Supporting information

Convergence of the interaction energies in noncovalent complexes in the coupled-cluster methods up to full configuration interaction.

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Optimized geometries of studied complexes:

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

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

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

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

H^- - LiH
H 0.000000 0.000000 0.114805
Li 0.000000 0.000000 1.877476
H 0.000000 0.000000 3.640119

LiH- H^+
H 0.000000 0.000000 0.000000
Li 0.000000 0.000000 -1.671611
Li 0.000000 0.000000 1.671611

	HF	MP2	CCSD
Li_2 ... H_2	0.0001	0.0429	0.0290
	0.0206	0.0912	0.0755
BH_3 ... H_2	**0.0477**	0.0416	0.0384
	0.0284	0.0999	0.1053
BeH_2 ... H_2	0.0069	0.0769	0.0667
	0.0563	0.1783	0.1776
CH_4 dimer	**0.4870**	0.0741	0.0182
	0.4995	0.2448	0.2091
LiH ... H_2	0.2460	0.3252	0.2524
	0.4051	0.6035	0.5458
NH_3 dimer	1.4772	2.3082	2.1504
	1.5818	2.6443	2.5061
H_2O dimer	3.9255	4.0415	3.8543
	4.0230	4.2176	4.0901
BeH_2 ... LiH	7.2100	6.8259	6.4590
	7.2951	7.1420	6.8666
LiH dimer	24.6124	23.7060	22.5135
	24.7429	24.4112	23.4869
H^- ... LiH	54.5285	52.8175	50.0513
	55.1792	54.0931	51.9983
LiH ... Li^+	57.2972	56.0861	54.8452
	57.2117	56.2702	55.1366

Table 1. Interaction energies [kcal/mol] calculated at the HF, MP2 and CCSD levels of theory. **Bold** printed data at HF level correspond to unstable interaction. The data shown in the first and second rows were obtained using the 6-31G*(0.25) and 6-31G**(0.25,0.15) basis sets, respectively.

	CCSD	CCSD(T)	CCSD[T]	CCDST	CCSDT(Q)	CCSDTQ	CCSDTQ(P)	CCSDTQP	FCI
LiH dimer	25.3917	25.4743	25.4749	25.5139	25.5174	25.5189	25.5189	25.5189	25.5189
	27.6212	27.7178	27.7206	27.7589	27.7607	27.7613	27.7613	27.7613	27.7613
Li_2 ... H_2	0.0641	0.0704	0.0703	0.0720	0.0724	0.0726	0.0726	0.0726	0.0726
	0.1617	0.1749	0.1748	0.1784	0.1790	0.1791	0.1791	0.1791	0.1791
LiH ... Li^+	57.1356	57.1355	57.1352	57.1356	57.1355	57.1355	57.1355	57.1355	57.1355
	57.6209	57.6229	57.6227	57.6234	57.6234	57.6234	57.6234	57.6234	57.6234

Table 2. Interaction energies [kcal/mol] of selected complexes evaluated without counterpoise correction.