

Supplementary Material

Assessing the applicability of the geometric counterpoise correction in B2PLYP/double- ζ calculations for thermochemistry, kinetics, and noncovalent interactions

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SI.1 BSSE in double-hybrid DFT and (SCS-)MP2 calculations of the S66x8 benchmark set

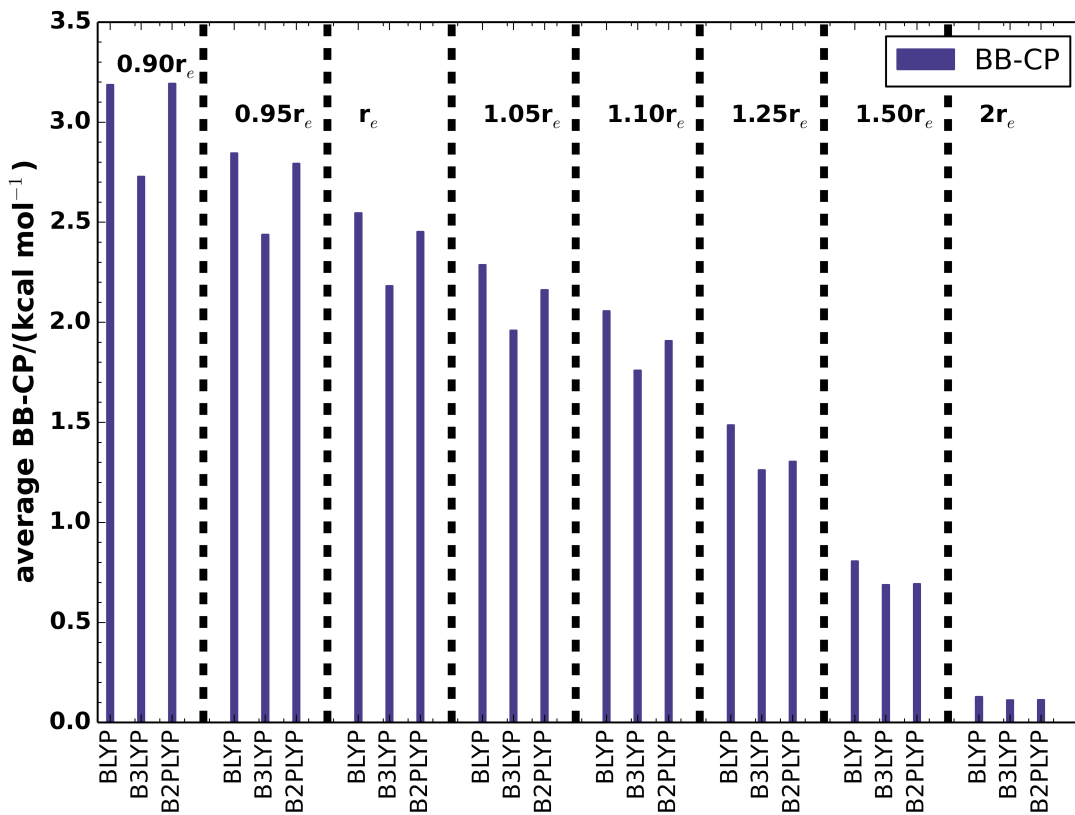


Figure S1: Average BB-CP corrections for different intermolecular distances in the S66x8 benchmark set. The def2-SVP basis set was used for all calculations.

Table S1: BB-CP corrections (kcal mol⁻¹) for different systems in the S66x8 benchmark set. The def2-SVP basis set was used for all calculations. Each dimer is assigned the same number as in the original set. The value after each dot represents 100 times pre-factor for r_e .

	BLYP	B3LYP	B2PLYP	PBE0-DH	PBE0-2	MP2	SCS-MP2
S66x8.01.100	3.537924240	2.965712396	2.869077053	2.269568159	2.411654068	2.872156508	2.809414561
S66x8.01.105	3.252175501	2.700331559	2.567128113	2.018220634	2.107953656	2.489367093	2.443244430
S66x8.01.110	3.000986284	2.464551085	2.295061534	1.794351782	1.834115030	2.171266985	2.111503975
S66x8.01.125	2.372989240	1.929649669	1.750888670	1.376570113	1.361410416	1.590650368	1.531867268
S66x8.01.150	1.384747677	1.167727436	1.110337125	0.912422110	0.935607608	1.089943382	1.044549374
S66x8.01.200	0.137124958	0.119678802	0.115659378	0.100533651	0.102878527	0.135848468	0.110204657
S66x8.01.90	4.206413951	3.554513296	3.511977941	2.798188692	3.039622101	3.660188215	3.576902535
S66x8.01.95	3.856848677	3.252294492	3.185843344	2.532422407	2.724616506	3.263677791	3.184185144
S66x8.02.100	3.380229583	2.910415398	3.000270148	2.418210691	2.714002667	3.303748791	3.201476403
S66x8.02.105	3.078217720	2.639478539	2.698889132	2.166258757	2.413135463	2.932431913	2.842604092
S66x8.02.110	2.814212546	2.399659491	2.429620190	1.942234141	2.145568965	2.601032908	2.512139445
S66x8.02.125	2.192863789	1.849419008	1.826435482	1.458798725	1.569552400	1.884304717	1.819875559
S66x8.02.150	1.334267298	1.147464938	1.150698196	0.941961191	1.017233023	1.209915964	1.167630025
S66x8.02.200	0.168065079	0.147874252	0.148374786	0.126833234	0.134843836	0.168781233	0.141674632
S66x8.02.90	4.090347353	3.529641791	3.689262433	2.983773749	3.399689366	4.171355249	4.024551420
S66x8.02.95	3.717848759	3.207914683	3.330654291	2.692271494	3.043455858	3.715973732	3.593400798
S66x8.03.100	3.244283560	2.755954264	2.814161344	2.189542215	2.485220069	3.105877074	3.018168836
S66x8.03.105	2.994644407	2.547770926	2.597272918	2.014804303	2.280381965	2.845393735	2.768459548
S66x8.03.110	2.777894349	2.360152581	2.394584503	1.849911454	2.083301290	2.597675464	2.526561460
S66x8.03.125	2.275941237	1.907571052	1.876384347	1.439092569	1.568766378	1.942019467	1.882127444
S66x8.03.150	1.561760692	1.325042848	1.296613783	1.029345110	1.097791806	1.323506741	1.276302215
S66x8.03.200	0.256790096	0.227005263	0.226374772	0.193235804	0.204328532	0.247658233	0.226550036
S66x8.03.90	3.866952286	3.258733250	3.329621316	2.593404912	2.960489585	3.727587338	3.586527614
S66x8.03.95	3.531429897	2.989024897	3.052909004	2.378307714	2.706107206	3.392351633	3.291884873
S66x8.04.100	4.024609746	3.467674748	3.599461645	2.866689681	3.253747401	3.994354638	3.866482463
S66x8.04.105	3.738408793	3.214246994	3.309378459	2.632463597	2.960585470	3.619571320	3.491410128
S66x8.04.110	3.464543340	2.967090197	3.026301197	2.402312848	2.675266003	3.260428438	3.139717963
S66x8.04.125	2.735992969	2.315496242	2.295284024	1.821467781	1.965593149	2.368524494	2.271987704
S66x8.04.150	1.689193783	1.444203214	1.432712541	1.163903087	1.243583269	1.477509844	1.412193730
S66x8.04.200	0.180051149	0.153067741	0.148652988	0.125646658	0.129102240	0.157691029	0.133874579
S66x8.04.90	4.635618435	3.984582095	4.187457884	3.323631118	3.841899499	4.777555991	4.624222766
S66x8.04.95	4.321320510	3.722969830	3.891063797	3.097167456	3.547541436	4.379881592	4.230068601
S66x8.05.100	3.641971968	3.152123273	3.276697490	2.642773219	2.991233991	3.641527647	3.525997461
S66x8.05.105	3.309016948	2.852289668	2.938266978	2.61831568	2.651523836	3.219539259	3.115544386
S66x8.05.110	3.013130150	2.581537685	2.630302733	2.105966473	2.341656965	2.836907427	2.742451221
S66x8.05.125	2.321013917	1.957818489	1.931804869	1.540917881	1.660130233	1.989821079	1.930084832
S66x8.05.150	1.430569985	1.229246876	1.226192633	1.003131720	1.082354625	1.280793666	1.245600462
S66x8.05.200	0.202057560	0.177977448	0.177602655	0.152414976	0.161378888	0.191804332	0.187185018
S66x8.05.90	4.401878813	3.814372345	4.024975383	3.248781489	3.736614432	4.596736222	4.457117790
S66x8.05.95	4.006989449	3.474005104	3.639654129	2.940362272	3.354611954	4.100661672	3.981398522
S66x8.06.100	3.479565781	2.966178791	3.092648092	2.418332957	2.804160235	3.529715506	3.446398340
S66x8.06.105	3.203276473	2.733048218	2.833537871	2.213202933	2.547268583	3.192474138	3.121185188
S66x8.06.110	2.960871892	2.521013479	2.591434019	2.018225273	2.302684580	2.877128225	2.814564070
S66x8.06.125	2.392168261	2.008268519	1.994941102	1.539782051	1.697002655	2.101050232	2.053229864
S66x8.06.150	1.661146386	1.399119237	1.361201188	1.076403583	1.146022926	1.380107395	1.347346818
S66x8.06.200	0.330110750	0.288070286	0.282749985	0.239902355	0.251000975	0.294474496	0.287976578
S66x8.06.90	4.135572501	3.498715248	3.679060345	2.863915102	3.373680827	4.304288845	4.189167043
S66x8.06.95	3.788185469	3.218601939	3.369957604	2.631797303	3.074292234	3.893147537	3.794693434
S66x8.07.100	5.103582777	4.385593980	4.566846622	3.645756057	4.134694649	5.067045795	4.881185442
S66x8.07.105	4.754893947	4.079284838	4.219411397	3.370166886	3.790304334	4.619455185	4.447855263
S66x8.07.110	4.420860683	3.789372098	3.900956361	3.118375552	3.488422391	4.234709479	4.075425688
S66x8.07.125	3.514761604	3.024524565	3.109268807	2.501074740	2.779608388	3.346728120	3.219218257
S66x8.07.150	1.981514456	1.722122085	1.761939736	1.446846354	1.581621309	1.873490604	1.802513353
S66x8.07.200	0.093711852	0.084196851	0.091519541	0.079338971	0.089945066	0.110191749	0.106689819
S66x8.07.90	5.835761806	5.027411895	5.336456351	4.236947608	4.916891697	6.128621872	5.907545119
S66x8.07.95	5.463186725	4.702184720	4.941328231	3.937320888	4.512086889	5.573105318	5.370635311
S66x8.08.100	3.690668825	3.113450569	3.041897500	2.412614410	2.587909771	3.084404347	3.026389545
S66x8.08.105	3.373862683	2.821225556	2.710691479	2.138256335	2.256785233	2.667916309	2.617385368

Table S1: BB-CP corrections (kcal mol⁻¹) for different systems in the S66x8 benchmark set. The def2-SVP basis set was used for all calculations. Each dimer is assigned the same number as in the original set. The value after each dot represents 100 times pre-factor for r_e .

	BLYP	B3LYP	B2PLYP	PBE0-DH	PBE0-2	MP2	SCS-MP2
S66x8.08.110	3.093568871	2.557679595	2.406153331	1.886945883	1.949677732	2.302491824	2.256884082
S66x8.08.125	2.415709129	1.964206644	1.779079527	1.395004094	1.378684302	1.603933854	1.567114750
S66x8.08.150	1.437775702	1.210192707	1.144914365	0.935902405	0.956256768	1.106473773	1.082198724
S66x8.08.200	0.161742128	0.140825471	0.134924843	0.116498048	0.118614722	0.145708410	0.142617943
S66x8.08.90	4.415524691	3.746739760	3.734655556	2.974244323	3.259955255	3.933363104	3.850135649
S66x8.08.95	4.039290935	3.424057210	3.385073574	2.694126300	2.924520378	3.506056927	3.437145849
S66x8.09.100	2.744150104	2.299485438	2.305375705	1.808240952	2.002566746	2.460812659	2.389151243
S66x8.09.105	2.556019613	2.136041990	2.118362454	1.665697976	1.819401016	2.218023168	2.151030265
S66x8.09.110	2.374680293	1.988225652	1.965048648	1.553957284	1.685206411	2.039881624	1.977562125
S66x8.09.125	1.814123186	1.548022095	1.550608904	1.253795104	1.362036389	1.625431974	1.578084115
S66x8.09.150	0.830293912	0.727482402	0.738321134	0.617593678	0.668911606	0.784773865	0.763423430
S66x8.09.200	0.028196444	0.027873068	0.033126635	0.029135815	0.035814265	0.050437788	0.049685788
S66x8.09.90	3.192095871	2.714699711	2.816023095	2.218995563	2.543617194	3.169358042	3.086032779
S66x8.09.95	2.951484912	2.489945187	2.537695457	1.992823196	2.246334691	2.780628258	2.703890144
S66x8.10.100	3.011163789	2.557485498	2.641382595	2.052644264	2.356755782	2.959124339	2.879135663
S66x8.10.105	2.764906760	2.346585124	2.403293855	1.872255808	2.126099808	2.653553480	2.582633555
S66x8.10.110	2.535249553	2.149827461	2.183372501	1.706811907	1.916267422	2.376365664	2.313077073
S66x8.10.125	1.907513638	1.622035709	1.618122278	1.289259860	1.405510202	1.704659130	1.660031567
S66x8.10.150	0.729994332	0.635909766	0.633721354	0.530596385	0.565494575	0.664331458	0.649515112
S66x8.10.200	0.014434859	0.010999519	0.008791770	0.007038465	0.006408300	0.014599367	0.014875301
S66x8.10.90	3.586009728	3.041583073	3.188678408	2.466296227	2.891472163	3.678070567	3.572342726
S66x8.10.95	3.281364068	2.786574265	2.900157206	2.248800667	2.608877626	3.295685434	3.204407778
S66x8.11.100	3.963835262	3.396074829	3.523260774	2.736324510	3.141801788	3.946531389	3.792733426
S66x8.11.105	3.675197902	3.144102255	3.228798016	2.519360871	2.854764080	3.557667213	3.418068030
S66x8.11.110	3.397240506	2.905499661	2.960644408	2.323787106	2.604416551	3.220693024	3.092997168
S66x8.11.125	2.086949841	1.799501147	1.814005205	1.462972689	1.599454929	1.930447411	1.852785823
S66x8.11.150	0.474256762	0.407216932	0.394199951	0.332339470	0.343533630	0.368574457	0.383262339
S66x8.11.200	0.007562554	0.003109892	-0.001232505	-0.002042697	-0.005095320	-0.033669776	-0.017020675
S66x8.11.90	4.611856787	3.966080030	4.207372517	3.250859364	3.836787298	4.893187062	4.710525427
S66x8.11.95	4.275641431	3.671178703	3.851385120	2.982806530	3.471915987	4.393804742	4.229072493
S66x8.12.100	3.174163616	2.712223998	2.812598037	2.222566859	2.547948737	3.188538984	3.091576989
S66x8.12.105	2.873270164	2.452001451	2.526327328	1.992920668	2.269697673	2.830467854	2.745255870
S66x8.12.110	2.613471489	2.228398240	2.286459554	1.799646559	2.040728924	2.539706379	2.477200237
S66x8.12.125	2.036826857	1.741186358	1.781218412	1.401325082	1.577152770	1.952689577	1.897935284
S66x8.12.150	1.383315281	1.187826642	1.192567265	0.955898566	1.041505165	1.262026077	1.224516987
S66x8.12.200	0.264062537	0.229343020	0.224353516	0.190234459	0.197845068	0.239868462	0.220767833
S66x8.12.90	3.917363556	3.360405456	3.553639635	2.809673950	3.286302346	4.156974954	4.028313816
S66x8.12.95	3.519531478	3.012438596	3.151820220	2.492418622	2.883431290	3.626366865	3.511703486
S66x8.13.100	3.979965206	3.432258563	3.555417513	2.817139845	3.205896160	3.951999316	3.821694948
S66x8.13.105	3.695554868	3.170136117	3.243106822	2.566365454	2.885283575	3.539500375	3.427486637
S66x8.13.110	3.431001781	2.926886196	2.955323947	2.337248111	2.593466682	3.163736375	3.061260189
S66x8.13.125	2.710531576	2.301263907	2.269522866	1.811402429	1.952847621	2.337635847	2.260927603
S66x8.13.150	1.570255361	1.368252975	1.368252564	1.127437879	1.213698444	1.424022075	1.383280831
S66x8.13.200	0.164283008	0.145038839	0.141477443	0.123140332	0.127172341	0.146097472	0.142141049
S66x8.13.90	4.612951984	3.999548456	4.230190785	3.351620480	3.895422714	4.855513702	4.706444234
S66x8.13.95	4.285893907	3.709541974	3.884012278	3.079891639	3.543288249	4.389245608	4.254687085
S66x8.14.100	3.257204451	2.816632657	3.047824474	2.383402684	2.850700423	3.649653029	3.538913257
S66x8.14.105	3.018133244	2.605799909	2.797216207	2.186044090	2.591829987	3.304336015	3.208032001
S66x8.14.110	2.813630819	2.417651798	2.562823965	2.000108408	2.343522809	2.975447772	2.890594135
S66x8.14.125	2.335067749	1.964936542	1.977680720	1.540226392	1.714764164	2.135189598	2.074722951
S66x8.14.150	1.606285469	1.361100288	1.337542309	1.072007384	1.147434983	1.376241216	1.342172896
S66x8.14.200	0.247642517	0.203792822	0.179833365	0.151920507	0.142414912	0.160101382	0.155226574
S66x8.14.90	3.842033804	3.308771853	3.618757852	2.818089881	3.426254835	4.440341818	4.290890867
S66x8.14.95	3.530716948	3.049563467	3.318473944	2.591819246	3.124914304	4.022301593	3.893853177
S66x8.15.100	4.055812890	3.549481145	3.868698350	3.019113235	3.616904554	4.620937275	4.444116179
S66x8.15.105	3.813250693	3.318792470	3.571331888	2.783236683	3.298457339	4.191551373	4.026384447
S66x8.15.110	3.589779985	3.105440279	3.296100886	2.567266282	3.002288776	3.795719018	3.641830735
S66x8.15.125	2.970556723	2.548087333	2.623897389	2.061338689	2.325351897	2.877884484	2.757455621

Table S1: BB-CP corrections (kcal mol⁻¹) for different systems in the S66x8 benchmark set. The def2-SVP basis set was used for all calculations. Each dimer is assigned the same number as in the original set. The value after each dot represents 100 times pre-factor for r_e .

	BLYP	B3LYP	B2PLYP	PBE0-DH	PBE0-2	MP2	SCS-MP2
S66x8_15.150	1.895118434	1.658659129	1.715984852	1.392971447	1.548677815	1.865210292	1.794545604
S66x8_15.200	0.173796735	0.154408259	0.160017606	0.137401990	0.149575742	0.172943735	0.166643053
S66x8_15.90	4.595134546	4.042855128	4.500633178	3.513459531	4.300300609	5.545827659	5.342350081
S66x8_15.95	4.317378898	3.792705840	4.180273141	3.266153734	3.954591798	5.073766177	4.884304590
S66x8_16.100	3.824773292	3.209070468	3.099283719	2.434985038	2.592226707	3.082836077	3.021978041
S66x8_16.105	3.523664246	2.927796730	2.771288831	2.167979289	2.260174330	2.657288139	2.601694360
S66x8_16.110	3.251270715	2.679203284	2.488456539	1.942964915	1.982887587	2.336498662	2.285088898
S66x8_16.125	2.520834760	2.081973986	1.911323842	1.515559363	1.515678544	1.756742279	1.716322062
S66x8_16.150	1.364241760	1.171819891	1.120542790	0.928107377	0.952545042	1.092714497	1.069803197
S66x8_16.200	0.103095897	0.091914833	0.089207704	0.078725850	0.079915823	0.099447348	0.097509784
S66x8_16.90	4.519321782	3.835331244	3.806436692	3.010162062	3.295289868	3.980245178	3.902288712
S66x8_16.95	4.157051384	3.514404537	3.449218347	2.721251941	2.944117642	3.532673171	3.464654994
S66x8_17.100	4.867031082	4.208847063	4.733414092	3.642414859	4.509547696	5.818539988	5.626951194
S66x8_17.105	4.640969950	4.001921556	4.443983562	3.409384984	4.171799519	5.356216771	5.173359735
S66x8_17.110	4.438327377	3.799595530	4.147774582	3.166065494	3.817015696	4.879822186	4.704789444
S66x8_17.125	3.918296859	3.243594901	3.312443476	2.485856978	2.821704343	3.549768138	3.397115059
S66x8_17.150	3.050783916	2.535267460	2.536757749	1.951800892	2.138176700	2.598497719	2.485914285
S66x8_17.200	0.925052142	0.800918371	0.822467385	0.674736086	0.731814896	0.840268058	0.803214339
S66x8_17.90	5.412028591	4.657053662	5.321895568	4.079902997	5.161010609	6.750276104	6.540881385
S66x8_17.95	5.122614102	4.424829290	5.021257585	3.862088160	4.833104580	6.273489168	6.072635410
S66x8_18.100	2.834408875	2.375475436	2.475860893	1.892822014	2.215794618	2.814366527	2.725337279
S66x8_18.105	2.597850169	2.179637243	2.267395549	1.723258659	2.013400017	2.557053827	2.476579051
S66x8_18.110	2.389305999	2.001237396	2.071772307	1.562538111	1.818806045	2.312046930	2.238245137
S66x8_18.125	1.887914088	1.556804153	1.563390027	1.154193100	1.306503321	1.660571611	1.602133642
S66x8_18.150	1.236279142	1.028845783	1.023734026	0.775062938	0.852148879	1.061975431	1.024403927
S66x8_18.200	0.211389645	0.185529845	0.189406939	0.156454839	0.169746218	0.204420209	0.197575948
S66x8_18.90	3.422740374	2.847395190	2.965563655	2.280421927	2.676173914	3.412108233	3.300017342
S66x8_18.95	3.105584967	2.594284240	2.704020404	2.075030194	2.432181497	3.093393870	2.993651376
S66x8_19.100	3.178245137	2.700563653	2.869716792	2.214589972	2.620864416	3.319790725	3.207295164
S66x8_19.105	2.918722536	2.482206013	2.626240453	2.020924662	2.380139985	3.005821204	2.905284496
S66x8_19.110	2.698106324	2.291856886	2.411105892	1.847065764	2.164456055	2.729814697	2.638213566
S66x8_19.125	2.091711196	1.746404007	1.779555930	1.336291199	1.524535927	1.916218271	1.847452543
S66x8_19.150	1.363439777	1.133178046	1.127637728	0.853588050	0.939468121	1.163245923	1.121044438
S66x8_19.200	0.272741414	0.238868999	0.244656018	0.200780655	0.219506655	0.257466390	0.248940866
S66x8_19.90	3.799239021	3.211681035	3.438209780	2.654238831	3.176584219	4.062815196	3.921002844
S66x8_19.95	3.468148924	2.940009715	3.135798046	2.422056684	2.881474986	3.665688102	3.539179225
S66x8_20.100	6.091602793	5.284584843	5.796452626	4.555850508	5.485117146	6.953113246	6.762647531
S66x8_20.105	5.785339960	5.030077982	5.475636783	4.314227212	5.139059842	6.468225732	6.288277451
S66x8_20.110	5.501831511	4.779486528	5.145982151	4.058049426	4.779150752	5.979385801	5.809561592
S66x8_20.125	4.730629838	4.009311499	4.108450945	3.194259974	3.596255993	4.445567229	4.299162545
S66x8_20.150	3.564848379	2.959103214	2.881967427	2.245456478	2.392358171	2.886127026	2.778070288
S66x8_20.200	1.275420988	1.103741935	1.118130030	0.921332993	0.993841937	1.157490290	1.129563390
S66x8_20.90	6.801616843	5.837937421	6.469577008	5.025493874	6.184030913	7.979454732	7.782776678
S66x8_20.95	6.428363175	5.551825464	6.124976393	4.791123326	5.830019805	7.443521760	7.253683742
S66x8_21.100	5.405323458	4.719187843	5.152518173	4.028437651	4.816198590	6.085996687	5.927004590
S66x8_21.105	5.154761825	4.475490991	4.815094882	3.753457181	4.425197258	5.563669961	5.406590719
S66x8_21.110	4.917115390	4.232144008	4.475739042	3.471967637	4.030985545	5.047443637	4.898673227
S66x8_21.125	4.290089104	3.600933926	3.620578246	2.786212752	3.075049945	3.786446533	3.652953108
S66x8_21.150	3.233620668	2.750148697	2.764504743	2.196933573	2.386383150	2.859236674	2.763628584
S66x8_21.200	0.551710502	0.474329939	0.478910550	0.401587222	0.427555641	0.492546129	0.471658311
S66x8_21.90	5.968460771	5.210300657	5.812969160	4.533058772	5.560841432	7.129752754	6.946498726
S66x8_21.95	5.672176351	4.960450490	5.481150525	4.286286991	5.191208629	6.602633215	6.429802806
S66x8_22.100	5.381162997	4.652222173	5.149156589	4.000272491	4.880988828	6.250662214	6.090155748
S66x8_22.105	5.136467049	4.440461152	4.862306436	3.780197252	4.556032536	5.794790005	5.630897018
S66x8_22.110	4.906377294	4.226526689	4.567120096	3.543119085	4.214631646	5.331230565	5.177634517
S66x8_22.125	4.256764412	3.568418931	3.652368054	2.788668058	3.157705672	3.944752625	3.801420345
S66x8_22.150	3.299894428	2.733538953	2.685439838	2.073952852	2.233234530	2.710135476	2.602819593
S66x8_22.200	1.172757811	1.014879983	1.029972227	0.848794417	0.914216483	1.073865045	1.035519469

Table S1: BB-CP corrections (kcal mol⁻¹) for different systems in the S66x8 benchmark set. The def2-SVP basis set was used for all calculations. Each dimer is assigned the same number as in the original set. The value after each dot represents 100 times pre-factor for r_e .

	BLYP	B3LYP	B2PLYP	PBE0-DH	PBE0-2	MP2	SCS-MP2
S66x8_22.90	5.958598680	5.110782775	5.744455785	4.420352949	5.526430852	7.207341858	7.010205045
S66x8_22.95	5.651092964	4.871547342	5.438275586	4.209369745	5.199024609	6.713064556	6.523495321
S66x8_23.100	5.035844314	4.369362454	4.858917991	3.758408028	4.601398349	5.905282598	5.729608964
S66x8_23.105	4.822074588	4.172737193	4.580602150	3.538251515	4.275472011	5.455485982	5.287552273
S66x8_23.110	4.628139471	3.979486074	4.298461964	3.307947309	3.937742341	4.999245302	4.838282278
S66x8_23.125	4.099748189	3.426533257	3.495527018	2.654663551	2.994296159	3.742442734	3.600774513
S66x8_23.150	3.228397087	2.701529860	2.695325348	2.093323458	2.276590903	2.758829063	2.651599376
S66x8_23.200	1.077800433	0.931925877	0.944752308	0.782616557	0.840638523	0.971871678	0.934131173
S66x8_23.90	5.561691572	4.801367094	5.426654994	4.177885462	5.233979346	6.818493211	6.626854809
S66x8_23.95	5.279039415	4.575851969	5.136675919	3.969488360	4.917465607	6.353861693	6.169953414
S66x8_24.100	1.702257410	1.495343712	1.932855673	1.408349736	2.084198827	3.055072036	2.940455383
S66x8_24.105	1.459598602	1.289855780	1.573956772	1.157985015	1.619657133	2.323032657	2.248217131
S66x8_24.110	1.203025498	1.067211567	1.251517015	0.928587010	1.246542789	1.764617341	1.716002979
S66x8_24.125	0.614100735	0.570353125	0.626797196	0.506204360	0.604426907	0.774977164	0.762913229
S66x8_24.150	0.071067870	0.073930327	0.087689982	0.079405647	0.095915917	0.129354582	0.130048373
S66x8_24.200	0.000245810	0.003515754	0.008496646	0.008436887	0.012501087	0.028977961	0.030170765
S66x8_24.90	2.581773619	2.224285157	3.111067229	2.255674636	3.575449424	5.415929086	5.154007702
S66x8_24.95	2.042680060	1.771250330	2.397131296	1.736214724	2.685157791	4.022100333	3.848119377
S66x8_25.100	1.884346527	1.643329416	2.123936450	1.566970781	2.301482370	3.343404902	3.222384109
S66x8_25.105	1.557671427	1.365767099	1.695966985	1.243821753	1.772888906	2.532037088	2.449970518
S66x8_25.110	1.293380754	1.137991538	1.355416187	0.997833076	1.366362019	1.914049945	1.858478113
S66x8_25.125	0.697927826	0.625830400	0.672721733	0.521119350	0.625372541	0.798111015	0.782298450
S66x8_25.150	0.116666380	0.108762045	0.108833192	0.096035881	0.100381180	0.099967579	0.099018103
S66x8_25.200	-0.000459392	0.000838408	0.002211653	0.002763538	0.003312670	-0.007330445	-0.008108337
S66x8_25.90	2.804210099	2.428265362	3.399681946	2.483668676	3.910330061	5.831280406	5.574583042
S66x8_25.95	2.299087475	1.991632827	2.672885330	1.955894336	2.986501590	4.402959364	4.225679577
S66x8_26.100	4.117102606	3.622607024	4.392223253	3.360757129	4.542074301	6.235417587	5.983922825
S66x8_26.105	3.483304088	3.063291168	3.646003834	2.786874440	3.705980714	5.052043249	4.852501976
S66x8_26.110	2.913305850	2.559862801	2.995256030	2.286644453	2.994686300	4.055396268	3.897541064
S66x8_26.125	1.651969722	1.454438948	1.621267808	1.255757129	1.550594302	2.024053902	1.950161627
S66x8_26.150	0.429857763	0.371253263	0.381472359	0.310306411	0.349399876	0.416380090	0.400875532
S66x8_26.200	0.001042905	-0.005652831	-0.014131394	-0.013811306	-0.019697266	-0.039298229	-0.040283344
S66x8_26.90	5.609541386	4.943609871	6.262781860	4.781692863	6.712210410	9.370687200	8.966587225
S66x8_26.95	4.817576154	4.242922674	5.254706658	4.020156094	5.533336580	7.657129865	7.338847235
S66x8_27.100	1.782520323	1.556355756	2.020121404	1.473330018	2.186779268	3.197102007	3.076074858
S66x8_27.105	1.502176211	1.316040721	1.616152335	1.185550707	1.676180887	2.391131402	2.311496171
S66x8_27.110	1.242764221	1.090566954	1.280296195	0.944701954	1.280395314	1.796589960	1.744214803
S66x8_27.125	0.651415782	0.583739165	0.620947091	0.487115326	0.574663330	0.736533715	0.722613810
S66x8_27.150	0.091154780	0.083827273	0.083180252	0.073462535	0.077306250	0.090076457	0.089913265
S66x8_27.200	-0.000673127	-0.000349403	-0.000192851	0.000466720	0.000220952	0.001420495	0.001742206
S66x8_27.90	2.753034569	2.371438658	3.321945897	2.412117241	3.823322761	5.750447730	5.477803737
S66x8_27.95	2.200566690	1.901865738	2.559791495	1.863162429	2.861185038	4.256723078	4.073973312
S66x8_28.100	2.841555219	2.518619957	3.182994524	2.420574874	3.418490162	4.809640134	4.622404182
S66x8_28.105	2.390760460	2.133054302	2.615625704	2.013793149	2.747139243	3.792790125	3.658639616
S66x8_28.110	1.977870995	1.766126668	2.102721000	1.630865261	2.160857733	2.937194445	2.841344250
S66x8_28.125	0.995970961	0.889836341	0.995095214	0.780943812	0.966764618	1.272851404	1.239374774
S66x8_28.150	0.232596329	0.211703102	0.219680281	0.185303162	0.207053949	0.240024821	0.235566536
S66x8_28.200	0.001216160	0.001053286	0.000804846	0.001631286	0.001842325	-0.001747330	-0.003032890
S66x8_28.90	4.097592887	3.610466389	4.835163051	3.618092758	5.389487426	7.800607674	7.445296381
S66x8_28.95	3.425884109	3.015924088	3.903959098	2.942244509	4.259196275	6.092298503	5.832762887
S66x8_29.100	3.034770481	2.675080207	3.284977507	2.510342040	3.456558974	4.814476827	4.636123019
S66x8_29.105	2.469424483	2.184111853	2.597124169	2.003834293	2.667614656	3.648224800	3.524969084
S66x8_29.110	1.950461222	1.727344510	2.008218160	1.553228294	2.016833866	2.735680983	2.636106969
S66x8_29.125	0.908919264	0.806361642	0.877234249	0.689146572	0.830608824	1.072526919	1.029252685
S66x8_29.150	0.166879296	0.146067712	0.142283310	0.119907958	0.127531604	0.149313791	0.129871438
S66x8_29.200	0.000140144	-0.002521305	-0.006471163	-0.005717007	-0.008509011	-0.011377176	-0.028242891
S66x8_29.90	4.567485514	4.020926511	5.288904219	3.972865642	5.826343513	8.367848179	7.991300713
S66x8_29.95	3.722618573	3.272130428	4.149347538	3.142364997	4.465402835	6.333170171	6.063251031

Table S1: BB-CP corrections (kcal mol⁻¹) for different systems in the S66x8 benchmark set. The def2-SVP basis set was used for all calculations. Each dimer is assigned the same number as in the original set. The value after each dot represents 100 times pre-factor for r_e .

	BLYP	B3LYP	B2PLYP	PBE0-DH	PBE0-2	MP2	SCS-MP2
S66x8_30.100	1.272375683	1.125004980	1.331229299	0.984324844	1.345087268	1.880745179	1.828478660
S66x8_30.105	1.064685048	0.950162787	1.085002561	0.813149381	1.063628586	1.452239204	1.418630819
S66x8_30.110	0.886577556	0.798769753	0.884442304	0.677581403	0.846350465	1.125102883	1.104823494
S66x8_30.125	0.436960119	0.403443591	0.415674864	0.346056636	0.385321696	0.449871195	0.452268112
S66x8_30.150	0.050464130	0.047955842	0.049113608	0.045673723	0.050393965	0.058114231	0.072048398
S66x8_30.200	0.000135394	0.000831584	0.001732665	0.002304440	0.003224172	0.003158626	0.017710244
S66x8_30.90	1.826465764	1.587974560	2.040405904	1.479002951	2.202982056	3.230780672	3.113254088
S66x8_30.95	1.520908748	1.332321504	1.640259309	1.200988742	1.714970713	2.458028562	2.379294723
S66x8_31.100	1.672547843	1.493643011	1.811702296	1.356223924	1.855441716	2.573674158	2.472101694
S66x8_31.105	1.415502175	1.270195673	1.505343807	1.140965495	1.516309995	2.066798962	1.990257147
S66x8_31.110	1.187860632	1.071384792	1.243560027	0.955154411	1.235419589	1.653490572	1.580840236
S66x8_31.125	0.651257121	0.597794905	0.662214807	0.532200406	0.640701665	0.809055476	0.792457415
S66x8_31.150	0.151352569	0.141073745	0.150178529	0.129529036	0.145487677	0.171301150	0.168182111
S66x8_31.200	-0.000299647	0.000890617	0.003381149	0.003402738	0.005242225	0.006355743	0.008046299
S66x8_31.90	2.296762769	2.043410236	2.613313500	1.924068324	2.779785396	3.961279541	3.805907717
S66x8_31.95	1.969211835	1.751294967	2.173406288	1.611526484	2.263987249	3.186817211	3.062232103
S66x8_32.100	1.561474841	1.342906825	1.550773309	1.149583128	1.542391430	2.157410652	2.082978277
S66x8_32.105	1.323613628	1.141034975	1.281864716	0.961492738	1.249193467	1.714434945	1.659894806
S66x8_32.110	1.113956264	0.962395114	1.052964315	0.799419649	1.005724636	1.351814713	1.306047345
S66x8_32.125	0.613816771	0.535496618	0.552557126	0.436097085	0.507321352	0.638148810	0.614350372
S66x8_32.150	0.159061174	0.139946788	0.134731111	0.114218325	0.120991340	0.143484743	0.135971780
S66x8_32.200	0.000897055	0.000353535	-0.000022484	0.000222233	-0.000011145	-0.008097326	-0.011129566
S66x8_32.90	2.119510169	1.824904710	2.249068714	1.636127702	2.341666604	3.374931382	3.264510331
S66x8_32.95	1.826802955	1.568866982	1.866392838	1.368549628	1.895877128	2.695558072	2.606917008
S66x8_33.100	1.287479717	1.107141243	1.307377923	0.944619037	1.310897036	1.880538472	1.806952548
S66x8_33.105	1.094822666	0.947618140	1.076055247	0.786481332	1.043287467	1.463108360	1.408530347
S66x8_33.110	0.923333849	0.807538194	0.890280608	0.662506868	0.842832627	1.151156093	1.110440774
S66x8_33.125	0.508548138	0.454941120	0.462659037	0.369696495	0.416652808	0.513578190	0.497115363
S66x8_33.150	0.096085596	0.089535233	0.089323008	0.079258361	0.084128408	0.096667160	0.094349389
S66x8_33.200	0.000457158	0.000614264	0.001112109	0.001059974	0.002092123	0.004954332	0.004577890
S66x8_33.90	1.785194457	1.517272464	1.946813582	1.380351641	2.084789232	3.098203628	2.963061823
S66x8_33.95	1.512042059	1.291794633	1.589367808	1.137486994	1.648339342	2.412029198	2.312310563
S66x8_34.100	0.956632383	0.674623660	0.918076971	0.588569753	1.003707253	1.577429153	1.507449632
S66x8_34.105	0.861139307	0.574169201	0.683018289	0.425921220	0.687386705	1.104966990	1.044371506
S66x8_34.110	0.778243963	0.526334994	0.586424451	0.380661196	0.571057406	0.905316828	0.852089085
S66x8_34.125	0.457610901	0.283486881	0.257995296	0.163185543	0.207746863	0.351171947	0.314010008
S66x8_34.150	0.162116963	0.113870595	0.122488592	0.095624324	0.118089327	0.172011333	0.156182308
S66x8_34.200	0.013518164	0.006857538	0.000206977	-0.002650699	-0.007827997	-0.010272271	-0.010650291
S66x8_34.90	1.419995516	1.136961575	1.713393741	1.186137278	2.011385899	3.022467705	2.923076267
S66x8_34.95	1.159792841	0.892069701	1.308168931	0.886627389	1.502093249	2.282896582	2.200335306
S66x8_35.100	0.924203873	0.734526796	0.989250102	0.729767057	1.116168761	1.624098964	1.551198339
S66x8_35.105	0.697573050	0.573557801	0.821846657	0.616385138	0.956107051	1.388932420	1.327076895
S66x8_35.110	0.560773745	0.481504061	0.714219087	0.549857911	0.848428244	1.219592556	1.166423215
S66x8_35.125	0.343740882	0.302022015	0.430766145	0.347126812	0.506523788	0.707673147	0.672501029
S66x8_35.150	0.140550461	0.132758509	0.184983748	0.160072252	0.218826591	0.290924073	0.277749690
S66x8_35.200	0.007092885	0.012337417	0.022869343	0.020258956	0.029901120	0.041687730	0.041756465
S66x8_35.90	1.303235226	1.043358998	1.516803317	1.096800768	1.785461572	2.633619676	2.526894585
S66x8_35.95	1.120633926	0.888138215	1.217963418	0.889474934	1.391248605	2.035259247	1.947855508
S66x8_36.100	0.694919464	0.670512343	1.010016231	0.812635413	1.208784399	1.667109796	1.608063205
S66x8_36.105	0.591702458	0.578315486	0.874226035	0.715992720	1.052589006	1.442347299	1.389456992
S66x8_36.110	0.510617068	0.509452439	0.775482948	0.647244242	0.943330067	1.282885434	1.235271685
S66x8_36.125	0.321888495	0.338645697	0.528595984	0.458079504	0.659387461	0.881448090	0.847929948
S66x8_36.150	0.123073526	0.144175535	0.237748463	0.211896294	0.305591911	0.403685232	0.390682799
S66x8_36.200	0.005653211	0.021821739	0.049610499	0.044752825	0.069364448	0.096665489	0.096975668
S66x8_36.90	0.884329383	0.892585238	1.451234094	1.145822330	1.789456863	2.496604362	2.417255332
S66x8_36.95	0.788615776	0.775424436	1.206746224	0.960769117	1.463520726	2.030887778	1.963445143
S66x8_37.100	0.847439698	0.748681056	1.137642592	0.875059927	1.362974071	1.917168878	1.836875779
S66x8_37.105	0.715295763	0.617303726	0.899257453	0.693147442	1.053086895	1.474982610	1.408523502

Table S1: BB-CP corrections (kcal mol⁻¹) for different systems in the S66x8 benchmark set. The def2-SVP basis set was used for all calculations. Each dimer is assigned the same number as in the original set. The value after each dot represents 100 times pre-factor for r_e .

	BLYP	B3LYP	B2PLYP	PBE0-DH	PBE0-2	MP2	SCS-MP2
S66x8_37.110	0.615375256	0.525005642	0.735788633	0.572238217	0.844852336	1.175027240	1.117633206
S66x8_37.125	0.394100519	0.339348894	0.451583069	0.369826777	0.512396725	0.687602466	0.646184447
S66x8_37.150	0.174697143	0.160430080	0.216452098	0.189573490	0.255482303	0.319712518	0.299361920
S66x8_37.200	0.015713415	0.020193864	0.032484023	0.028928420	0.040979605	0.037416157	0.034053889
S66x8_37.90	1.348696812	1.201578173	1.842600499	1.411223952	2.229312833	3.148555289	3.020168311
S66x8_37.95	1.059209795	0.948217689	1.459066638	1.122545244	1.763072732	2.481656452	2.380846000
S66x8_38.100	0.844173374	0.608202213	0.809215541	0.555144401	0.885288543	1.327411469	1.233459983
S66x8_38.105	0.695324415	0.542167868	0.773716094	0.561567661	0.884352170	1.284063060	1.201499257
S66x8_38.110	0.669979188	0.548696380	0.746750967	0.571482679	0.840260422	1.168189463	1.094600327
S66x8_38.125	0.390684626	0.346870266	0.494418328	0.411852500	0.585095764	0.769757566	0.718220139
S66x8_38.150	0.144789172	0.126992345	0.172662357	0.155104826	0.208693958	0.243151798	0.220718268
S66x8_38.200	0.010703616	0.011368915	0.015014371	0.012699119	0.016346424	-0.011131056	-0.016371792
S66x8_38.90	1.149928773	0.791889236	1.058127154	0.688215972	1.160001067	1.801722548	1.675668350
S66x8_38.95	1.017130962	0.698432771	0.887773339	0.583166107	0.942340139	1.450229682	1.341434720
S66x8_39.100	1.392028233	1.194687914	1.753799593	1.243556847	2.036152177	3.067995445	2.912918968
S66x8_39.105	1.196505071	1.037152249	1.466604216	1.053610827	1.661390986	2.442283136	2.347666226
S66x8_39.110	1.027918319	0.897805192	1.226697601	0.892297774	1.360724606	1.996383342	1.898290561
S66x8_39.125	0.649180744	0.563650309	0.684480841	0.505598978	0.698026125	0.989264635	0.943420722
S66x8_39.150	0.248321224	0.222769458	0.246029521	0.194029778	0.235584380	0.300774727	0.286143781
S66x8_39.200	0.003198994	0.003951312	0.005708459	0.004831541	0.006348546	0.007117406	-0.000895866
S66x8_39.90	1.918664549	1.601376302	2.485106908	1.728638050	2.989138400	4.633463727	4.374624240
S66x8_39.95	1.625989731	1.378452364	2.092545440	1.467533740	2.479974270	3.801303885	3.595543316
S66x8_40.100	1.159951164	1.068581388	1.674663161	1.232695754	2.018396782	2.989440670	2.870711888
S66x8_40.105	1.012346510	0.939036494	1.414597722	1.053309888	1.670388079	2.433293603	2.346671310
S66x8_40.110	0.898229814	0.832308875	1.193437422	0.895065112	1.368371495	1.964194317	1.901912729
S66x8_40.125	0.622149572	0.566381257	0.707414593	0.533520947	0.737301594	1.019382059	1.000489144
S66x8_40.150	0.241395473	0.243149497	0.299465570	0.251716355	0.319416041	0.397661382	0.403933892
S66x8_40.200	0.000932609	0.010996675	0.026924152	0.025619272	0.039476863	0.048427824	0.060005385
S66x8_40.90	1.553168145	1.397435886	2.357774072	1.677066756	2.929840757	4.484156212	4.271737300
S66x8_40.95	1.358347401	1.238316266	2.001030707	1.454353333	2.446116939	3.676428985	3.516371667
S66x8_41.100	2.803844742	2.342452670	2.791207217	2.050359145	2.809533864	3.964119442	3.775351858
S66x8_41.105	2.412564391	2.025114252	2.366207982	1.752746226	2.341159192	3.263771206	3.109331342
S66x8_41.110	2.002878922	1.681934470	1.908390246	1.425580345	1.839997165	2.525052848	2.407276553
S66x8_41.125	1.038519334	0.863702747	0.923208663	0.700593244	0.843606571	1.117587633	1.073224386
S66x8_41.150	0.254825072	0.203374731	0.190483506	0.150396588	0.155319298	0.189978872	0.178336573
S66x8_41.200	0.000877772	-0.008041717	-0.022273096	-0.020692154	-0.033412515	-0.052236868	-0.054516980
S66x8_41.90	3.771577637	3.133915154	3.879910191	2.815960610	4.031842889	5.791483077	5.511048647
S66x8_41.95	3.270694141	2.720875808	3.293823942	2.404657042	3.363241763	4.788919204	4.556550461
S66x8_42.100	2.362606059	2.060917146	2.565834614	1.950249422	2.685188391	3.697430476	3.541262316
S66x8_42.105	2.037979855	1.785037578	2.176038294	1.670922620	2.244227548	3.045297323	2.918420668
S66x8_42.110	1.741665059	1.527925613	1.826573129	1.414486818	1.857403610	2.476499528	2.373324661
S66x8_42.125	1.004156346	0.880976890	1.018125642	0.796987963	1.003435745	1.290689645	1.235921917
S66x8_42.150	0.305599106	0.269489387	0.299089189	0.243723864	0.290723244	0.337983583	0.319968611
S66x8_42.200	0.004824329	0.003418149	0.002416448	0.002534638	0.001863219	-0.024730218	-0.030395978
S66x8_42.90	3.212688405	2.798393217	3.647169130	2.743788065	3.959815284	5.566587756	5.330037656
S66x8_42.95	2.751917219	2.391995066	3.037156285	2.292978918	3.231920822	4.497157283	4.304918635
S66x8_43.100	1.974384957	1.687087428	2.014956664	1.500795886	2.034425327	2.833183943	2.708260721
S66x8_43.105	1.668209025	1.433376134	1.683030208	1.268775868	1.674698124	2.296280975	2.197193975
S66x8_43.110	1.381565541	1.186715106	1.367209717	1.039174108	1.339207843	1.814268921	1.735736945
S66x8_43.125	0.732507181	0.633710892	0.709089856	0.554034967	0.684016822	0.898167125	0.860344584
S66x8_43.150	0.192918278	0.175276810	0.201257753	0.165352055	0.200419434	0.248113334	0.238741932
S66x8_43.200	0.002045890	0.004174886	0.007927202	0.006681108	0.010308636	0.009535802	0.013153613
S66x8_43.90	2.776666559	2.392133134	3.005274787	2.214350052	3.151055061	4.464555571	4.269059913
S66x8_43.95	2.352116049	2.008463864	2.445542586	1.805899326	2.505315068	3.525044019	3.368447910
S66x8_44.100	0.786158532	0.608682121	0.698522219	0.471708563	0.676906374	1.012205932	0.956025574
S66x8_44.105	0.665692099	0.521025870	0.591410121	0.407578202	0.569187000	0.839901690	0.791577487
S66x8_44.110	0.576080872	0.460531900	0.519596479	0.369578540	0.501687441	0.724037679	0.682604762
S66x8_44.125	0.373505517	0.296774966	0.300589244	0.227024022	0.269880546	0.366030156	0.340481944

Table S1: BB-CP corrections (kcal mol⁻¹) for different systems in the S66x8 benchmark set. The def2-SVP basis set was used for all calculations. Each dimer is assigned the same number as in the original set. The value after each dot represents 100 times pre-factor for r_e .

	BLYP	B3LYP	B2PLYP	PBE0-DH	PBE0-2	MP2	SCS-MP2
S66x8_44.150	0.128472227	0.105282165	0.103440519	0.086228785	0.093286418	0.121180597	0.113313072
S66x8_44.200	0.005922800	0.001758367	-0.003044149	-0.003922714	-0.007536451	-0.002939082	-0.002762970
S66x8_44.90	1.138886451	0.890413983	1.071822699	0.723501091	1.085234582	1.629565820	1.551466537
S66x8_44.95	0.972828305	0.761902718	0.887404435	0.605312142	0.874786037	1.301752621	1.236125207
S66x8_45.100	0.912223074	0.732583290	0.796053773	0.539248194	0.740826207	1.088978066	1.047424797
S66x8_45.105	0.810984264	0.657385814	0.685331378	0.477684935	0.618093933	0.880942258	0.845919188
S66x8_45.110	0.723323642	0.591334280	0.592539030	0.425703058	0.518760531	0.712168346	0.682731840
S66x8_45.125	0.468397311	0.394619139	0.369388258	0.287665104	0.308510669	0.382978467	0.367360934
S66x8_45.150	0.141693804	0.126065251	0.118077750	0.101781307	0.102810959	0.115212490	0.111909546
S66x8_45.200	0.000043020	0.001006435	0.002124672	0.002203469	0.002710316	0.003912753	0.004090011
S66x8_45.90	1.212527361	0.932633989	1.057918958	0.678564468	1.018704795	1.567758106	1.506180478
S66x8_45.95	1.039232682	0.820416449	0.919611874	0.605591455	0.876260485	1.320856203	1.270772097
S66x8_46.100	2.699968400	2.182147076	2.371827250	1.730156898	2.220246521	3.069725838	2.927029474
S66x8_46.105	2.393891039	1.962097725	2.123660009	1.576731701	1.987206247	2.706192150	2.585344940
S66x8_46.110	2.104286070	1.744384093	1.876958626	1.415901091	1.754534890	2.356237337	2.254050923
S66x8_46.125	1.285585140	1.071536526	1.118866176	0.870187165	1.029161646	1.308461673	1.246120615
S66x8_46.150	0.397713698	0.338812391	0.350427349	0.290612028	0.327471503	0.371928797	0.352272457
S66x8_46.200	0.007838103	0.004365182	0.002080366	0.002480527	0.001262536	-0.029681064	-0.032934172
S66x8_46.90	3.447301736	2.757734051	3.074122772	2.204598434	2.945848056	4.122657068	3.928016323
S66x8_46.95	3.056941893	2.447741955	2.678213943	1.930595201	2.521264995	3.492685831	3.325513080
S66x8_47.100	0.959662327	0.844581493	1.293877936	0.933433816	1.553606936	2.351914856	2.240116637
S66x8_47.105	0.804019254	0.713414966	1.062628494	0.775839291	1.258017883	1.878796050	1.796780526
S66x8_47.110	0.680113129	0.607947161	0.879468484	0.649807964	1.025618434	1.509010937	1.449115095
S66x8_47.125	0.422012761	0.369749101	0.474992412	0.350382744	0.504437921	0.726137038	0.703884140
S66x8_47.150	0.190228556	0.166536509	0.184323672	0.139217581	0.173174001	0.227296813	0.223692837
S66x8_47.200	0.005302217	0.005165876	0.005484948	0.005192820	0.005467869	0.004706085	0.004929480
S66x8_47.90	1.313463751	1.120334004	1.847370078	1.280599503	2.286843748	3.592053217	3.387926888
S66x8_47.95	1.110363803	0.965035514	1.544357565	1.091606939	1.890398666	2.918899751	2.767096102
S66x8_48.100	1.572728504	1.324270511	1.659454684	1.203846173	1.728412487	2.480778276	2.369319859
S66x8_48.105	1.397686840	1.180481754	1.438646299	1.054321729	1.468852177	2.074186453	1.985638532
S66x8_48.110	1.240532476	1.057284882	1.263775041	0.938582613	1.271964397	1.761130769	1.691189485
S66x8_48.125	0.821406044	0.703390969	0.787699164	0.593077997	0.747970480	0.992510503	0.959093322
S66x8_48.150	0.331193818	0.281739003	0.286095542	0.220212678	0.249416898	0.306229227	0.298367488
S66x8_48.200	0.010987559	0.005359332	-0.001211335	-0.001286507	-0.006650433	-0.020450325	-0.021093563
S66x8_48.90	1.961106339	1.657640582	2.246398390	1.607653119	2.474002714	3.657043676	3.482329772
S66x8_48.95	1.758380382	1.485133442	1.935066315	1.394380230	2.073259214	3.019356502	2.879593997
S66x8_49.100	0.912070486	0.806097194	1.285301350	0.926263996	1.572512592	2.404891891	2.292253962
S66x8_49.105	0.771972770	0.688363022	1.061890432	0.775309142	1.277421989	1.926509945	1.843802576
S66x8_49.110	0.655324765	0.590535709	0.885018819	0.654543914	1.048383489	1.565318881	1.497352484
S66x8_49.125	0.426547857	0.372844526	0.482148870	0.355741629	0.515038975	0.742395859	0.721547581
S66x8_49.150	0.198912720	0.171459433	0.186352276	0.140181441	0.172330411	0.228306318	0.226249958
S66x8_49.200	0.006120251	0.005407435	0.005010434	0.005091037	0.004665870	0.003785014	0.005725435
S66x8_49.90	1.280836262	1.096146243	1.850618699	1.289354203	2.318672531	3.651196805	3.448871652
S66x8_49.95	1.064034911	0.929438735	1.541295705	1.091239517	1.917949521	2.979675621	2.828912890
S66x8_50.100	0.833434548	0.730970656	1.127737840	0.809915815	1.361662498	2.081997858	2.002234525
S66x8_50.105	0.693798237	0.618601611	0.936069503	0.691788800	1.126886653	1.689734028	1.634747087
S66x8_50.110	0.566877801	0.512871951	0.769553357	0.580138662	0.926167927	1.367809582	1.331136450
S66x8_50.125	0.317656152	0.276697835	0.382311724	0.281870999	0.432230699	0.633987656	0.627938472
S66x8_50.150	0.153660646	0.131170152	0.151541180	0.108120353	0.141686995	0.195700259	0.202716135
S66x8_50.200	0.006148409	0.007001439	0.007291922	0.007046517	0.006106732	0.002892437	0.012853579
S66x8_50.90	1.129367049	0.966599130	1.606034480	1.086388697	1.974344138	3.137875954	2.984111859
S66x8_50.95	0.975122733	0.840382008	1.338198465	0.928514879	1.626727601	2.544767548	2.432346048
S66x8_51.100	0.554261677	0.482212757	0.620429091	0.423283915	0.663737478	1.001674895	0.974575479
S66x8_51.105	0.488789216	0.417413632	0.512118898	0.345685587	0.528944245	0.799454345	0.774369055
S66x8_51.110	0.436588070	0.366595543	0.425323716	0.285156089	0.421071490	0.634802800	0.614437644
S66x8_51.125	0.332090482	0.277376857	0.278319212	0.194344240	0.243983347	0.344810410	0.331125238
S66x8_51.150	0.182163837	0.161727419	0.151734139	0.124405841	0.128808419	0.154225357	0.143656079
S66x8_51.200	0.005927053	0.005996132	0.005441716	0.005534984	0.004287986	0.007892182	0.006575031

Table S1: BB-CP corrections (kcal mol⁻¹) for different systems in the S66x8 benchmark set. The def2-SVP basis set was used for all calculations. Each dimer is assigned the same number as in the original set. The value after each dot represents 100 times pre-factor for r_e .

	BLYP	B3LYP	B2PLYP	PBE0-DH	PBE0-2	MP2	SCS-MP2
S66x8_51.90	0.723035813	0.629370112	0.843152092	0.576832859	0.928214795	1.411879131	1.374347060
S66x8_51.95	0.633097643	0.555924338	0.737356859	0.506673863	0.806649321	1.217455383	1.185203399
S66x8_52.100	2.107545292	1.828034073	2.161627074	1.721556869	2.240621005	3.020765669	2.910932636
S66x8_52.105	1.711596710	1.487306311	1.751673667	1.408419055	1.820355675	2.438918373	2.334367296
S66x8_52.110	1.369369111	1.192642257	1.405118131	1.137461132	1.465832079	1.956117533	1.877992373
S66x8_52.125	0.662305877	0.579516587	0.693026422	0.558027779	0.725430438	0.973971532	0.938129265
S66x8_52.150	0.222717228	0.189128549	0.217512241	0.161512840	0.208831396	0.296075984	0.280295524
S66x8_52.200	0.020994721	0.021499730	0.026801841	0.023451524	0.029890783	0.050075339	0.038047059
S66x8_52.90	3.019938375	2.625909270	3.202955233	2.490885239	3.351545393	4.604162578	4.388491609
S66x8_52.95	2.538614384	2.203479889	2.641012239	2.079260241	2.746426303	3.736150723	3.561387321
S66x8_53.100	2.493723385	2.089089659	2.241544893	1.712752755	2.064298770	2.705820517	2.592382661
S66x8_53.105	2.239654067	1.874371424	1.985249242	1.523070878	1.811661233	2.344916401	2.243735267
S66x8_53.110	1.994192641	1.674485403	1.763637851	1.360615384	1.602560080	2.053156896	1.967404784
S66x8_53.125	1.309717269	1.114380688	1.166087234	0.911967322	1.050255331	1.318993183	1.268909011
S66x8_53.150	0.493530842	0.423224106	0.428715936	0.340616026	0.377228524	0.452941524	0.437139688
S66x8_53.200	0.012403157	0.008288739	0.003877694	0.002532610	-0.000333369	-0.009166603	-0.010222412
S66x8_53.90	3.008635234	2.558391690	2.886776729	2.200288622	2.784369479	3.712305844	3.550286798
S66x8_53.95	2.750940336	2.317804412	2.541099205	1.938293758	2.387764939	3.148960675	3.010047220
S66x8_54.100	1.542839943	1.328152055	1.485225290	1.210487891	1.491794964	1.952616726	1.888771126
S66x8_54.105	1.149154496	0.987499586	1.114267325	0.902566996	1.125799499	1.488384426	1.444560266
S66x8_54.110	0.852026427	0.729968260	0.832603710	0.667469194	0.844782552	1.132031710	1.102292988
S66x8_54.125	0.377549579	0.319316669	0.369093267	0.279147730	0.364756866	0.516195377	0.507083479
S66x8_54.150	0.144635823	0.123533043	0.134973923	0.099176383	0.123344174	0.189727235	0.187527241
S66x8_54.200	0.007098160	0.006962606	0.008249894	0.007330287	0.008746496	0.033139919	0.033245422
S66x8_54.90	2.704356585	2.338191756	2.591878199	2.116497228	2.573166543	3.324245036	3.196969534
S66x8_54.95	2.058055701	1.773995291	1.968378826	1.608183235	1.961988172	2.547262729	2.456259584
S66x8_55.100	1.862888239	1.621735515	1.944955000	1.534441818	2.045693325	2.785332443	2.688020290
S66x8_55.105	1.473168351	1.290137311	1.562113059	1.232927634	1.653642161	2.255422378	2.182747579
S66x8_55.110	1.161052158	1.026293906	1.258976805	0.994100283	1.343380452	1.835509148	1.781976107
S66x8_55.125	0.594044992	0.533394513	0.657926408	0.515783975	0.695051070	0.947988393	0.927233346
S66x8_55.150	0.223155670	0.200642240	0.234476545	0.181033553	0.231444507	0.313145664	0.308551511
S66x8_55.200	0.015170233	0.018668834	0.028077440	0.024626069	0.034924911	0.054662559	0.054350338
S66x8_55.90	2.820058496	2.444338745	2.948687828	2.303687172	3.094612349	4.239101365	4.069029811
S66x8_55.95	2.310472857	2.004381881	2.401364433	1.887784739	2.518967543	3.435491152	3.306415877
S66x8_56.100	1.335219728	1.173201104	1.542388551	1.185922623	1.715990928	2.441217475	2.350901120
S66x8_56.105	1.064871238	0.941156906	1.234551881	0.952521571	1.369974449	1.940349963	1.874128899
S66x8_56.110	0.846795208	0.753209043	0.984596654	0.761982557	1.088768191	1.535835668	1.488350087
S66x8_56.125	0.449195568	0.391507647	0.477257759	0.361669420	0.492541717	0.692345997	0.676224409
S66x8_56.150	0.164982961	0.146097958	0.165419898	0.126509103	0.158775799	0.219277211	0.216601810
S66x8_56.200	0.003410148	0.006120137	0.011492468	0.010322337	0.015658915	0.030239828	0.030775558
S66x8_56.90	1.966754484	1.703030071	2.263107545	1.708440760	2.524166194	3.649439569	3.492163620
S66x8_56.95	1.620593882	1.412805929	1.867650230	1.424048206	2.087659011	2.988137889	2.868430981
S66x8_57.100	1.637365294	1.422306311	1.961415332	1.453946454	2.221426973	3.266947132	3.109147136
S66x8_57.105	1.370204204	1.192324324	1.596444034	1.198124147	1.781690484	2.588552681	2.470802114
S66x8_57.110	1.121223950	0.977584459	1.284505002	0.971429872	1.420115375	2.048386735	1.961824852
S66x8_57.125	0.643979637	0.553341917	0.659924949	0.501337680	0.674224223	0.957380629	0.926071170
S66x8_57.150	0.246406588	0.204033963	0.207495156	0.155653287	0.181170037	0.245358703	0.240349205
S66x8_57.200	0.009828847	0.005790140	0.001901825	0.001791866	-0.000827250	0.004321622	0.004336240
S66x8_57.90	2.376561486	2.048024450	2.955924545	2.135932945	3.412295480	5.129663911	4.855600288
S66x8_57.95	1.962580661	1.696722950	2.398763283	1.753295576	2.745915814	4.089375843	3.880382383
S66x8_58.100	2.824667186	2.357359595	2.560367935	1.844157116	2.287050289	3.045203875	2.932046578
S66x8_58.105	2.557752350	2.109973441	2.215588627	1.601941578	1.915982428	2.514996262	2.417533628
S66x8_58.110	2.312214315	1.907680434	1.969079618	1.444075219	1.683028362	2.169768177	2.085717674
S66x8_58.125	1.546769985	1.317544160	1.363788873	1.059392079	1.199164806	1.473996642	1.422572130
S66x8_58.150	0.455828090	0.395811076	0.402137502	0.333523394	0.362330090	0.413845127	0.399143156
S66x8_58.200	0.004592806	0.002087074	-0.000393813	-0.000304070	-0.001966565	-0.017238435	-0.018675537
S66x8_58.90	3.430109223	2.942776124	3.389230642	2.483890332	3.240275853	4.360265059	4.216918355
S66x8_58.95	3.158464539	2.686026925	3.032994609	2.203781300	2.827996573	3.793396371	3.662744175

Table S1: BB-CP corrections (kcal mol⁻¹) for different systems in the S66x8 benchmark set. The def2-SVP basis set was used for all calculations. Each dimer is assigned the same number as in the original set. The value after each dot represents 100 times pre-factor for r_e .

	BLYP	B3LYP	B2PLYP	PBE0-DH	PBE0-2	MP2	SCS-MP2
S66x8_59.100	2.848512355	2.333134285	2.135768241	1.611398468	1.646812204	1.978021047	1.948519586
S66x8_59.105	2.634799516	2.133803933	1.907735367	1.433461012	1.423769433	1.695202164	1.667563889
S66x8_59.110	2.448182123	1.977272610	1.752436096	1.322122374	1.295500949	1.529556116	1.503168861
S66x8_59.125	1.936537841	1.600758279	1.460847390	1.142630010	1.140898394	1.328268861	1.304765566
S66x8_59.150	1.024682255	0.882845375	0.841213097	0.695520223	0.710408875	0.813736203	0.798124498
S66x8_59.200	0.053364016	0.047042003	0.044561625	0.039303957	0.039451798	0.052228286	0.051068576
S66x8_59.90	3.391069441	2.865862266	2.777556128	2.139660232	2.317539602	2.800608473	2.763036762
S66x8_59.95	3.099467490	2.580879461	2.436335694	1.856719147	1.960905556	2.345294696	2.312798001
S66x8_60.100	2.313095604	1.942875190	2.065590362	1.575303336	1.900259958	2.477673463	2.395321987
S66x8_60.105	2.082906365	1.749380064	1.839187007	1.410955572	1.680012724	2.171948664	2.100650452
S66x8_60.110	1.857920181	1.558222307	1.619685820	1.247026852	1.467346702	1.884415001	1.822662010
S66x8_60.125	1.247929220	1.044060172	1.054030132	0.815835469	0.931640282	1.176128880	1.136636627
S66x8_60.150	0.548075070	0.465121617	0.453170309	0.360218723	0.391683704	0.475355293	0.459120917
S66x8_60.200	0.045872467	0.040241613	0.036571668	0.031353272	0.031365458	0.035756036	0.035548129
S66x8_60.90	2.792948755	2.338016389	2.548019187	1.905698328	2.375317892	3.171327905	3.062150613
S66x8_60.95	2.547701248	2.136716682	2.299326924	1.736890363	2.126542769	2.802914340	2.707907835
S66x8_61.100	2.290536170	1.942167430	2.117683096	1.644103800	2.014715545	2.637427048	2.540520200
S66x8_61.105	2.023227946	1.715283462	1.838708495	1.437726819	1.727721732	2.237902207	2.146731444
S66x8_61.110	1.764516622	1.494305274	1.577222384	1.240842169	1.465069615	1.879965241	1.806064841
S66x8_61.125	1.065428174	0.901622309	0.929462922	0.743757504	0.848916713	1.066834470	1.017829055
S66x8_61.150	0.306097198	0.263986245	0.270904542	0.227321267	0.252664628	0.306479998	0.313537742
S66x8_61.200	0.006233246	0.006148435	0.007711196	0.007307953	0.009007906	0.013378102	0.014388732
S66x8_61.90	2.934136165	2.464254523	2.728028763	2.082841632	2.619838158	3.491622152	3.354712811
S66x8_61.95	2.586783862	2.186216906	2.411093032	1.856576975	2.311676867	3.056055033	2.937865974
S66x8_62.100	3.169885829	2.698544478	2.901081498	2.241327783	2.701432043	3.509051953	3.360051108
S66x8_62.105	2.803053083	2.402944077	2.567343445	2.005459362	2.386234291	3.065725553	2.937731377
S66x8_62.110	2.454337628	2.115331116	2.246805232	1.772063832	2.084351902	2.651153422	2.540764622
S66x8_62.125	1.531556056	1.336578726	1.403896240	1.136822196	1.302171413	1.610696787	1.546119488
S66x8_62.150	0.520717136	0.460575067	0.480007747	0.405355254	0.452051428	0.538395707	0.518523120
S66x8_62.200	0.012430250	0.009358592	0.007665430	0.006161479	0.005694553	0.005492855	0.004878012
S66x8_62.90	4.033031791	3.383191898	3.671220736	2.781219297	3.436002202	4.552054555	4.352966171
S66x8_62.95	3.575571529	3.019994171	3.261816747	2.492882201	3.042253494	3.992737993	3.820168363
S66x8_63.100	1.787619308	1.577747389	1.970115062	1.519138011	2.117761865	2.969908733	2.873152994
S66x8_63.105	1.439138568	1.269957546	1.563060603	1.203987776	1.658497811	2.318578374	2.247059473
S66x8_63.110	1.182053548	1.043725754	1.256959288	0.971130814	1.309838022	1.817574012	1.764902674
S66x8_63.125	0.605250232	0.529506100	0.600242522	0.461857344	0.590372084	0.813931330	0.794943513
S66x8_63.150	0.171189022	0.154354340	0.168481067	0.133977670	0.159721335	0.218102726	0.216657283
S66x8_63.200	0.002237957	0.002983180	0.004304157	0.003781940	0.005214463	0.022046410	0.023879876
S66x8_63.90	2.658363860	2.356121979	3.074375187	2.359948298	3.416541998	4.846880053	4.672033963
S66x8_63.95	2.210668191	1.956052767	2.485856250	1.918826188	2.716476446	3.817396504	3.686919812
S66x8_64.100	2.179007878	1.873282876	2.038621488	1.532629436	1.896250195	2.515556490	2.398742445
S66x8_64.105	1.964891098	1.704777532	1.843939469	1.406301807	1.711427970	2.237829325	2.135643209
S66x8_64.110	1.749446404	1.531628759	1.651686942	1.275498523	1.533509078	1.995175013	1.906006744
S66x8_64.125	1.153283721	1.023666335	1.082057746	0.861016675	0.999715891	1.246472918	1.189980969
S66x8_64.150	0.365686104	0.328074821	0.335768815	0.280938509	0.309300757	0.363704181	0.346877357
S66x8_64.200	0.003013906	0.002167603	0.001565736	0.001761887	0.001069228	-0.002374617	-0.003155229
S66x8_64.90	2.656388684	2.260436121	2.524274610	1.854288517	2.392818871	3.266845551	3.114764506
S66x8_64.95	2.404216265	2.052652901	2.257751317	1.675628952	2.114667709	2.848135692	2.714967098
S66x8_65.100	2.171603573	1.818733491	1.946225474	1.401770592	1.732154126	2.295526639	2.217698890
S66x8_65.105	2.068418792	1.723461882	1.821954657	1.305021073	1.592511826	2.103233200	2.030312128
S66x8_65.110	1.974451591	1.637621737	1.708953273	1.221207197	1.468621833	1.929523492	1.861547381
S66x8_65.125	1.710644792	1.421303235	1.452217381	1.055745571	1.219991125	1.567564304	1.513293356
S66x8_65.150	1.123270322	0.961212664	0.986168815	0.760880464	0.853632963	1.049011091	1.014734048
S66x8_65.200	0.101868186	0.089209872	0.089202151	0.075599746	0.080276132	0.086650840	0.083283630
S66x8_65.90	2.403882407	2.019078274	2.196590894	1.596620195	2.009165533	2.682391885	2.593153740
S66x8_65.95	2.283525392	1.918586000	2.073270903	1.501542755	1.873773478	2.490720693	2.407677664
S66x8_66.100	2.172096181	1.876317064	2.151894337	1.633929046	2.100108055	2.797892335	2.695257900
S66x8_66.105	1.941376426	1.681087902	1.910533249	1.455732595	1.848987137	2.444406307	2.355732277

Table S1: BB-CP corrections (kcal mol⁻¹) for different systems in the S66x8 benchmark set. The def2-SVP basis set was used for all calculations. Each dimer is assigned the same number as in the original set. The value after each dot represents 100 times pre-factor for r_e .

	BLYP	B3LYP	B2PLYP	PBE0-DH	PBE0-2	MP2	SCS-MP2
S66x8_66.110	1.730864724	1.499878442	1.686506411	1.288817495	1.612728135	2.121078879	2.044902524
S66x8_66.125	1.196306342	1.027029886	1.103880479	0.845982417	1.011301139	1.304677507	1.257627106
S66x8_66.150	0.550508345	0.475785477	0.490729735	0.384341004	0.434644124	0.538569274	0.521507955
S66x8_66.200	0.038128573	0.032339645	0.029845914	0.024633098	0.024529038	0.025708611	0.024764186
S66x8_66.90	2.711226064	2.322804776	2.706441554	2.040131400	2.682366869	3.632042114	3.495511183
S66x8_66.95	2.427907103	2.089636645	2.415564103	1.827724654	2.375390346	3.189286329	3.070930106

SI.2 DFT-D3(BJ) and gCP parameters

Table S2: Damping parameters for the DFT-D3(BJ) correction for B2PLYP/def2-SVP with various BSSE corrections.

method	s ₆	a ₁	s ₈	a ₂
for B2PLYP-gCP-D3(BJ)	0.830	0.0400	0.5297	5.0471
for B2PLYP-(damped)gCP-D3(BJ)	0.830	-0.2217	0.3799	6.1387
for B2PLYP-CP-D3(BJ) ^a	0.830	0.1943	0.8686	4.8049

^aParameters for the BB-CP variant.

Table S3: Parameters for the gCP correction.

method	σ	η	α	β
for B2PLYP-gCP-D3(BJ)	0.31	1.25	0.65	1.35
for B2PLYP-(damped)gCP-D3(BJ)	0.303	1.2640	0.6403	1.3523

SI.3 Analysis of the damped-gCP variant

Table S4: Mean absolute deviations (MADs) and mean deviations (MDs) in parentheses for the S66x8 benchmark set and its categories. The def2-SVP basis set was used for all calculations. All values are reported in kcal mol⁻¹.

Level of theory	All	Hydrogen-bonded	Dispersion-driven	Mix
B2PLYP-gCP-D3(BJ)	0.56 (0.11)	0.80 (0.62)	0.52 (-0.39)	0.33 (0.10)
B2PLYP-(damped)gCP-D3(BJ)	0.65 (-0.19)	0.69 (0.30)	0.79 (-0.74)	0.45(-0.13)

^aDFT-D3(BJ) parameters are optimised in the presence of gCP.

^bDFT-D3(BJ) parameters are optimised in the presence of damped-gCP.

SI.4 Statistical results for all test sets in GMTKN55

Table S5: Statistical analysis of B2PLYP/(aug')-def2-SVP for all 55 categories and for the entire GMTKN55 benchmark set. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), deviation span (Δ_{error}), maximum (max) and minimum deviation (min). All values are in kcal mol⁻¹.

	MD	MAD	RMSD	Δ_{error}	max	min
ACONF	0.43	0.44	0.51	1.00	0.94	-0.06
ADIM6	-2.88	2.88	3.22	4.36	-0.82	-5.17
AHB21	-0.15	0.60	0.72	2.77	1.19	-1.58
AL2X6	-2.61	5.51	5.94	16.19	8.71	-7.48
ALK8	-1.75	3.05	4.50	13.65	4.89	-8.76
ALKBDE10	-9.09	9.09	9.63	10.36	-4.66	-15.02
AMINO20x4	0.17	0.56	0.71	3.43	2.27	-1.15
BH76	-3.23	4.00	5.90	27.61	6.37	-21.24
BHDIV10	-0.39	2.60	3.11	9.71	4.37	-5.33
BHPERI	-0.17	0.83	1.01	3.81	1.72	-2.09
BHROT27	0.27	0.45	0.62	2.36	1.57	-0.79
BSR36	-4.97	4.97	5.48	8.86	-1.61	-10.47
BUT14DIOL	2.28	2.29	2.38	3.73	3.41	-0.32
C60ISO	-6.72	6.78	9.02	17.54	0.31	-17.24
CARBHB12	0.93	1.09	1.41	3.84	3.47	-0.37
CDIE20	1.20	1.20	1.35	2.24	2.22	-0.02
CHB6	-3.04	4.26	5.31	10.42	2.08	-8.34
DARC	2.62	3.03	3.78	8.63	6.69	-1.95
DC13	7.72	8.18	14.63	52.34	49.33	-3.00
DIPCS10	-8.92	8.92	9.42	11.11	-1.54	-12.65
FH51	0.98	3.91	5.96	33.95	22.95	-11.00
G21EA	-1.77	3.04	3.85	17.12	12.00	-5.11
G21IP	-4.09	4.76	5.78	19.35	6.39	-12.97
G2RC	-0.01	7.90	10.03	43.70	30.86	-12.83
HAL59	0.34	1.06	1.44	6.47	4.14	-2.34
HEAVY28	-0.41	0.94	1.04	3.49	1.84	-1.65
HEAVYSB11	-7.45	7.45	7.92	9.01	-4.01	-13.03
ICONF	0.04	0.49	0.59	1.97	1.05	-0.92
IDISP	1.56	6.96	7.43	17.73	10.21	-7.53
IL16	2.75	2.75	2.83	2.99	3.95	0.96
INV24	0.24	1.68	2.49	11.17	8.17	-3.01
ISO34	-0.34	1.88	2.44	12.41	6.94	-5.47
ISOL24	-1.08	3.80	5.27	27.88	13.63	-14.25
MB16-43	-42.93	43.41	48.19	126.60	10.34	-116.26
MCONF	-0.32	0.42	0.50	1.69	0.63	-1.06
NBPRC	0.97	2.00	2.58	9.77	5.55	-4.22
PA26	3.31	3.57	4.13	9.54	7.84	-1.70
PArel	-0.29	1.94	3.33	13.83	2.01	-11.83
PCONF21	0.08	0.49	0.59	2.11	0.96	-1.15
PNICO23	-0.21	1.36	1.74	7.90	2.41	-5.49
PX13	-6.19	6.19	6.32	5.47	-2.78	-8.25
RC21	1.33	2.16	3.26	13.32	9.37	-3.94
RG18	-0.09	0.47	0.59	2.23	1.03	-1.20
RSE43	-0.92	1.03	1.29	4.48	1.08	-3.41
S22	-0.24	1.99	2.34	8.52	4.29	-4.23
S66	-0.07	1.81	2.02	7.85	4.37	-3.48
SCONF	1.22	2.51	2.88	9.98	4.46	-5.52
SIE4x4	11.12	11.12	12.54	20.13	21.14	1.02
TAUT15	0.03	1.40	1.60	5.34	3.18	-2.16
UPU23	0.76	0.94	1.22	4.01	3.03	-0.98
W4-11	-8.70	8.92	12.61	61.78	2.12	-59.66
WATER27	8.48	8.81	12.92	36.65	32.17	-4.48
WCPT18	-4.65	4.95	5.96	12.94	2.33	-10.61
YBDE18	-6.68	7.50	8.12	15.75	4.73	-11.01
BH76RC	-0.56	4.26	6.11	31.45	11.24	-20.20

Table S6: Statistical analysis of B2PLYP-D3(BJ)/(aug')-def2-SVP for all 55 categories and for the entire GMTKN55 benchmark set. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), deviation span (Δ_{error}), maximum (max) and minimum deviation (min). All values are in kcal mol⁻¹.

	MD	MAD	RMSD	Δ_{error}	max	min
ACONF	-0.04	0.16	0.20	0.72	0.31	-0.41
ADIM6	-0.26	0.32	0.39	0.95	0.16	-0.79
AHB21	-0.63	0.81	0.95	2.90	0.96	-1.93
AL2X6	0.75	3.57	4.72	12.74	10.46	-2.28
ALK8	2.01	2.67	4.16	11.66	9.02	-2.65
ALKBDE10	-8.73	8.73	9.27	10.41	-4.38	-14.79
AMINO20x4	0.21	0.68	0.86	3.90	2.59	-1.32
BH76	-3.59	4.24	6.13	27.92	6.36	-21.55
BHDIV10	-0.94	2.72	3.29	9.88	4.31	-5.57
BHPERI	-2.32	2.39	2.68	5.69	0.91	-4.78
BHROT27	0.29	0.46	0.62	2.32	1.54	-0.78
BSR36	-1.28	1.28	1.44	2.53	0.05	-2.48
BUT14DIOL	2.51	2.52	2.63	4.17	3.78	-0.39
C60ISO	-6.44	6.57	8.86	17.69	0.57	-17.12
CARBHB12	1.58	1.58	2.02	4.33	4.38	0.04
CDIE20	1.09	1.09	1.21	1.96	1.98	0.02
CHB6	-3.85	4.20	5.57	9.39	0.65	-8.74
DARC	-1.04	2.28	2.40	6.65	2.44	-4.22
DC13	6.52	6.54	12.11	38.92	38.84	-0.08
DIPCS10	-8.92	8.92	9.41	11.11	-1.54	-12.65
FH51	0.36	3.99	5.91	34.24	22.15	-12.09
G21EA	-1.77	3.03	3.85	17.07	11.95	-5.11
G21IP	-4.09	4.76	5.78	19.35	6.39	-12.97
G2RC	-0.20	8.16	10.32	45.78	31.41	-14.38
HAL59	1.51	1.51	1.96	5.26	5.20	-0.06
HEAVY28	0.49	0.52	0.97	3.04	2.75	-0.29
HEAVYSB11	-4.88	4.88	6.04	11.85	-0.53	-12.38
ICONF	-0.01	0.54	0.72	3.13	1.13	-2.00
IDISP	1.10	1.85	2.11	4.95	3.79	-1.16
IL16	1.14	1.23	1.32	2.57	1.86	-0.71
INV24	0.84	1.67	2.53	11.25	8.41	-2.83
ISO34	-0.20	1.68	2.17	11.02	6.48	-4.54
ISOL24	0.15	2.47	3.12	14.89	8.25	-6.65
MB16-43	-24.56	25.82	30.80	108.13	22.79	-85.34
MCONF	0.91	1.05	1.16	2.80	2.01	-0.79
NBPRC	-0.49	2.33	2.85	9.50	4.19	-5.31
PA26	3.58	3.82	4.37	9.70	8.08	-1.62
PArel	-0.30	1.88	3.26	13.52	1.89	-11.64
PCONF21	0.27	1.83	2.24	7.67	3.35	-4.31
PNICO23	0.94	1.32	1.80	7.86	4.07	-3.80
PX13	-6.51	6.51	6.65	5.37	-3.13	-8.50
RC21	2.38	3.02	4.06	14.19	10.38	-3.80
RG18	0.42	0.44	0.57	1.35	1.23	-0.12
RSE43	-0.81	0.96	1.22	4.47	1.17	-3.30
S22	1.81	1.86	2.51	5.87	5.44	-0.43
S66	1.69	1.71	2.17	5.93	5.61	-0.32
SCONF	1.33	2.93	3.37	11.55	4.76	-6.78
SIE4x4	11.31	11.31	12.71	20.07	21.16	1.10
TAUT15	-0.02	1.41	1.62	5.45	3.20	-2.25
UPU23	-0.07	1.05	1.48	7.81	3.31	-4.51
W4-11	-7.91	8.23	11.83	61.34	2.96	-58.38
WATER27	12.82	13.10	19.57	52.62	48.78	-3.85
WCPT18	-5.18	5.47	6.66	13.93	2.31	-11.62
YBDE18	-4.76	6.02	6.54	15.78	6.34	-9.43
BH76RC	-0.56	4.30	6.09	31.15	11.46	-19.69

Table S7: Statistical analysis of B2PLYP-gCP-D3(BJ)/(aug')-def2-SVP for all 55 categories and for the entire GMTKN55 benchmark set. The statistical key data are: mean deviation (MD), mean absolute deviation (MAD), root-mean-square deviation (RMSD), deviation span (Δ_{error}), maximum (max) and minimum deviation (min). All values are in kcal mol⁻¹.

	MD	MAD	RMSD	Δ_{error}	max	min
ACONF	0.04	0.19	0.21	0.68	0.39	-0.29
ADIM6	-0.98	0.98	1.14	1.85	-0.12	-1.98
AHB21	1.96	2.11	3.07	9.25	8.65	-0.60
AL2X6	4.65	5.10	6.24	13.74	12.41	-1.33
ALK8	11.61	12.23	16.17	40.25	37.79	-2.46
ALKBDE10	-8.40	8.40	9.42	13.37	-3.06	-16.43
AMINO20x4	-0.10	0.47	0.67	3.74	2.20	-1.54
BH76	-2.31	3.49	5.04	22.56	4.96	-17.60
BHDIV10	-0.89	2.75	3.37	10.01	4.11	-5.90
BHPERI	-2.46	2.52	3.07	6.75	0.81	-5.94
BHROT27	0.24	0.45	0.56	1.87	1.17	-0.70
BSR36	1.47	1.50	2.51	8.21	7.90	-0.31
BUT14DIOL	0.89	0.90	0.95	2.04	1.65	-0.39
C60ISO	-5.07	5.62	7.64	16.59	1.20	-15.39
CARBHB12	1.16	1.16	1.40	2.62	2.77	0.15
CDIE20	1.22	1.23	1.37	2.47	2.36	-0.11
CHB6	-5.72	5.72	6.54	7.53	-1.82	-9.36
DARC	1.34	2.75	3.49	9.74	6.28	-3.45
DC13	5.33	6.90	8.33	28.22	20.02	-8.20
DIPCS10	-9.41	9.41	9.93	12.13	-1.54	-13.67
FH51	1.87	3.97	5.78	34.37	22.75	-11.62
G21EA	-1.68	2.96	3.76	16.78	11.67	-5.11
G21IP	-4.17	4.86	5.92	19.76	6.39	-13.38
G2RC	3.39	9.35	11.79	48.88	33.14	-15.74
HAL59	0.82	1.22	1.55	6.83	4.26	-2.57
HEAVY28	0.51	0.61	0.93	2.95	2.45	-0.51
HEAVYSB11	2.04	6.30	7.52	22.55	11.34	-11.22
ICONF	-0.18	0.55	0.90	3.97	0.85	-3.12
IDISP	1.18	2.57	3.55	9.87	7.79	-2.08
IL16	5.13	5.13	5.53	6.63	8.44	1.82
INV24	1.26	1.83	2.76	11.86	9.14	-2.72
ISO34	0.07	2.03	2.75	13.28	7.34	-5.94
ISOL24	0.17	3.42	4.81	20.16	13.00	-7.16
MB16-43	16.63	27.54	33.59	117.32	67.02	-50.29
MCONF	-0.04	0.35	0.45	1.79	0.97	-0.82
NBPRC	0.17	4.87	6.48	23.67	12.85	-10.82
PA26	0.65	2.12	2.64	10.61	6.07	-4.54
PArel	-0.44	1.81	3.30	16.21	5.59	-10.63
PCONF21	0.47	0.57	0.75	2.14	1.85	-0.29
PNICO23	1.26	1.55	1.83	7.04	3.94	-3.09
PX13	-0.81	2.15	2.68	8.63	3.85	-4.78
RC21	0.83	2.14	3.03	12.72	7.56	-5.16
RG18	-0.83	0.96	1.36	3.21	0.41	-2.81
RSE43	-1.49	1.53	1.83	4.66	0.85	-3.80
S22	-0.01	0.60	0.85	3.87	1.48	-2.39
S66	0.21	0.65	0.86	4.37	1.90	-2.47
SCONF	0.02	0.52	0.69	2.89	1.31	-1.58
SIE4x4	10.49	10.49	11.93	20.08	20.87	0.79
TAUT15	-0.73	1.84	2.13	6.50	3.62	-2.88
UPU23	1.08	1.12	1.41	3.59	3.30	-0.29
W4-11	-13.60	13.72	17.34	71.70	4.66	-67.04
WATER27	-13.13	13.13	19.39	51.00	-0.82	-51.82
WCPT18	-2.62	3.09	3.68	9.75	2.81	-6.94
YBDE18	-4.86	5.50	6.44	14.82	3.05	-11.76
BH76RC	0.18	4.60	5.87	25.89	11.51	-14.38

SI.5 Weighted total mean absolute deviations for GMTKN55

Table S8: WTMAD-2 values (in kcal mol⁻¹) for B2PLYP, B2PLYP-D3(BJ), and B2PLYP-gCP-D3(BJ). The values are displayed for basic properties and reactions of small systems (A), isomerisations and reactions of large systems (B), barrier heights (C), intermolecular noncovalent interactions (D), intramolecular noncovalent interactions (E), all noncovalent interactions (F), and the entire GMTKN55 database (G). The (aug')-def2-SVP basis set was used for all calculations.

	B2PLYP-SVP	B2PLYP-D3(BJ)	B2PLYP-gCP-D3(BJ)
A	5.59	5.40	6.05
B	10.79	7.64	9.10
C	7.65	8.64	6.96
D	18.09	16.47	16.77
E	20.04	25.58	11.30
F	19.04	20.93	14.09
G	12.01	12.32	9.84