0.27534
1.6798	113.4712	107.4712	107.4004	0.11123	-0.27291
1.6798	115.4712	107.4712	105.3063	0.16706	-0.26798
1.6798	117.4712	107.4712	103.1610	0.22281	-0.26045
1.6798	109.4712	109.4712	109.4712	0.00000	-0.27656
1.6798	111.4712	109.4712	107.4462	0.05551	-0.27533
1.6798	113.4712	109.4712	105.3695	0.11149	-0.27157
1.6798	115.4712	109.4712	103.2380	0.16754	-0.26519
1.6798	117.4712	109.4712	101.0473	0.22350	-0.25608
1.6798	111.4712	111.4712	105.3905	...[b]	-0.27277
1.6798	113.4712	111.4712	103.2764	0.11225	-0.26756
1.6798	115.4712	111.4712	101.0995	0.16851	-0.25958
1.6798	117.4712	111.4712	98.8540	0.22463	-0.24872
1.6798	113.4712	113.4712	101.1169	...[b]	-0.26075
1.6798	115.4712	113.4712	98.8850	0.16995	-0.25101
1.6798	117.4712	113.4712	96.5730	0.22618	-0.23819
1.6798	115.4712	115.4712	96.5866	...[b]	-0.23932
1.6798	117.4712	115.4712	94.1935	0.22813	-0.22430
1.6798	117.4712	117.4712	91.7008	...[b]	-0.20680
1.7798	101.4712	101.4712	124.5866	...[b]	-0.36729
1.7798	103.4712	101.4712	122.7613	-0.15993	-0.37892
1.7798	105.4712	101.4712	120.9027	-0.10595	-0.38854
1.7798	107.4712	101.4712	119.0116	-0.05123	-0.39608
1.7798	109.4712	101.4712	117.0886	0.00411	-0.40149
1.7798	111.4712	101.4712	115.1340	0.05987	-0.40470

1.7798	113.4712	101.4712	113.1474	0.11591	-0.40566
1.7798	115.4712	101.4712	111.1284	0.17208	-0.40431
1.7798	117.4712	101.4712	109.0759	0.22822	-0.40059
1.7798	103.4712	103.4712	120.9388	...[b]	-0.38982
1.7798	105.4712	103.4712	119.0798	-0.10844	-0.39865
1.7798	107.4712	103.4712	117.1851	-0.05339	-0.40535
1.7798	109.4712	103.4712	115.2549	0.00226	-0.40984
1.7798	111.4712	103.4712	113.2893	0.05834	-0.41206
1.7798	113.4712	103.4712	111.2876	0.11469	-0.41196
1.7798	115.4712	103.4712	109.2489	0.17116	-0.40945
1.7798	117.4712	103.4712	107.1716	0.22758	-0.40448
1.7798	105.4712	105.4712	117.2173	...[b]	-0.40663
1.7798	107.4712	105.4712	115.3154	-0.05507	-0.41241
1.7798	109.4712	105.4712	113.3744	0.00090	-0.41592
1.7798	111.4712	105.4712	111.3937	0.05729	-0.41707
1.7798	113.4712	105.4712	109.3724	0.11394	-0.41580
1.7798	115.4712	105.4712	107.3089	0.17070	-0.41203
1.7798	117.4712	105.4712	105.2010	0.22739	-0.40568
1.7798	107.4712	107.4712	113.4028	...[b]	-0.41720
1.7798	109.4712	107.4712	111.4468	0.00006	-0.41963
1.7798	111.4712	107.4712	109.4465	0.05675	-0.41961
1.7798	113.4712	107.4712	107.4004	0.11369	-0.41707
1.7798	115.4712	107.4712	105.3063	0.17072	-0.41192
1.7798	117.4712	107.4712	103.1610	0.22765	-0.40405
1.7798	109.4712	109.4712	109.4712	0.00000	-0.42089
1.7798	111.4712	109.4712	107.4462	0.05676	-0.41960
1.7798	113.4712	109.4712	105.3695	0.11397	-0.41566

1.7798	115.4712	109.4712	103.2380	0.17125	-0.40898
1.7798	117.4712	109.4712	101.0473	0.22840	-0.39943
1.7798	111.4712	111.4712	105.3905	...[b]	-0.41691
1.7798	113.4712	111.4712	103.2764	0.11479	-0.41145
1.7798	115.4712	111.4712	101.0995	0.17230	-0.40308
1.7798	117.4712	111.4712	98.8540	0.22964	-0.39166
1.7798	113.4712	113.4712	101.1169	...[b]	-0.40429
1.7798	115.4712	113.4712	98.8850	0.17388	-0.39404
1.7798	117.4712	113.4712	96.5730	0.23136	-0.38053
1.7798	115.4712	115.4712	96.5866	...[b]	-0.38170
1.7798	117.4712	115.4712	94.1935	0.23353	-0.36583
1.7798	117.4712	117.4712	91.7008	...[b]	-0.34726
1.8798	101.4712	101.4712	124.5866	...[b]	-0.50799
1.8798	103.4712	101.4712	122.7613	-0.16327	-0.52021
1.8798	105.4712	101.4712	120.9027	-0.10808	-0.53030
1.8798	107.4712	101.4712	119.0116	-0.05212	-0.53822
1.8798	109.4712	101.4712	117.0886	0.00444	-0.54389
1.8798	111.4712	101.4712	115.1340	0.06143	-0.54725
1.8798	113.4712	101.4712	113.1474	0.11869	-0.54826
1.8798	115.4712	101.4712	111.1284	0.17606	-0.54684
1.8798	117.4712	101.4712	109.0759	0.23338	-0.54295
1.8798	103.4712	103.4712	120.9388	...[b]	-0.53167
1.8798	105.4712	103.4712	119.0798	-0.11076	-0.54095
1.8798	107.4712	103.4712	117.1851	-0.05446	-0.54798
1.8798	109.4712	103.4712	115.2549	0.00244	-0.55270
1.8798	111.4712	103.4712	113.2893	0.05978	-0.55503
1.8798	113.4712	103.4712	111.2876	0.11737	-0.55492

1.8798	115.4712	103.4712	109.2489	0.17507	-0.55229
1.8798	117.4712	103.4712	107.1716	0.23269	-0.54707
1.8798	105.4712	105.4712	117.2173	...[b]	-0.54935
1.8798	107.4712	105.4712	115.3154	-0.05626	-0.55543
1.8798	109.4712	105.4712	113.3744	0.00098	-0.55911
1.8798	111.4712	105.4712	111.3937	0.05865	-0.56032
1.8798	113.4712	105.4712	109.3724	0.11656	-0.55898
1.8798	115.4712	105.4712	107.3089	0.17457	-0.55502
1.8798	117.4712	105.4712	105.2010	0.23248	-0.54835
1.8798	107.4712	107.4712	113.4028	...[b]	-0.56047
1.8798	109.4712	107.4712	111.4468	0.00008	-0.56302
1.8798	111.4712	107.4712	109.4465	0.05807	-0.56301
1.8798	113.4712	107.4712	107.4004	0.11629	-0.56033
1.8798	115.4712	107.4712	105.3063	0.17459	-0.55490
1.8798	117.4712	107.4712	103.1610	0.23277	-0.54662
1.8798	109.4712	109.4712	109.4712	0.00000	-0.56435
1.8798	111.4712	109.4712	107.4462	0.05807	-0.56299
1.8798	113.4712	109.4712	105.3695	0.11659	-0.55884
1.8798	115.4712	109.4712	103.2380	0.17516	-0.55179
1.8798	117.4712	109.4712	101.0473	0.23358	-0.54172
1.8798	111.4712	111.4712	105.3905	...[b]	-0.56016
1.8798	113.4712	111.4712	103.2764	0.11748	-0.55438
1.8798	115.4712	111.4712	101.0995	0.17629	-0.54554
1.8798	117.4712	111.4712	98.8540	0.23492	-0.53347
1.8798	113.4712	113.4712	101.1169	...[b]	-0.54682
1.8798	115.4712	113.4712	98.8850	0.17800	-0.53597
1.8798	117.4712	113.4712	96.5730	0.23680	-0.52166

1.8798	115.4712	115.4712	96.5866	...[b]	-0.52288
1.8798	117.4712	115.4712	94.1935	0.23918	-0.50603
1.8798	117.4712	117.4712	91.7008	...[b]	-0.48627

[a] Only the M_x and M_z components were calculated. The M_y components can be derived by symmetry considerations. See text for details.

[b] No value for M_x available due to technical problems in the CCSD(T) calculation. The total number of data points is thus only 333 for M_x, compared with 405 for M_z.