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Evaluation of composite schemes for CCSDT(Q) calculations of interaction energies in noncovalent complexes

Supplementary information

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	MP2	CCSD	CCSD[T]	CCSD(T)	CCSDT	CCSDT[Q]	CCSDT(Q)
Li_2 ... H_2	-0.071	-0.055	-0.072	-0.068	-0.071	-0.071	**-0.072**
	-0.096	-0.082	-0.100	-0.100	-0.105	-0.105	**-0.106**
	-0.111	-0.094	-0.117	-0.117	-0.122	-0.122	**-0.123**
BH_3 ... H_2	-0.128	-0.134	-0.148	-0.148	-0.151	-0.151	**-0.151**
	-0.145	-0.150	-0.168	-0.168	-0.172	-0.172	**-0.173**
	-0.154	-0.155	-0.176	-0.176	-0.180	-0.180	**-0.181**
BeH_2 ... H_2	-0.122	-0.121	-0.136	-0.136	-0.140	-0.140	**-0.140**
	-0.144	-0.144	-0.162	-0.162	-0.167	-0.167	**-0.167**
	-0.156	-0.152	-0.173	-0.173	-0.178	-0.178	**-0.179**
CH_4 dimer	-0.744	-0.709	-0.795	-0.792	-0.795	-0.792	**-0.798**
	-0.847	-0.778	-0.887	-0.885	-0.888	-0.885	**-0.894**
	-0.940	-0.850	-0.980	-0.981	-0.982	-0.979	**-0.990**
LiH ... H_2	-0.198	-0.141	-0.173	-0.172	-0.182	-0.183	**-0.183**
	-0.260	-0.227	-0.268	-0.267	-0.280	-0.280	**-0.281**
	-0.302	-0.258	-0.308	-0.308	-0.320	-0.320	**-0.322**
Ne dimer	-0.041	-0.047	-0.052	-0.051	-0.052	-0.051	**-0.051**
	-0.057	-0.061	-0.068	-0.068	-0.068	-0.068	**-0.068**
	-0.084	-0.093	-0.106	-0.105	-0.106	-0.105	**-0.106**

Table S1: *Correlation interaction energies of dispersion-bound complexes [kcal/mol]. For each complex, the results obtained in 6-31G**(0.25,0.15), aug-cc-pVDZ and aug-cc-pVTZ basis sets are listed.*

	MP2	CCSD	CCSD[T]	CCSD(T)	CCSDT	CCSDT[Q]	CCSDT(Q)
H^- ... LiH	1.086	3.181	3.015	3.021	2.944	2.946	**2.939**
	0.422	2.240	2.077	2.079	2.008	2.010	**2.003**
	-0.353	1.380	1.167	1.168	1.092	1.094	**1.085**
LiH ... Li^+	0.942	2.075	2.075	2.074	2.074	2.074	**2.074**
	0.027	0.461	0.459	0.459	0.458	0.458	**0.458**
	-0.208	0.300	0.290	0.289	0.287	0.287	**0.287**
F^- ... HF	10.137	120.019	11.654	10.995	11.187	11.042	**11.214**
	6.840	6.284	7.418	6.852	6.989	6.805	**7.080**
	5.341	4.293	5.384	4.940	4.976	4.808	**5.069**
HCN ... Li^+	2.240	1.981	2.061	2.175	2.122	2.244	**2.229**
	1.984	1.883	2.105	2.166	2.130	2.222	**2.213**
	1.844	1.502	1.762	1.811	1.769	1.863	**1.861**
C_2H_2 ... Li^+	2.214	2.038	2.130	2.116	2.093	2.166	**2.162**
	2.124	1.810	2.018	2.005	1.985	2.034	**2.040**
	1.782	1.294	1.528	1.508	1.471	1.517	**1.528**
C_2H_2 ... H^-	-0.578	0.177	-0.258	-0.222	-0.284	-0.219	**-0.261**
	-1.007	0.487	-0.040	-0.029	-0.078	-0.042	**-0.099**
	-1.543	-0.071	-0.646	-0.635	-0.684	-0.651	**-0.717**

Table S2: *Correlation interaction energies of complexes stabilized by electrostatic interaction [kcal/mol]. For each complex, the results obtained in 6-31G**(0.25,0.15), aug-cc-pVDZ and aug-cc-pVTZ basis sets are listed.*

	MP2	CCSD	CCSD[T]	CCSD(T)	CCSDT	CCSDT[Q]	CCSDT(Q)
NH_3 dimer	-1.063	-0.924	-1.080	-1.072	-1.072	-1.063	**-1.076**
	-1.269	-1.020	-1.223	-1.216	-1.217	-1.208	**-1.227**
	-1.552	-1.299	-1.545	-1.546	-1.541	-1.533	**-1.558**
H_2O dimer	-0.195	-0.067	-0.178	-0.196	-0.180	-0.174	**-0.184**
	-0.776	-0.567	-0.738	-0.738	-0.731	-0.722	**-0.740**
	-1.122	-0.930	-1.153	-1.153	-1.149	-1.137	**-1.163**
LiH dimer	0.332	1.256	1.164	1.167	1.127	1.128	**1.124**
	-0.305	0.090	-0.007	-0.007	-0.045	-0.045	**-0.045**
	-0.572	-0.086	-0.207	-0.208	-0.247	-0.246	**-0.251**
HF dimer	0.463	0.515	0.492	0.442	0.469	0.460	**0.460**
	-0.185	-0.120	-0.204	-0.224	-0.211	-0.210	**-0.217**
	-0.470	-0.434	-0.565	-0.573	-0.571	-0.564	**-0.580**
HCN ... HF	-0.075	0.102	0.088	0.113	0.108	0.115	**0.110**
	-0.696	-0.362	-0.420	-0.407	-0.411	-0.404	**-0.412**
	-1.447	-0.987	-1.290	-1.255	-1.256	-1.228	**-1.268**
BeH_2 ... LiH	0.153	0.429	0.398	0.400	0.392	0.393	**0.392**
	-0.329	-0.297	-0.329	-0.328	-0.335	-0.335	**-0.336**
	-0.319	-0.203	-0.245	-0.246	-0.255	-0.255	**-0.257**

Table S3: *Correlation interaction energies os hydrogen-bonded and lithium-bonded complexes [kcal/mol].For each complex, the results obtained in 6-31G**(0.25,0.15), aug-cc-pVDZ and aug-cc-pVTZ basis sets are listed.*

Optimized geometries used

Li_2-H_2

Li	-1.370000	1.369244	0.000000
Li	-1.370000	-1.369244	0.000000
H	4.470845	0.000000	0.000000
H	3.731708	0.000000	0.000000

BH_3-H_2

B	0.000000	0.000000	0.893908
H	0.000000	0.000000	-0.293284
H	0.000000	1.028365	1.487062
H	0.000000	-1.028365	1.487062
H	0.000000	0.000000	-3.205643
H	0.000000	0.000000	-3.944736

BeH_2-H_2

H	0.000000	0.000000	2.495481
Be	0.000000	0.000000	1.168445
H	0.000000	0.000000	-0.158980
H	0.000000	0.000000	-3.135511
H	0.000000	0.000000	-3.874769

CH_4 dimer

C	-0.000000000	0.000000000	1.819014570
H	0.512741150	0.888093730	1.454767430
H	0.512741150	-0.888093730	1.454767430
H	-1.025482300	0.000000000	1.454767430
H	0.000000000	-0.000000000	2.907220720
C	0.000000000	-0.000000000	-1.819014570
H	-0.000000000	0.000000000	-2.907220720
H	-0.512741150	0.888093730	-1.454767430
H	-0.512741150	-0.888093730	-1.454767430
H	1.025482300	-0.000000000	-1.454767430

LiH-H_2

Li	0.000000	0.000000	1.886217
H	0.000000	0.000000	0.256553
H	0.000000	0.000000	-2.587475
H	0.000000	0.000000	-3.327729

Ne dimer

Ne	0.000000	0.000000	1.547000
Ne	0.000000	0.000000	-1.547000

H^- - LiH

H	0.000000	0.000000	0.114805
Li	0.000000	0.000000	1.877476
H	0.000000	0.000000	3.640119

LiH- Li^+

H	0.000000	0.000000	0.000000
Li	0.000000	0.000000	-1.671611
Li	0.000000	0.000000	1.671611

F^- HF

F	0.000000	0.000000	1.143697938
H	0.000000	0.000000	0.004335379
F	0.000000	0.000000	-1.135033317

HCN – Li^+

Li	0.00000000	0.000000000	-3.004029931
N	0.00000000	0.000000001	-1.070231139
C	0.00000000	0.000000000	0.078848146
H	0.00000000	0.000000000	1.153412924

C_2H_2 – Li^+

H	0.000000	-0.211076	-1.677162
H	0.000000	-0.211076	1.677162
C	0.000000	-0.116500	-0.610156
C	0.000000	-0.116500	0.610156
LI	0.000000	2.155152	0.000000

C_2H_2 – H^-

H	0.000000	0.000000	1.921399
H	0.000000	0.000000	-1.455889
C	0.000000	0.000000	0.857647
C	0.000000	0.000000	-0.363572
H	0.000000	0.000000	-3.429963

NH_3 dimer

N	-0.049981290	-1.587093230	0.000000000
H	0.122962650	-2.168460180	0.811059760
H	0.122962650	-2.168460180	-0.811059760
H	0.659885800	-0.862352980	0.000000000
N	0.049981290	1.587093230	0.000000000
H	-0.122962650	2.168460180	0.811059760
H	-0.659885800	0.862352980	0.000000000
H	-0.122962650	2.168460180	-0.811059760

H_2O dimer

O	-0.066999140	0.000000000	1.494354740
H	0.815734270	0.000000000	1.865866390
H	0.068855100	0.000000000	0.539142770
O	0.062547750	0.000000000	-1.422632080
H	-0.406965400	-0.760178410	-1.771744500
H	-0.406965400	0.760178410	-1.771744500

LiH dimer

Li	0.000000	0.000000	0.000000
H	0.000000	0.000000	-1.667100
Li	0.000000	0.000000	3.375700
H	0.000000	0.000000	1.767800

HF dimer

H	0.000000000	0.802679820	1.695293290
F	0.000000000	-0.045966660	1.340348180
H	0.000000000	-0.120407870	-0.490828400
F	0.000000000	0.009769450	-1.404249780

HCN – HF

H	0.000000000	0.000000000	-2.956181146
C	0.000000000	0.000000000	-1.888298711
N	0.000000000	0.000000000	-0.737148859
H	0.000000000	0.000000000	1.096599407
F	0.000000000	0.000000000	2.026255026

BeH_2-LiH

H	0.000000	0.000000	2.759972
Be	0.000000	0.000000	1.443257
H	0.000000	0.000000	0.114802
Li	0.000000	0.000000	-1.752962
H	0.000000	0.000000	-3.388917