Supplemental Material (ESI) to: Electron correlation effects in boron clusters B_n^Q (for $Q = -1, 0, 1$ and $n \leq 13$) based on quantum Monte Carlo simulations

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S1. ATOMIC STRUCTURE: CLUSTERS COORDINATES

The optimized structures of the boron clusters B_n^Q (for $Q = -1, 0, 1$ and $n \leq 13$) were obtained from DFT with B3LYP exchange-correlation functional as implemented in the Gaussian09 program[1] with the basis set 6-311+G* from the site EMSL basis set exchange[2]. The atomic coordinates and spin contamination of the clusters are shown in Table S1.

TABLE S1: Cartesian coordinates (x, y and z) describe the atomic coordinates relative to the origin (in Å) of the boron clusters B_n^Q (for $Q = -1, 0, 1$ and $n \leq 13$). We provide also for each clusters the $< S^2 >$ expectation value of the Kohn-Sham determinant as an approximate measure of spin contamination.

Cluster	B_n				B_n^+				B_n^-			
size, n	x	y	z	$< S^2 >$	x	y	z	$< S^2 >$	x	y	z	$< S^2 >$
2	−0.808046	−0.001756	0.00000	2.0048	−0.810445	−0.001756	0.00000	0.7527	−0.911724	−0.001756	0.00000	3.7591
	0.808046	−0.001756	0.00000		0.810445	1.823448	0.00000		0.911724	−0.001756	0.00000	
2⋆	−0.820610	−0.001756	0.00000	0.0	–	–	–		–	–	–	
	−0.820610	−0.001756	0.00000		–	–	–		–	–	–	
3	−0.774095	−0.001756	0.00000	0.8144	−0.781776	−0.006192	0.000000	0.0	−0.771064	−0.000007	0.000000	0.0
	0.774095	−0.001756	0.00000		0.781776	−0.006192	0.000000		0.771064	−0.000007	0.000000	
	0.000000	0.000000	1.339019		0.000000	1.347891	0.000000		0.000000	1.335521	0.000000	
4	1.219972	−0.049867	0.000000	0.0	0.000000	0.000000	0.000000	0.7585	1.358482	−0.049851	0.000000	0.9853
	−1.169972	−0.050133	0.000000		1.162344	1.019348	0.000000		−1.308490	−0.050149	0.000000	
	0.024895	0.893649	0.000000		1.162344	−1.019348	0.000000		0.024912	0.774642	0.000000	
	0.025105	−0.993649	0.000000		2.324688	0.000000	0.000000		0.025096	−0.874642	0.000000	
5	−4.573899	2.846036	−0.002372	0.8902	−4.270204	2.781220	−0.002098	0.0	−4.624404	2.864418	−0.002404	0.0
	−3.033086	3.203480	−0.000211		−3.050251	3.738293	0.000437		−3.029820	3.114052	−0.000250	
	−1.472142	2.948356	0.001618		−1.769096	2.864759	0.001122		−1.422218	2.970351	0.001637	
	−3.753304	1.516266	−0.002770		−3.746908	1.321680	−0.003022		−3.766440	1.539763	−0.002838	
	−2.201239	1.566331	−0.000945		−2.197211	1.374517	−0.001119		−2.190787	1.591884	−0.000825	
6	1.767923	−0.458974	−0.168076	0.0	1.758586	−0.410283	−0.317819	0.7760	−4.637233	2.856491	−0.002824	3.7759
	0.240514	1.648573	−0.131750		0.230185	1.611462	−0.202767		−3.066170	3.062604	−0.005636	
	1.771295	2.144010	−0.162579		1.794347	2.124311	−0.214266		−1.413767	3.013967	−0.007280	
	0.238017	0.039553	−0.134992		0.214804	0.050526	−0.039804		−3.692002	1.419205	0.003581	
	2.716109	0.841322	−0.182371		2.733094	0.876165	−0.057396		−2.120940	1.625318	0.001263	
	1.365743	0.841495	0.779769		1.368586	0.803796	0.832054		−5.344407	1.467837	0.004557	
6⋆	−4.617675	2.880833	−0.003064	2.0421	–	–	–		−4.462592	2.783535	−0.002462	0.8562
	−3.065757	3.197189	−0.006509		–	–	–		−2.960421	3.377753	−0.007516	
	−1.502594	2.977103	−0.006744		–	–	–		−1.469451	2.996488	−0.007153	
	−3.692420	1.284583	0.004121		–	–	–		−3.797752	1.104053	0.005213	
	−2.140506	1.600998	0.001317		–	–	–		−2.295580	1.698276	0.001186	
	−5.255567	1.504715	0.004539		–	–	–		−5.288723	1.485315	0.004393	
7	0.011186	0.013098	−0.657147	0.7687	0.011588	0.013369	−0.721266	0.0	0.010457	0.011958	−0.452639	2.0093
	1.668815	0.010789	−0.152696		1.591941	0.009964	0.003193		1.614159	0.010201	−0.041283	
	0.818696	1.310422	0.069308		0.800037	1.381279	0.007447		0.811084	1.400299	−0.037283	
	−0.802278	1.309371	0.062367		−0.783605	1.380911	0.000774		−0.794283	1.399923	−0.044040	
	−1.650840	0.010048	−0.166807		−1.574813	0.009231	−0.010145		−1.596659	0.009459	−0.054815	
	−0.801824	−1.291526	0.048805		−0.782910	−1.362089	−0.013635		−0.793577	−1.380633	−0.058643	
	0.819215	−1.291262	0.055581		0.800730	−1.361723	−0.006957		0.811788	−1.380266	−0.051885	
7⋆	–	–	–		–	–	–		0.011229	0.012937	−0.638753	0.0
	–	–	–		–	–	–		1.707793	0.011365	−0.258149	
	–	–	–		–	–	–		0.838187	1.247929	0.117199	
	–	–	–		–	–	–		−0.822612	1.247548	0.110199	
	–	–	–		–	–	–		−1.688456	0.010579	−0.272460	
	–	–	–		–	–	–		−0.821985	−1.229904	0.097189	
	–	–	–		–	–	–		0.838813	−1.229513	0.104186	
8	0.000216	−0.000053	0.000000	2.0094	0.000099	−0.000056	0.000000	0.7588	0.000130	−0.000053	0.000000	0.7595

	1.790837	−0.000230	0.000001		1.790276	−0.002948	0.000001		1.766187	−0.002610	0.000001	
	1.116455	1.399947	0.000001		1.107500	1.433577	0.000000		1.094917	1.411738	0.000000	
	−0.398251	1.745673	−0.000001		−0.397137	1.784331	0.000000		−0.392792	1.759181	0.000000	
	−1.613102	0.777172	0.000000		−1.609608	0.802032	0.000000		−1.588973	0.788675	0.000000	
	−1.613244	−0.777080	0.000001		−1.608715	−0.797752	0.000000		−1.587978	−0.784859	0.000000	
	−0.398479	−1.745759	0.000000		−0.392333	−1.783776	0.000000		−0.388641	−1.758529	0.000000	
	1.116279	−1.400230	0.000000		1.110628	−1.435968	0.000001		1.097860	−1.414104	0.000001	
9	1.758925	−0.006585	−0.011055	0.7687	1.711153	0.017080	−0.050012	0.0	0.000000	0.000000	0.000000	0.0
	1.096470	1.368471	−0.018387		1.179405	1.500707	−0.104265		1.974961	−0.000120	0.000000	
	−0.391442	1.708061	−0.017047		−0.388959	1.825657	−0.102707		1.397626	1.397642	0.000000	
	−1.585024	0.757346	−0.008323		−1.503348	0.725233	−0.019758		−0.000121	1.975014	0.000000	
	−1.584373	−0.769247	0.000955		−1.634745	−0.830061	0.080100		−1.397729	1.397750	0.000000	
	−0.391418	−1.720401	0.004883		−0.436950	−1.884748	0.092402		−1.974961	0.000120	0.000000	
	1.096663	−1.381562	−0.000655		1.072702	−1.403148	0.056460		−1.397626	−1.397642	0.000000	
	0.000082	−0.006999	−0.869754		0.121712	0.323764	−0.754077		0.000121	−1.975014	0.000000	
	0.001197	−0.003175	0.843664		−0.119889	−0.328575	0.726138		1.397729	−1.397750	0.000000	
10	−0.176565	0.309350	−0.388888	0.0	−0.165067	0.290476	−0.220815	0.7601	−0.157257	0.277747	−0.204822	0.7848
	1.444187	0.303946	−0.023773		1.483873	0.271838	−0.071579		1.480572	0.315396	−0.080312	
	0.771862	1.771037	−0.074924		0.772005	1.771128	−0.074729		0.791786	1.783252	−0.074568	
	−0.961372	1.588482	0.237131		−0.972682	1.607449	0.067365		−0.980551	1.620304	0.053255	
	−1.909534	0.127144	−0.076098		−1.909855	0.126968	−0.076713		−1.929654	0.114830	−0.076476	
	−0.907336	−1.137810	−0.025716		−0.896675	−1.187593	−0.073397		−0.933988	−1.164875	−0.082216	
	0.669971	−1.071693	−0.118483		0.685348	−1.096825	−0.112990		0.668062	−1.068644	−0.106977	
	−2.582203	1.594261	−0.127180		−2.621813	1.626287	−0.078445		−2.618427	1.582690	−0.070351	
	−1.807774	2.969785	−0.031832		−1.823200	2.994917	−0.036451		−1.805917	2.966730	−0.043463	
	−0.230467	3.035917	−0.124617		−0.241165	3.085775	−0.076629		−0.203858	3.062990	−0.068451	
11	−4.603442	2.858928	0.036733	0.7662	−4.608203	2.843901	−0.049275	0.0	−4.588063	2.846622	0.036919	0.0
	−3.046900	3.084275	−0.012827		−3.041527	3.038619	−0.014371		−3.058621	3.178288	−0.010752	
	−1.483175	3.256969	−0.064711		−1.475336	3.237529	0.020659		−1.495253	3.241062	−0.065507	
	−3.693128	1.387436	−0.027037		−3.665275	1.376172	0.159381		−3.720749	1.351631	−0.028889	
	−1.999016	1.606233	−0.087368		−2.025596	1.595429	−0.274471		−1.964630	1.577092	−0.087337	
	−5.381734	1.521559	0.034496		−5.416829	1.527415	0.061683		−5.376551	1.527392	0.035028	
	−0.397449	2.155848	−0.130466		−0.365914	2.171184	−0.156730		−0.404447	2.159880	−0.130084	
	−1.840636	−0.280315	−0.135468		−1.840278	−0.268536	−0.114585		−1.830702	−0.262796	−0.135349	
	−3.382508	−0.479800	−0.083846		−3.383399	−0.463825	−0.104127		−3.394951	−0.462901	−0.083286	
	−0.588006	0.619134	−0.159556		−0.575691	0.646535	−0.131876		−0.568458	0.598591	−0.160632	
	−4.817376	0.080492	−0.018908		−4.835324	0.106334	−0.045247		−4.830946	0.055897	−0.019070	
12	−0.047676	−0.136640	0.285850	0.0	−0.084868	−0.139677	0.307817	0.7865	−0.078839	−0.119561	0.276395	0.7584
	1.709626	−0.147956	−0.155339		1.755054	−0.172999	−0.211314		1.822320	−0.209844	−0.152078	
	0.762470	1.335743	0.280204		0.746115	1.367627	0.302406		0.732248	1.351395	0.270960	
	−0.917251	1.300926	0.283819		−0.924202	1.305755	0.342624		−0.932586	1.309931	0.190796	
	−1.806126	−0.217853	−0.149880		−1.777674	−0.182318	−0.122759		−1.789388	−0.207572	−0.152303	
	−0.799285	−1.477689	−0.277759		−0.792330	−1.485193	−0.278849		−0.786332	−1.466685	−0.256758	
	0.753732	−1.447160	−0.279952		0.757704	−1.429478	−0.284547		0.788810	−1.419328	−0.276314	
	2.297442	1.353281	−0.289380		2.284934	1.340744	−0.293862		2.292964	1.309169	−0.285515	
	−2.452468	1.259525	−0.282448		−2.459609	1.253064	−0.327090		−2.496208	1.289908	−0.250231	
	1.494823	2.683168	−0.291886		1.504418	2.681068	−0.293122		1.491973	2.666244	−0.270841	
	−0.107696	2.861984	−0.160439		−0.122914	2.819589	−0.133380		−0.107910	2.842784	−0.163174	
	−1.702192	2.619500	−0.286790		−1.701230	2.628644	−0.331926		−1.751653	2.640386	−0.254937	
13	−0.070977	0.060071	−0.106027	0.7596	−0.040725	0.042369	−0.106103	0.0	0.008139	0.025827	−0.244109	0.0
	1.642714	0.104586	−0.113159		1.666290	0.080420	−0.112473		1.561473	0.041935	0.222637	
	0.624701	1.724877	−0.116636		0.615828	1.749102	−0.115824		0.799828	1.592341	−0.051693	
	−0.956861	1.453156	−0.109114		−0.943949	1.454777	−0.108918		−0.816566	1.574932	−0.049870	
	−1.720297	0.137203	−0.100598		−1.715307	0.125166	−0.100446		−1.544179	0.008732	0.225970	
	−1.170328	−1.370622	−0.095241		−1.196439	−1.375017	−0.095915		−0.783211	−1.541100	−0.053277	
	0.739141	−1.450091	−0.102616		0.772480	−1.458740	−0.102623		0.833204	−1.523735	−0.054888	
	2.447427	−2.293801	−0.105676		2.404986	−2.293308	−0.104935		−2.437206	1.376093	−0.046176	
	3.222073	−0.958059	−0.113774		3.201453	−0.921576	−0.113831		2.424304	1.428163	−0.051545	
	2.196099	1.714717	−0.120581		2.202047	1.736096	−0.121738		2.453880	−1.324831	−0.054316	

	−0.382659	−2.730342	−0.092628		−0.398200	−2.745875	−0.092840	−2.407691	−1.376860	−0.049236
	3.243771	0.600412	−0.120123		3.258668	0.622980	−0.120781	−3.167683	−0.008512	0.079678
	1.105039	−3.085837	−0.096897		1.092710	−3.110122	−0.096641	3.184600	0.059548	0.072816
13*	−0.021155	−0.395748	−0.086616	0.7631	–	–	–	–	–	–
	2.160032	−0.083440	−0.091845		–	–	–	–	–	–
	0.794264	1.173661	−0.113431		–	–	–	–	–	–
	−0.901752	1.133977	−0.110613		–	–	–	–	–	–
	−2.186719	−0.190549	−0.085558		–	–	–	–	–	–
	−1.405651	−1.529881	−0.068528		–	–	–	–	–	–
	1.439485	−1.453046	−0.072512		–	–	–	–	–	–
	2.419752	1.481260	−0.115627		–	–	–	–	–	–
	−2.538473	1.358398	−0.109316		–	–	–	–	–	–
	1.493396	2.691797	−0.136223		–	–	–	–	–	–
	−0.093111	2.786330	−0.138998		–	–	–	–	–	–
	−1.676631	2.613676	−0.132465		–	–	–	–	–	–
	0.031014	−2.077526	−0.062278		–	–	–	–	–	–
13**	0.008638	0.025391	0.240509	0.7610	–	–	–	–	–	–
	1.588487	0.042191	0.334870		–	–	–	–	–	–
	0.804803	1.620738	0.085255		–	–	–	–	–	–
	−0.822078	1.604679	0.085754		–	–	–	–	–	–
	−1.571002	0.008210	0.338067		–	–	–	–	–	–
	−0.787822	−1.570248	0.082657		–	–	–	–	–	–
	0.838773	−1.553317	0.081262		–	–	–	–	–	–
	−2.383679	1.386949	−0.193350		–	–	–	–	–	–
	2.370297	1.437869	−0.198903		–	–	–	–	–	–
	2.399851	−1.335173	−0.201534		–	–	–	–	–	–
	−2.354092	−1.386328	−0.196233		–	–	–	–	–	–
	−3.118994	−0.007841	−0.252789		–	–	–	–	–	–
	3.135709	0.059412	−0.259574		–	–	–	–	–	–

S2. THE CBS EXTRAPOLATION SCHEMES

We use the Gaussian program[1] to carry out the HF calculations with subsequent extrapolation to the CBS limit. To do this, we employed a hierarchically designed correlated basis set, aug-cc-pVXZ, where X is a cardinal number, the highest angular momentum included in the basis set. For the HF/CBS energy extrapolation we use five schemes[3] which will denoted as CBS$_n$ where $n = 1, 2, ..., 5$. The first one, CBS$_1$, is an exponential scheme[4],

$$Y(X) = Y_{CBS} + A \exp(-BX) \tag{S1}$$

where Y_{CBS} is the energy in the CBS limit, $Y(X)$ the energy with a given basis set. Y_{CBS}, A and B are fitting parameters. The second one, CBS$_2$, is a power extrapolation scheme[5]

$$Y(X) = Y_{CBS} + AX^{-B} \tag{S2}$$

the third one, CBS$_3$, is a mixed exponential scheme[5]

$$Y(X) = Y_{CBS} + A \exp(-(X-1)) + B \exp(-(X-1)^2), \tag{S3}$$

the fourth one[6, 7], CBS$_4$, is given by

$$Y(X) = Y_{CBS} + \frac{A}{(X+1/2)^B}, \tag{S4}$$

the last one[6, 7] CBS$_5$, is

$$Y(X) = Y_{CBS} + \frac{A}{(X+1/2)^4} + \frac{B}{(X+1/2)^6}. \tag{S5}$$

The CBS extrapolations of the HF energies of ${B_n}^Q$ (for $Q = -1, 0, 1$ and $n \leq 13$) clusters according to the above schemes Eqs. (S1)-(S5) are shown in Table S2. It can be seen that the five adopted extrapolation schemes work well for clusters with up to five atoms, whereas, for larger clusters, we found good fitting results with the schemes CBS_3 and CBS_5.

TABLE S2: The HF energies of the B_n^Q (for $Q = -1, 0, 1$ and $n \leq 13$) clusters at different basis set calculated using Gaussian program[1] and the CBS extrapolation of the HF energies using the methods denoted as CBS_n where $n = 1, 2, ..., 5$.

Cluster size, n	Basis set	B_n	B_n^+	B_n^-
1				
	aug-cc-pVDZ	−24.53057377	−24.23501373	−24.51954239
	aug-cc-pVTZ	−24.53217153	−24.23681573	−24.52094707
	aug-cc-pVQZ	−24.53298389	−24.23747329	−24.52178338
	aug-cc-pV5Z	−24.53313019	−24.23754633	−24.52194427
	CBS_1	−24.5334	−24.2377	−24.5223
	CBS_2	−24.5339	−24.2379	−24.5230
	CBS_3	−24.5333	−24.2377	−24.5222
	CBS_4	−24.5337	−24.2378	−24.5228
	CBS_5	−24.5334	−24.2378	−24.5223
2	aug-cc-pVDZ	−49.08766994	−48.76340558	−49.16993215
	aug-cc-pVTZ	−49.09264235	−48.76844821	−49.17480280
	aug-cc-pVQZ	−49.09457495	−48.77032570	−49.17678100
	aug-cc-pV5Z	−49.09488696	−48.77062018	−49.17712554
	CBS_1	−49.0953	−48.7710	−49.1775
	CBS_2	−49.0960	−48.7716	−49.1784
	CBS_3	−49.0954	−48.7712	−49.1776
	CBS_4	−49.0959	−48.7715	−49.1782
	CBS_5	−49.0956	−48.7713	−49.1778
2∗	aug-cc-pVDZ	−49.03890972	−	−
	aug-cc-pVTZ	−49.04375611	−	−
	aug-cc-pVQZ	−49.04566991	−	−
	aug-cc-pV5Z	−49.04597036	−	−
	CBS_1	−49.0464	−	−
	CBS_2	−49.0471	−	−
	CBS_3	−49.0465	−	−
	CBS_4	−49.0469	−	−
	CBS_5	−49.0466	−	−
3	aug-cc-pVDZ	−73.77983557	−73.43296012	−73.82014472
	aug-cc-pVTZ	−73.79555343	−73.44556281	−73.83438643
	aug-cc-pVQZ	−73.79968694	−73.44932157	−73.83821354
	aug-cc-pV5Z	−73.80033485	−73.44992715	−73.83882411
	CBS_1	−73.8008	−73.4504	−73.8392
	CBS_2	−73.8018	−73.4515	−73.8402
	CBS_3	−73.8013	−73.4508	−73.8397
	CBS_4	−73.8016	−73.4512	−73.8400
	CBS_5	−73.8015	−73.4511	−73.8400
4	aug-cc-pVDZ	−98.43989048	−98.14816045	−98.52748143
	aug-cc-pVTZ	−98.45924494	−98.16649325	−98.54674035
	aug-cc-pVQZ	−98.46423315	−98.17157859	−98.55169773
	aug-cc-pV5Z	−98.46513747	−98.17249174	−98.55261104
	CBS_1	−98.4656	−98.1731	−98.5531
	CBS_2	−98.4668	−98.1758	−98.5543
	CBS_3	−98.4663	−98.1752	−98.5537
	CBS_4	−98.4666	−98.1749	−98.5541
	CBS_5	−98.4666	−98.1734	−98.5540
5	aug-cc-pVDZ	−123.15227140	−122.83571838	−123.15377873

	aug-cc-pVTZ	−123.17436796	−122.85739648	−123.17493761
	aug-cc-pVQZ	−123.18027427	−122.86318736	−123.18066563
	aug-cc-pV5Z	−123.18138860	−122.86429776	−123.18174708
	CBS_3	−123.1827	−122.8656	−123.1830
	CBS_5	−123.1831	−122.8660	−123.1834
6	aug-cc-pVDZ	−147.76319869	−147.48717237	−147.87803539
	aug-cc-pVTZ	−147.79017225	−147.51313297	−147.90445261
	aug-cc-pVQZ	−147.79737620	−147.52031461	−147.91137507
	aug-cc-pV5Z	−147.79878584	−147.52169885	−147.91271401
	CBS_3	−147.8004	−147.5233	−147.9143
	CBS_5	−147.8009	−147.5239	−147.9147
6∗	aug-cc-pVDZ	−147.80143161	–	−147.83667918
	aug-cc-pVTZ	−147.82888500	–	−147.86437640
	aug-cc-pVQZ	−147.83589621	–	−147.87142761
	aug-cc-pV5Z	−147.83723797	–	−147.87275897
	CBS_3	−147.8388	–	−147.8743
	CBS_5	−147.8392	–	−147.8748
7	aug-cc-pVDZ	−172.48112730	−172.22154661	−172.53475769
	aug-cc-pVTZ	−172.51303088	−172.25186286	−172.56792644
	aug-cc-pVQZ	−172.52131038	−172.26004120	−172.57633832
	aug-cc-pV5Z	−172.52291920	−172.26163308	−172.57795736
	CBS_3	−172.5248	−172.2635	−172.5798
	CBS_5	−172.5253	−172.2641	−172.5804
7∗	aug-cc-pVDZ	–	–	−172.51550737
	aug-cc-pVTZ	–	–	−172.54777036
	aug-cc-pVQZ	–	–	−172.55603704
	aug-cc-pV5Z	–	–	−172.55764341
	CBS_3	–	–	−172.5595
	CBS_5	–	–	−172.5600
8	aug-cc-pVDZ	−197.19110703	−196.91019526	−197.24912507
	aug-cc-pVTZ	−197.22774609	−196.94485270	−197.28661156
	aug-cc-pVQZ	−197.23697413	−196.95394358	−197.29590363
	CBS_3	−197.2419	−196.9589	−197.3009
	CBS_5	−197.2426	−196.9596	−197.3016
9	aug-cc-pVDZ	−221.82186050	−221.54740028	−221.89635257
	aug-cc-pVTZ	−221.86192843	−221.58643569	−221.93880291
	aug-cc-pVQZ	−221.87225965	−221.59680346	−221.94914155
	CBS_3	−221.8779	−221.6025	−221.9547
	CBS_5	−221.8787	−221.6033	−221.9554
10	aug-cc-pVDZ	−246.50683338	−246.22722364	−246.58056522
	aug-cc-pVTZ	−246.55325972	−246.27350908	−246.62857419
	aug-cc-pVQZ	−246.56483211	−246.28505647	−246.64023476
	CBS_3	−246.5710	−246.2913	−246.6465
	CBS_5	−246.5719	−246.2921	−246.6473
11	aug-cc-pVDZ	−271.18462827	−270.92479966	−271.27608286
	aug-cc-pVTZ	−271.23631534	−270.97407869	−271.32684132
	aug-cc-pVQZ	−271.24888667	−270.98648913	−271.33932128
	CBS_3	−271.2556	−270.9932	−271.3460
	CBS_5	−271.2565	−270.9941	−271.3469
12	aug-cc-pVDZ	−295.87496079	−295.58802694	−295.91991489
	aug-cc-pVTZ	−295.93099327	−295.64367079	−295.97647807
	aug-cc-pVQZ	−295.9448853	−295.65762905	−295.990396
	CBS_3	−295.9523	−295.6651	−295.9978
	CBS_5	−295.9534	−295.6662	−295.9989

13	aug-cc-pVDZ	−320.53345755	−320.30108995	−320.59841749
	aug-cc-pVTZ	−320.59407279	−320.35980147	−320.65943769
	aug-cc-pVQZ	−320.60881158	−320.37440282	−320.67434864
	CBS_3	−320.6167	−320.3822	−320.6823
	CBS_5	−320.6177	−320.3833	−320.6834
13∗	aug-cc-pVDZ	−320.53144825	–	–
	aug-cc-pVTZ	−320.59199321	–	–
	aug-cc-pVQZ	−320.60674255	–	–
	CBS_3	−320.6146	–	–
	CBS_5	−320.6157	–	–
13 ∗ ∗	aug-cc-pVDZ	−320.50633686	–	–
	aug-cc-pVTZ	−320.56605607	–	–
	aug-cc-pVQZ	−320.5809227	–	–
	CBS_3	−320.5889	–	–
	CBS_5	−320.5900	–	–

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