Supplement to the paper:

Interactions in diatomic dimers involving closed-shell metals

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TABLE 1: Comparison of the beryllium dimer interaction energies at $R = 2.44$ Å obtained using various methods and basis sets. The symbols "AE" and "FC" denote all-electron and frozen-core results, respectively.

method	AE/FC	$E^{[2]}_{\mathrm{SAPT}}$	MP2	MP4	CCSD(T)	CCSDT	CCSDTQ	FCI
aDZ	AE	-1227	348	-154	93	-104	-181	-181
aDZ	FC	-1177	358	-146	110	-90	-166	-166
aDZ+(332)	AE	-2124	-184	-718	-542	-721		
aDZ+(332)	FC	-2048	-109	-637	-443	-625	-709	-709
aTZ	AE	-1973	-150	-696	-519	-693		
aTZ	FC	-1901	-63	-597	-399	-576	-662	-662
aTZ+(332)	AE	-2075	-246	-768	-610	-771		
aTZ+(332)	FC	-2056	-196	-715	-538	-701		-787
aTZ+(33221)	AE	-2115	-287	-797	-646	-797		
aTZ+(33221)	FC	-2109	-233	-741	-571	-726		-812
aQZ	AE	-2043	-268	-798	-642	-798		
aQZ	FC	-2045	-201	-724	-548	-707		-793
aQZ+(33221)	AE	-2105	-338	-849	-701			
aQZ+(33221)	FC	-2107	-262	-766	-601			-837
a5Z	AE	-2084	-330	-846	-696			
a5Z	FC	-2097	-255	-764	-599			
a5Z+(33221)	AE	-2102	-351	-857	-709			
a5Z+(33221)	FC	-2117	-276	-776	-614			
aCVTZ+(33221)	AE	-2077	-280	-783	-618			
aCVTZ+(33221)	FC	-2105	-238	-745	-576			
aCVQZ+(33221)	AE	-2072	-326	-829	-667			
aCVQZ+(33221)	FC	-2107	-264	-768	-603			

TABLE 2: Components of the SAPT and SAPT(DFT) (denoted 'SDFT') beryllium dimer interaction energy at $R = 2.44$ Å as well as supermolecular interaction energies for different basis sets. The columns marked "AE" and "FC" list all-electron and frozen-core results, respectively. For the description of scaled $E^{[2]}_{\rm SAPT}/E^{[2]}_{\rm SDFT}$, see text. SAPT(DFT) results were obtained with the a5ZM basis set. The letter "M" in a basis set symbol denotes the (33221) set of midbond functions. In the first column, the first symbol refers to SAPT and the second one to SAPT(DFT).

method	aQZ		aQZM		a5Z		a5ZM		SDFT
	AE	FC	AE	FC	AE	FC	AE	FC	AE
$E^{\rm HF}_{\rm int}$	2680	2680	2679	2679	2677	2677	2677	2677	
$E^{(1)}_{\rm elst,resp}(3)/E^{(1)}_{\rm elst}$(KS)	-6193	-6222	-6190	-6220	-6179	-6220	-6174	-6220	-6242
$E^{(1)}_{\rm exch}(2)$	15808	15837	15798	15831	15774	15810	15768	15808	
$E^{(1)}_{\rm exch}$(CCSD)$/E^{(1)}_{\rm exch}$(KS)	13947	13966	13947	13972	13939	13969	13936	13972	13853
$E^{(10)}_{\rm exch}(S^{k>2})/\ E^{(1)}_{\rm exch}(S^{k>2})$(KS)	1780	1780	1780	1780	1780	1780	1780	1780	1464
$E^{(20)}_{\rm ind,resp}/E^{(2)}_{\rm ind}$(CKS)	-13479	-13466	-13494	-13480	-13496	-13482	-13497	-13483	-12667
$E^{(20)}_{\rm exch-ind,resp}/\widetilde{E}^{(2)}_{\rm ex-ind}$(CKS)	8166	8152	8184	8169	8186	8172	8187	8173	7980
${}^tE^{(22)}_{\rm ind}$	526	454	545	460	574	476	583	477	
${}^tE^{(22)}_{\rm exch-ind}$	-319	-275	-330	-279	-348	-288	-353	-289	
$E^{(2)}_{\rm disp}(2)/E^{(2)}_{\rm disp}$(CKS)	-5066	-5019	-5154	-5107	-5149	-5100	-5178	-5129	-4944
$E^{(20)}_{\rm exch-disp}/\widetilde{E}^{(2)}_{\rm exch-disp}$(CKS)	374	364	388	378	388	378	393	382	285
$\delta E^{\rm HF}_{\rm int,resp}$	-841	-840	-846	-845	-848	-846	-848	-847	-848
$E^{[2]}_{\rm SAPT}/E^{[2]}_{\rm SDFT}$	-2043	-2045	-2105	-2107	-2084	-2097	-2102	-2117	-1735
$E^{[2]}_{\rm SAPT+HF}/E^{[2]}_{\rm SDFT+HF}$	-2885	-2885	-2951	-2952	-2932	-2943	-2950	-2964	-2583
scaled $E^{[2]}_{\rm SAPT}/E^{[2]}_{\rm SDFT}$	-1106	-1098	-1161	-1151	-1146	-1143	-1163	-1161	-759
MP2	-268	-201	-338	-262	-330	-255	-351	-276	
MP3	-560	-499	-604	-534	-599	-530	-607	-538	
MP4	-798	-724	-849	-766	-846	-764	-857	-776	
CCSD	310	392	269	357	276	359	268	349	
CCSD(T)	-642	-548	-701	-601	-696	-599	-709	-614	
FCI		-793		-837					

TABLE 3: SAPT and supermolecular Be_2 interaction energies, calculated in the aQZ+(33221) basis set, as functions of the interatomic separation R. 'Asymp.' corresponds to $-C_6/R^6 - C_8/R^8 - C_{10}/R^{10}$. The C_6, C_8, and C_{10} coefficients equal to 214, 10230, and 504300 a.u., respectively, were taken from Ref. 1.

R [Å]	$E^{[2]}_{\rm SAPT}$	$E^{[2]}_{\rm SDFT}$	MP2	MP4	CCSD	CCSD(T)	Asymp.
2.44	-2105	-1805	-338	-849	269	-701	-41355
3.00	-300	-463	-423	-580	121	-358	-6747
4.00	-255	-287	-234	-267	-46	-170	-644
5.00	-116	-112	-100	-111	-46	-79	-121
6.00	-41.6	-37.5	-36.5	-40.2	-19.5	-28.9	-33.5
7.00	-15.5	-13.6	-13.8	-15.2	-7.6	-10.9	-11.8
8.00	-6.46	-5.62	-5.79	-6.40	-3.20	-4.53	-4.93
9.00	-3.02	-2.62	-2.71	-3.00	-1.50	-2.11	-2.32
10.00	-1.55	-1.34	-1.39	-1.54	-0.77	-1.08	-1.19

TABLE 4: Comparison of the magnesium dimer interaction energies at $R = 3.9$ Å obtained using various methods and basis sets. The symbols "AE" and "FC" denote all-electron and frozen-core results, respectively.

method	AE/FC	$E^{[2]}_{\mathrm{SAPT}}$	MP2	MP4	CCSD(T)	FCI
aTZ	AE	-503	-309	-438	-315	
aTZ	FC	-520	-293	-442	-321	-412
aTZ+(33221)	AE	-595	-383	-496	-375	
aTZ+(33221)	FC	-612	-362	-496	-380	-463
aQZ	AE	-559	-360	-475	-355	
aQZ	FC	-586	-342	-484	-368	-453
aQZ+(33221)	AE	-597	-401	-504	-384	
aQZ+(33221)	FC	-616	-369	-500	-386	-467
5Z	AE	-533	-371	-460	-344	
5Z	FC	-577	-344	-479	-365	
5Z+(33221)	AE	-586	-428	-511	-392	
5Z+(33221)	FC	-607	-367	-495	-383	
a5Z	AE	-568	-395	-483	-366	
a5Z	FC	-609	-361	-496	-383	
a5Z+(33221)	AE	-675	-535	-619	-498[a]	
a5Z+(33221)	FC	-621	-374	-503	-390	
aCVTZ+(33221)	AE	-565	-395	-482	-361	
aCVTZ+(33221)	FC	-614	-364	-498	-382	
aCVQZ+(33221)	AE	-563	-406	-483	-363	
aCVQZ+(33221)	FC	-618	-371	-502	-388	

[a]Result excluded from considerations, see text.

TABLE 5: SAPT/SAPT(DFT) interaction energy components and supermolecular interaction energies for the magnesium dimer at R = 3.9 Å. The letter "M" in a basis set symbol denotes the (33221) set of midbond functions. The columns marked "AE" and "FC" list all-electron and frozen-core results, respectively. SAPT(DFT) results were obtained with aCVQZ basis set and denoted as 'SDFT'.

method	aQZ		aQZM		a5Z		a5ZM	aCVQZM		SDFT
	AE	FC	AE	FC	AE	FC	FC	AE	FC	AE
$E_{\rm int}^{\rm HF}$	582	582	582	582	581	581	581	581	581	
$E_{\rm elst,resp}^{(1)}(3)/E_{\rm elst}^{(1)}$(KS)	-1049	-1100	-1052	-1097	-1018	-1100	-1098	-1002	-1096	-1034
$E_{\rm exch}^{(1)}(2)$	2706	2725	2702	2721	2662	2717	2715	2641	2720	
$E_{\rm exch}^{(1)}$(CCSD)$/E_{\rm exch}^{(1)}$(KS)	2367	2416	2364	2415	2314	2416	2415	2295	2415	2007
$E_{\rm exch}^{(10)}(S^{k>2})/E_{\rm exch}^{(1)}(S^{k>2})$(KS)	77	77	77	77	77	77	77	77	77	49
$E_{\rm ind,resp}^{(20)}/E_{\rm ind}^{(2)}$(CKS)	-2591	-2590	-2597	-2595	-2601	-2599	-2608	-2628	-2626	-2092
$E_{\rm exch-ind,resp}^{(20)}/\widetilde{E}_{\rm exch-ind}^{(2)}$(CKS)	2088	2086	2095	2093	2097	2095	2105	2125	2123	1716
${}^tE_{\rm ind}^{(22)}$	269	223	272	226	332	226	229	371	230	
${}^tE_{\rm exch-ind}^{(22)}$	-216	-180	-219	-182	-267	-182	-185	-300	-186	
$E_{\rm disp}^{(2)}(2)/E_{\rm disp}^{(2)}$(CKS)	-1675	-1683	-1722	-1729	-1687	-1714	-1735	-1697	-1730	-1623
$E_{\rm exch-disp}^{(20)}/\widetilde{E}_{\rm exch-disp}^{(2)}$(CKS)	250	242	262	254	262	249	255	273	254	254
$\delta E_{\rm int,resp}^{\rm HF}$	-214	-213	-216	-215	-214	-214	-216	-216	-215	-216
$E_{\rm SAPT}^{[2]}/E_{\rm SDFT}^{[2]}$	-559	-586	-597	-616	-568	-609	-621	-563	-618	-772
$E_{\rm SAPT+HF}^{[2]}/E_{\rm SDFT+HF}^{[2]}$	-772	-799	-813	-831	-782	-823	-837	-779	-833	-988
scaled $E_{\rm SAPT}^{[2]}/\ E_{\rm SDFT}^{[2]}$	-457	-474	-494	-499	-477	-495	-506	-474	-499	-723
MP2	-360	-342	-401	-369	-395	-361	-374	-406	-371	
MP3	-449	-450	-472	-461	-462	-460	-463	-463	-463	
MP4	-475	-484	-504	-500	-483	-496	-503	-483	-502	
CCSD	-86	-85	-109	-96	-98	-94	-99	-101	-98	
CCSD(T)	-355	-368	-384	-386	-366	-383	-390	-363	-388	

TABLE 6: Comparison of the calcium dimer interaction energies at $R = 8.2$ bohr obtained using various methods and basis sets. The symbols "AE" and "FC" denote all-electron and frozen-core results, respectively.

method	AE/FC	$E^{[2]}_{\mathrm{SAPT}}$	MP2	MP4	CCSD(T)	FCI
aTZ	AE	-1926	-775	-925	-784	
aTZ	FC	-2262	-667	-996	-876	-1089
aTZ+(33221)	AE	-2149	-986	-1114	-972	
aTZ+(33221)	FC	-2460	-836	-1138	-1036	-1239
aQZ	AE	-2043	-930	-1076	-921	
aQZ	FC	-2399	-783	-1117	-1011	-1220
aQZ+(33221)	AE	-2120	-1010	-1128	-973	
aQZ+(33221)	FC	-2472	-850	-1153	-1054	-1253
a5Z+(33221)	AE	-2126	-1028	-1141	-983	
a5Z+(33221)	FC	-2493	-858	-1160	-1064	
aCVTZ+(33221)	AE	-2114	-1005	-1121	-964	
aCVTZ+(33221)	FC	-2468	-839	-1142	-1039	
aCVQZ+(33221)	AE	-2097	-1028	-1138	-976	
aCVQZ+(33221)	FC	-2481	-851	-1154	-1055	

TABLE 7: SAPT/SAPT(DFT) interaction energy components and supermolecular interaction energies for the calcium dimer at $R = 8.2$ bohr. The basis sets employed are described in the text; the letter "M" in a basis set symbol denotes the (33221) set of midbond functions. The columns marked "AE" and "FC" list all-electron and frozen-core results, respectively. SAPT(DFT) results (denoted as 'SDFT') were obtained with the a5ZM basis set.

method	Bussery		BusseryM		aQZM		a5ZM		SDFT
	AE	FC	AE	FC	AE	FC	AE	FC	AE
$E_{\rm int}^{\rm HF}$	737	737	656	656	590	590	590	590	
$E_{\rm elst,resp}^{(1)}(3)/E_{\rm elst}^{(1)}$(KS)	-2286	-2686	-2307	-2704	-2231	-2630	-2216	-2633	-2313
$E_{\rm exch}^{(1)}(2)$	5061	5262	5029	5259	4871	5176	4826	5156	
$E_{\rm exch}^{(1)}$(CCSD)$/E_{\rm exch}^{(1)}$(KS)	4354	4689	4354	4709	4248	4669	4223	4666	3741
$E_{\rm exch}^{(10)}(S^{k>2})/E_{\rm exch}^{(1)}(S^{k>2})$(KS)	329	329	329	329	328	328	328	328	196
$E_{\rm ind,resp}^{(20)}/E_{\rm ind}^{(2)}$(CKS)	-12619	-12583	-12694	-12657	-12575	-12535	-12593	-12553	-9328
$E_{\rm exch-ind,resp}^{(20)}/\widetilde{E}_{\rm exch-ind}^{(2)}$(CKS)	10453	10419	10497	10463	10398	10361	10414	10377	7847
${}^tE_{\rm ind}^{(22)}$	1740	573	1896	616	2258	803	2389	843	
${}^tE_{\rm exch-ind}^{(22)}$	-1441	-475	-1568	-509	-1867	-663	-1976	-697	
$E_{\rm disp}^{(2)}(2)/E_{\rm disp}^{(2)}$(CKS)	-2334	-2318	-2854	-2818	-2886	-2897	-2913	-2922	-2866
$E_{\rm exch-disp}^{(20)}/\widetilde{E}_{\rm exch-disp}^{(2)}$(CKS)	434	332	514	409	535	420	546	426	484
$\delta E_{\rm int,resp}^{\rm HF}$	851	849	806	803	722	719	724	721	724
$E_{\rm SAPT}^{[2]}/E_{\rm SDFT}^{[2]}$	-1700	-2048	-2162	-2492	-2120	-2472	-2126	-2493	-2437
$E_{\rm SAPT+HF}^{[2]}/E_{\rm SDFT+HF}^{[2]}$	-848	-1199	-1357	-1689	-1398	-1752	-1401	-1772	-1712
scaled $E_{\rm SAPT}^{[2]}/\ E_{\rm SDFT}^{[2]}$	-1095	-1277	-1519	-1668	-1519	-1663	-1535	-1683	-1977
MP2	-427	-335	-907	-739	-1010	-850	-1028	-858	
MP3	-441	-506	-906	-910	-981	-1011	-992	-1016	
MP4	-495	-562	-1033	-1033	-1128	-1153	-1141	-1160	
CCSD	-17	-33	-429	-409	-501	-507	-508	-510	
CCSD(T)	-350	-413	-866	-913	-973	-1054	-983	-1064	
FCI						-1253			
Experiment	-1102 (Refs. 2,3)								

TABLE 8: SAPT/SAPT(DFT) interaction energy components and supermolecular interaction energies for the zinc dimer at R = 3.847 Å. The letter "M" in a basis set symbol denotes the (33221) set of midbond functions. The columns marked "AE" and "FC" list all-electron and frozen-core results, respectively. SAPT(DFT) results (denoted as 'SDFT') are obtained with the aQZM basis set.

method	aTZ		aTZM		aQZ		aQZM		SDFT
	AE	FC	AE	FC	AE	FC	AE	FC	AE
$E_{\rm int}^{\rm HF}$	446	446	444	444	445	445	444	444	
$E_{\rm elst,resp}^{(1)}(3)/E_{\rm elst}^{(1)}$(KS)	-547	-534	-553	-538	-533	-520	-535	-521	-569
$E_{\rm exch}^{(1)}(2)/E_{\rm exch}^{(1)}$(KS)	1645	1609	1655	1619	1623	1590	1626	1593	1100
$E_{\rm exch}^{(1)}$(CCSD)	1306	1280	1319	1293	1290	1267	1295	1271	
$E_{\rm exch}^{(10)}(S^{k>2})/E_{\rm exch}^{(1)}(S^{k>2})$(KS)	29	29	29	29	29	29	29	29	12
$E_{\rm ind,resp}^{(20)}/E_{\rm ind}^{(2)}$(CKS)	-3150	-3150	-3189	-3189	-3157	-3156	-3208	-3208	-2003
$E_{\rm exch-ind,resp}^{(20)}/\widetilde{E}_{\rm exch-ind}^{(2)}$(CKS)	2853	2853	2888	2888	2858	2858	2907	2906	1841
${}^tE_{\rm ind}^{(22)}$	703	763	687	745	770	818	783	831	
${}^tE_{\rm exch-ind}^{(22)}$	-636	-691	-622	-675	-697	-741	-710	-753	
$E_{\rm disp}^{(2)}(2)/E_{\rm ind}^{(2)}$(CKS)	-913	-891	-1111	-1084	-986	-963	-1107	-1083	-950
$E_{\rm exch-disp}^{(20)}/\widetilde{E}_{\rm exch-disp}^{(2)}$(CKS)	150	145	187	182	164	160	189	184	124
$\delta E_{\rm int,resp}^{\rm HF}$	-85	-85	-85	-85	-87	-86	-85	-85	-85
$E_{\rm SAPT}^{[2]}/E_{\rm SDFT}^{[2]}$	-235	-224	-393	-376	-290	-278	-386	-371	-458
$E_{\rm SAPT+HF}^{[2]}/E_{\rm SDFT+HF}^{[2]}$	-320	-309	-478	-461	-377	-365	-471	-456	-543
scaled $E_{\rm SAPT}^{[2]}/E_{\rm SDFT}^{[2]}$	-216	-209	-368	-355	-274	-262	-363	-353	-436
MP2	-318	-308	-441	-427	-378	-367	-450	-438	
MP3	-191	-205	-300	-311	-246	-259	-308	-319	
MP4	-282	-248	-418	-377	-345	-311	-420	-382	
CCSD	2	1	-84	-81	-39	-40	-86	-85	
CCSD(T)	-109	-113	-223	-224	-164	-169	-228	-230	
Experiment	−279.1 (Ref. 4)								

TABLE 9: Comparison of the He–Mg interaction energies at $R = 5.0$ Å obtained using various methods and basis sets. The symbols "AE" and "FC" denote all-electron and frozen-core results, respectively.

method	AE/FC	$E^{[2]}_{\mathrm{SAPT}}$	MP2	MP4	CCSD(T)	FCI
aTZ	AE	-3.30	-2.21	-4.25	-3.38	
aTZ	FC	-3.05	-1.75	-3.92	-3.18	-3.54
aTZ+(332)	AE	-4.71	-3.32	-5.56	-4.58	
aTZ+(332)	FC	-4.33	-2.69	-5.06	-4.23	-4.61
aTZ+(33221)	AE	-4.82	-3.40	-5.63	-4.63	
aTZ+(33221)	FC	-4.48	-2.80	-5.18	-4.33	-4.71
aQZ	AE	-4.13	-3.03	-4.94	-4.00	
aQZ	FC	-3.77	-2.38	-4.53	-3.76	-4.12
aQZ+(332)	AE	-4.82	-3.56	-5.55	-4.57	
aQZ+(332)	FC	-4.44	-2.88	-5.11	-4.31	-4.68
aQZ+(33221)	AE	-4.92	-3.64	-5.62	-4.63	
aQZ+(33221)	FC	-4.54	-2.95	-5.18	-4.37	-4.74
a5Z	AE	-4.70	-3.74	-5.33	-4.35	
a5Z	FC	-4.08	-2.65	-4.77	-4.01	
a5Z+(33221)	AE	-5.25	-4.20	-5.82	-4.79[a]	
a5Z+(33221)	FC	-4.57	-3.02	-5.18	-4.39	
aCVTZ+(33221)[b]	AE	-4.98	-3.85	-5.61	-4.61	
aCVTZ+(33221)[b]	FC	-4.45	-2.78	-5.15	-4.31	
aCVQZ+(33221)[b]	AE	-5.17	-4.16	-5.68	-4.69	
aCVQZ+(33221)[b]	FC	-4.54	-2.95	-5.17	-4.37	

[a] Result with possible numerical errors, not included in the final estimates.

[b] Helium basis set was aXZ, with the same X as for Mg.

TABLE 10: SAPT/SAPT(DFT) interaction energy components and supermolecular interaction energies for the He–Mg dimer at R = 5.0 Å. The letter "M" in a basis set symbol denotes the (33221) set of midbond functions. The columns marked "AE" and "FC" list all-electron and frozen-core results, respectively. SAPT(DFT) results (denoted as 'SDFT') were obtained with the aCVQZ basis set for magnesium, a5Z for helium, and the (33221) midbond set.

method	aQZM		a5ZM	aCVQZM		SDFT
	AE	FC	FC	AE	FC	AE
$E_{\rm int}^{\rm HF}$	9.36	9.36	9.37	9.37	9.37	
$E_{\rm elst,resp}^{(1)}(3)/E_{\rm elst}^{(1)}$(KS)	-1.92	-2.05	-2.05	-1.77	-2.05	-2.07
$E_{\rm exch}^{(1)}(2)/E_{\rm exch}^{(1)}$(KS)	12.40	12.79	12.75	11.84	12.79	10.98
$E_{\rm exch}^{(1)}$(CCSD)	9.78	10.35	10.35	9.21	10.35	
$E_{\rm exch}^{(10)}(S^{k>2})/E_{\rm exch}^{(1)}(S^{k>2})$(KS)	0.00	0.00	0.00	0.00	0.00	0.00
$E_{\rm ind,resp}^{(20)}/E_{\rm ind}^{(2)}$(CKS)	-1.46	-1.46	-1.46	-1.46	-1.46	-1.03
$E_{\rm exch-ind,resp}^{(20)}/\widetilde{E}_{\rm exch-ind}^{(2)}$(CKS)	2.00	2.00	2.00	2.00	2.00	1.34
${}^tE_{\rm ind}^{(22)}$	0.28	0.24	0.24	0.34	0.24	
${}^tE_{\rm exch-ind}^{(22)}$	-0.38	-0.33	-0.33	-0.46	-0.33	
$E_{\rm disp}^{(2)}(2)/E_{\rm disp}^{(2)}$(CKS)	-13.83	-13.89	-13.95	-13.63	-13.89	-13.45
$E_{\rm exch-disp}^{(20)}/\widetilde{E}_{\rm exch-disp}^{(2)}$(CKS)	0.61	0.61	0.63	0.61	0.61	0.53
$\delta E_{\rm int,resp}^{\rm HF}$	-3.09	-3.09	-3.09	-3.09	-3.09	-3.09
$E_{\rm SAPT}^{[2]}/E_{\rm SDFT}^{[2]}$	-4.92	-4.54	-4.57	-5.17	-4.54	-3.70
$E_{\rm SAPT+HF}^{[2]}/E_{\rm SDFT+HF}^{[2]}$	-8.01	-7.63	-7.66	-8.26	-7.63	-6.79
scaled $E_{\rm SAPT}^{[2]}$	-4.84	-4.44	-4.47	-5.09	-4.44	
MP2	-3.64	-2.95	-3.02	-4.16	-2.95	
MP3	-5.64	-5.04	-5.05	-5.98	-5.04	
MP4	-5.62	-5.18	-5.18	-5.68	-5.17	
CCSD	-3.03	-2.70	-2.71	-3.12	-2.70	
CCSD(T)	-4.63	-4.37	-4.39	-4.69	-4.37	
FCI		-4.74				

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