Benchmarking of London dispersion-accounting density functional theory methods on very large molecular complexes

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Supporting Information

Table S1: Statistical Data of all methods referenced in the paper: Mean deviation (MD), mean absolute deviation (MAD), root mean square deviation (RMSD). The use of the three body dispersion correction (+EABC) and the use of the Counterpoise correction scheme (CP) have been indicated after the basis set. Values reported herein as PBE-XDM/cc-pVTZ(seq-opt) and their derivatives are referred to as PBE-XDM/mixedTZ in the paper.

	MD	MAD	RMS
MP2/CBS/CP	−16.5	16.5	23.4
SCS-MP2/CBS/CP	−3.5	6.2	10.9
SOS-MP2/CBS/CP	−3.8	6.8	11.9
SCS(MI)-MP2/CBS/CP	−10.1	10.1	15.4
SOS(MI)-MP2/CBS/CP	−10.2	10.2	18.3
SSS(MI)-MP2/CBS/CP	−9.5	9.5	14.3
MP2/6-31G*(0.25) $(N = 10)$	−6.4	12.2	17.6
PBE/def2-QZVP'	25.8	25.8	28.0
PBE/def2-TZVP	24.4	24.4	26.6
PBE/def2-TZVP/0.5CP	25.5	25.5	27.6
PBE-dDsC/QZ4P	−4.8	4.8	5.7
PBE-dDsC/QZ4P+EABC	−2.6	2.7	3.6
PBE-dDsC/TZ2P	−5.6	5.6	6.9
PBE-dDsC/TZ2P+EABC	−3.4	3.5	4.6
PBE-dDsC/TZ2P/0.5CP+EABC	−1.9	2.5	3.5
PBE-D2/def2-QZVP'	0.3	1.5	1.9
PBE-D2/def2-QZVP'+EABC	−1.9	2.3	3.0
PBE-D2/def2-TZVP	−3.3	3.3	4.1
PBE-D2/def2-TZVP+EABC	−1.1	1.6	2.1
PBE-D2/def2-TZVP/0.5CP+EABC	−0.1	1.6	2.0
PBE-D3/def2-QZVP'	−0.5	2.1	2.5
PBE-D3/def2-QZVP'+EABC	1.6	2.4	3.0
PBE-D3/def2-TZVP	−1.9	2.1	3.1
PBE-D3/def2-TZVP+EABC	0.3	1.7	2.3
PBE-D3/def2-TZVP/0.5CP+EABC	1.3	2.3	2.8
PBE+vdW/T2	−7.7	7.7	9.3
PBE+vdW/T2+EABC	−5.5	5.5	7.0
PBE+vdW/T2/0.5CP+EABC	−5.3	5.3	6.8
M06-2X/def2-TZVP	−0.1	1.4	2.0
M06-2X/def2-TZVP/0.5CP	0.8	1.9	2.3
M06-2X/def2-TZVP+EABC	2.0	2.6	3.4
M06-2X/def2-TZVP/0.5CP+EABC	2.9	3.3	4.1
M06-L/def2-QZVP	0.5	3.1	3.6
M06-L/def2-QZVP+EABC	2.7	4.1	4.4
M06-L/def2-TZVP	−0.3	2.7	3.4
M06-L/def2-TZVP/0.5CP	1.2	3.7	3.9
M06-L/def2-TZVP+EABC	1.9	3.6	3.8
M06-L/def2-TZVP/0.5CP+EABC	3.4	4.6	5.1
PBE-NL/def2-QZVP	−3.6	3.7	4.8
PBE-NL/def2-QZVP+EABC	−1.4	2.1	2.9
PBE-NL/def2-TZVP	−5.0	5.0	6.1
PBE-NL/def2-TZVP+EABC	−2.8	3.1	3.9
PBE-NL/def2-TZVP/0.5CP*+EABC	−1.8	2.3	3.2
PBE-XDM6/cc-pVTZ(seq-opt)	1.7	5.1	5.6
PBE-XDM6/cc-pVTZ(seq-opt)/0.5CP*	3.6	5.5	6.1
PBE-XDM6/cc-pVTZ(seq-opt)+EABC	3.9	5.3	6.4
PBE-XDM6/cc-pVTZ(seq-opt)/0.5CP*+EABC	5.8	6.1	7.4
PBE-XDM10/cc-pVTZ(seq-opt)	0.8	4.7	5.1
PBE-XDM10/cc-pVTZ(seq-opt)/0.5CP*	2.7	5.2	5.4
PBE-XDM10/cc-pVTZ(seq-opt)+EABC	3.0	4.9	5.4
PBE-XDM10/cc-pVTZ(seq-opt)/0.5CP*+EABC	4.9	5.4	6.4
PBE-XDM6/TZV	−2.3	4.2	5.6
PBE-XDM6/TZV/0.5CP*	−0.5	3.8	5.0
PBE-XDM6/TZV+EABC	−0.2	3.8	4.9

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	MD	MAD	RMS
PBE-XDM6/TZV/0.5CP*+EABC	1.7	4.2	5.0
PBE-XDM10/TZV	−3.1	4.6	6.0
PBE-XDM10/TZV/0.5CP*	−1.2	4.2	5.2
PBE-XDM10/TZV+EABC	−0.9	3.5	4.7
PBE-XDM10/TZV/0.5CP*+EABC	0.9	3.7	4.7
BLYP-NL/QZVP	−7.7	7.7	9.1
BLYP-NL/QZVP+EABC	−5.5	5.5	6.7
BLYP-dDsC/QZ4P	−3.6	3.9	4.8
BLYP-dDsC/QZ4P+EABC	−1.4	2.3	3.0
BLYP-D3/QZVP	−6.2	6.2	7.4
BLYP-D3/QZVP+EABC	−4.0	4.1	5.3
DFTB3	20.6	20.6	23.0
DFTB3-D3	−6.8	7.5	10.1
DFTB3-D3+EABC	−4.7	6.2	8.4
OM2	16.9	16.9	19.8
OM2-D3	−5.2	5.2	7.6
OM2-D3+EABC	−3.1	3.8	6.3
OM3	20.9	20.9	22.8
OM3-D3	−5.0	5.4	6.9
OM3-D3+EABC	−3.0	4.1	5.3
PM6-DH2	−7.4	7.4	8.7
PM6-DH2+EABC	−5.4	5.5	6.9
PM6	15.1	15.1	17.4
VDW3	−8.5	8.5	14.6
VDW3+EABC	−6.4	8.3	13.6

Table S2: MP2/CBS: interaction energies (ΔE), CP correction (ΔCP) and full CP corrected interaction energies ($\Delta(E + 1.0CP)$). All energies in kcal/mol.

	ΔE	ΔCP	$\Delta(E + 1.0CP)$
2a	−52.8	6.3	−46.5
2b	−36.1	4.6	−31.5
3a	−46.5	13.3	−33.2
3b	−32.8	9.5	−23.4
4a	−90.4	11.6	−78.8
4b	−95.6	12.6	−83.1
5a	−45.4	6.0	−39.5
5b	−33.7	5.0	−28.7
6a	−91.7	4.5	−87.2
6b	−87.0	3.7	−83.2
7a	−159.2	9.1	−150.0
7b	−40.0	7.4	−32.6

Table S3: SCS-MP2/CBS: interaction energies (ΔE), CP correction (ΔCP) and full CP corrected interaction energies ($\Delta(E + 1.0CP)$). All energies in kcal/mol.

	ΔE	ΔCP	$\Delta(E + 1.0CP)$
2a	−38.6	6.6	−32.1
2b	−26.1	4.8	−21.3
3a	−34.3	13.4	−20.9
3b	−26.0	9.5	−16.5
4a	−65.3	12.1	−53.3
4b	−68.8	13.0	−55.8
5a	−36.1	6.1	−30.0
5b	−25.2	5.0	−20.2
6a	−84.3	4.6	−79.7
6b	−80.8	3.8	−77.0
7a	−141.8	9.5	−132.3
7b	−29.8	7.6	−22.3

Table S4: SOS-MP2/CBS: interaction energies (ΔE), CP correction (ΔCP) and full CP corrected interaction energies ($\Delta(E + 1.0CP)$). All energies in kcal/mol.

	ΔE	ΔCP	$\Delta(E + 1.0CP)$
2a	−40.2	7.8	−32.4
2b	−27.5	5.7	−21.8
3a	−36.3	15.4	−20.9
3b	−26.9	10.8	−16.1
4a	−70.0	14.4	−55.6
4b	−73.8	15.5	−58.4
5a	−36.4	7.1	−29.3
5b	−25.6	5.8	−19.8
6a	−84.6	5.4	−79.2
6b	−81.0	4.5	−76.5
7a	−143.8	11.3	−132.6
7b	−31.3	8.7	−22.5

Table S5: SCS(MI)-MP2/CBS: interaction energies (ΔE), CP correction (ΔCP) and full CP corrected interaction energies ($\Delta(E + 1.0CP)$). All energies in kcal/mol.

	ΔE	ΔCP	$\Delta(E + 1.0CP)$
2a	−43.1	3.6	−39.5
2b	−28.4	2.6	−25.8
3a	−36.7	8.8	−27.9
3b	−27.8	6.4	−21.4
4a	−68.8	6.5	−62.3
4b	−72.5	7.0	−65.5
5a	−40.7	3.8	−36.9
5b	−29.0	3.2	−25.8
6a	−88.0	2.8	−85.2
6b	−84.0	2.3	−81.7
7a	−147.1	5.3	−141.8
7b	−32.4	4.8	−27.6

Table S6: SOS(MI)-MP2/CBS: interaction energies (ΔE), CP correction (ΔCP) and full CP corrected interaction energies ($\Delta(E + 1.0CP)$). All energies in kcal/mol.

	ΔE	ΔCP	$\Delta(E + 1.0CP)$
2a	−48.3	8.8	−39.5
2b	−33.7	6.5	−27.2
3a	−43.9	17.3	−26.6
3b	−31.0	12.1	−18.9
4a	−86.3	16.4	−69.9
4b	−91.2	17.7	−73.6
5a	−41.0	8.0	−33.1
5b	−30.0	6.6	−23.5
6a	−88.2	6.1	−82.1
6b	−84.0	5.0	−78.9
7a	−153.8	12.7	−141.1
7b	−37.4	9.8	−27.6

Table S7: SSS(MI)-MP2/CBS: interaction energies (ΔE), CP correction (ΔCP) and full CP corrected interaction energies ($\Delta(E + 1.0CP)$). All energies in kcal/mol.

	ΔE	ΔCP	$\Delta(E + 1.0CP)$
2a	−41.4	2.6	−38.8
2b	−26.9	1.9	−25.0
3a	−34.7	7.1	−27.6
3b	−26.9	5.3	−21.6
4a	−64.1	4.5	−59.6
4b	−67.5	4.9	−62.6
5a	−40.2	2.9	−37.3
5b	−28.4	2.5	−25.9
6a	−87.6	2.1	−85.5
6b	−83.8	1.8	−82.0
7a	−144.9	3.8	−141.1
7b	−30.9	3.8	−27.1

Table S8: MP2/6-31G*(0.25): interaction energies (ΔE), CP correction (ΔCP) and full CP corrected interaction energies ($\Delta(E + 1.0CP)$). All energies in kcal/mol.

	ΔE	ΔCP	$\Delta(E + 1.0CP)$
2a	−64.0	28.9	−35.1
2b	−43.1	19.9	−23.2
3a	−62.9	46.3	−16.6
3b	−43.5	34.2	−9.2
4a	−113.8	49.9	−63.9
4b	−119.7	52.1	−67.6
5a	−62.3	32.9	−29.4
5b	−46.9	27.4	−19.6
6a	−107.0	23.2	−83.9
6b	−100.2	18.7	−81.5

Table S9: PBE/def2-QZVP': uncorrected interaction energies (ΔE). All energies in kcal/mol.

	ΔE
2a	−0.5
2b	1.8
3a	0.3
3b	−6.5
4a	12.3
4b	13.7
5a	−14.8
5b	−5.1
6a	−63.1
6b	−62.6
7a	−86.6
7b	1.3

Table S10: PBE-dDsC/QZ4P: interaction energies, uncorrected (ΔE) and three body energy corrected ($\Delta(E + E^{ABC})$). All energies in kcal/mol.

	ΔE	$\Delta(E + E^{ABC})$
2a	−33.1	−31.3
2b	−21.8	−20.6
3a	−28.1	−26.3
3b	−21.4	−20.7
4a	−34.9	−31.7
4b	−39.7	−36.2
5a	−38.1	−37.1
5b	−26.7	−25.7
6a	−84.7	−82.5
6b	−80.1	−78.2
7a	−135.8	−131.2
7b	−33.1	−29.9

Table S11: PBE-NL/def2-QZVP: interaction energies, uncorrected (ΔE) and three body energy corrected ($\Delta(E + E^{ABC})$). All energies in kcal/mol.

	ΔE	$\Delta(E + E^{ABC})$
2a	−30.3	−28.5
2b	−19.6	−18.4
3a	−27.0	−25.1
3b	−21.8	−21.1
4a	−34.9	−31.7
4b	−36.2	−32.8
5a	−35.4	−34.4
5b	−23.8	−22.8
6a	−85.3	−83.1
6b	−81.0	−79.2
7a	−136.1	−131.5
7b	−31.5	−28.2

Table S12: PBE-D2/def2-QZVP': interaction energies, uncorrected (ΔE) and three body energy corrected ($\Delta(E + E^{ABC})$). All energies in kcal/mol.

	ΔE	$\Delta(E + E^{ABC})$
2a	−30.6	−28.9
2b	−20.3	−19.1
3a	−23.9	−22.1
3b	−19.4	−18.7
4a	−31.8	−28.6
4b	−33.0	−29.5
5a	−35.9	−34.9
5b	−23.6	−22.6
6a	−83.4	−81.2
6b	−79.7	−77.9
7a	−133.2	−128.6
7b	−27.8	−24.5

Table S13: PBE-D3/def2-QZVP': interaction energies, uncorrected (ΔE) and three body energy corrected ($\Delta(E + E^{ABC})$). All energies in kcal/mol.

	ΔE	$\Delta(E + E^{ABC})$
2a	−29.8	−28.0
2b	−19.4	−18.2
3a	−23.7	−21.9
3b	−19.3	−18.6
4a	−29.8	−26.6
4b	−31.2	−27.7
5a	−33.3	−32.3
5b	−22.3	−21.3
6a	−82.9	−80.7
6b	−79.2	−77.4
7a	−128.2	−123.6
7b	−26.8	−23.5

Table S14: M06-L/def2-QZVP: interaction energies, uncorrected (ΔE) and three body energy corrected ($\Delta(E + E^{ABC})$). All energies in kcal/mol.

	ΔE	$\Delta(E + E^{ABC})$
2a	−27.8	−26.1
2b	−18.1	−16.8
3a	−23.2	−21.4
3b	−19.0	−18.2
4a	−25.4	−22.3
4b	−24.2	−20.7
5a	−31.4	−30.4
5b	−20.5	−19.5
6a	−84.1	−81.9
6b	−80.3	−78.5
7a	−131.5	−126.9
7b	−28.4	−25.2

Table S15: BLYP-NL/def2-QZVP: interaction energies, uncorrected (ΔE) and three body energy corrected ($\Delta(E+E^{ABC})$). All energies in kcal/mol.

	ΔE	$\Delta(E+E^{ABC})$
2a	−33.4	−31.7
2b	−21.7	−20.5
3a	−31.3	−29.5
3b	−24.0	−23.3
4a	−41.8	−38.6
4b	−43.9	−40.4
5a	−37.4	−36.4
5b	−26.4	−25.4
6a	−88.5	−86.3
6b	−83.6	−81.8
7a	−143.9	−139.3
7b	−36.0	−32.8

Table S16: BLYP-dDsC/QZ4P: interaction energies, uncorrected (ΔE) and three body energy corrected ($\Delta(E+E^{ABC})$). All energies in kcal/mol.

	ΔE	$\Delta(E+E^{ABC})$
2a	−31.6	−29.8
2b	−20.3	−19.1
3a	−25.6	−23.8
3b	−19.1	−18.4
4a	−30.6	−27.4
4b	−34.7	−31.2
5a	−39.8	−38.8
5b	−28.3	−27.3
6a	−84.1	−81.9
6b	−79.4	−77.6
7a	−136.9	−132.3
7b	−32.6	−29.3

Table S17: BLYP-D3/def2-QZVP: interaction energies, uncorrected (ΔE) and three body energy corrected ($\Delta(E+E^{ABC})$). All energies in kcal/mol.

	ΔE	$\Delta(E+E^{ABC})$
2a	−36.2	−34.5
2b	−24.2	−23.0
3a	−30.4	−28.6
3b	−22.7	−22.0
4a	−39.8	−36.6
4b	−44.5	−41.1
5a	−35.1	−34.1
5b	−25.2	−24.2
6a	−85.6	−83.4
6b	−81.8	−80.0
7a	−136.7	−132.1
7b	−31.3	−28.1

Table S18: PBE-dDsC/TZ2P: uncorrected interaction energies (ΔE), CP correction (ΔCP), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$), and three body energy and CP corrected interaction energies ($\Delta(E+0.5CP+E^{ABC})$). Note that half the CP correction was used to obtain these values. All energies in kcal/mol.

	ΔE	ΔCP	$\Delta(E+E^{ABC})$	$\Delta(E+0.5CP+E^{ABC})$
2a	−33.4	2.5	−31.7	−30.4
2b	−22.1	2.0	−20.9	−19.9
3a	−27.9	4.2	−26.1	−24.0
3b	−21.3	2.9	−20.6	−19.1
4a	−37.6	4.2	−34.4	−32.3
4b	−39.1	4.4	−35.6	−33.4
5a	−36.4	2.4	−35.4	−34.2
5b	−24.8	2.1	−23.8	−22.8
6a	−86.6	2.4	−84.4	−83.2
6b	−81.9	2.1	−80.1	−79.0
7a	−140.3	4.9	−135.7	−133.3
7b	−35.6	3.4	−32.3	−30.6

Table S19: PBE-D2/def2-TZVP: uncorrected interaction energies (ΔE), CP correction (ΔCP), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$), and three body energy and CP corrected interaction energies ($\Delta(E+0.5CP+E^{ABC})$). Note that half the CP correction was used to obtain these values. All energies in kcal/mol.

	ΔE	ΔCP	$\Delta(E+E^{ABC})$	$\Delta(E+0.5CP+E^{ABC})$
2a	−31.6	1.5	−29.8	−29.1
2b	−21.0	1.1	−19.8	−19.3
3a	−25.4	3.4	−23.6	−21.9
3b	−20.4	2.7	−19.7	−18.3
4a	−33.1	2.2	−29.9	−28.8
4b	−34.4	2.3	−30.9	−29.8
5a	−37.5	2.3	−36.5	−35.4
5b	−24.8	1.7	−23.8	−22.9
6a	−84.7	1.2	−82.5	−81.8
6b	−80.9	1.0	−79.1	−78.6
7a	−136.1	3.1	−131.5	−129.9
7b	−29.3	2.2	−26.0	−25.0

Table S20: PBE-D3/def2-TZVP: uncorrected interaction energies (ΔE), CP correction (ΔCP), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$), and three body energy and CP corrected interaction energies ($\Delta(E+0.5CP+E^{ABC})$). Note that half the CP correction was used to obtain these values. All energies in kcal/mol.

	ΔE	ΔCP	$\Delta(E+E^{ABC})$	$\Delta(E+0.5CP+E^{ABC})$
2a	−30.7	1.5	−28.9	−28.2
2b	−20.1	1.1	−18.9	−18.4
3a	−25.2	3.4	−23.4	−21.7
3b	−20.3	2.7	−19.6	−18.2
4a	−31.1	2.2	−27.9	−26.9
4b	−32.6	2.3	−29.1	−28.0
5a	−35.0	2.3	−34.0	−32.8
5b	−23.5	1.7	−22.5	−21.7
6a	−84.2	1.2	−82.0	−81.3
6b	−80.4	1.0	−78.6	−78.1
7a	−131.1	3.1	−126.5	−125.0
7b	−28.3	2.2	−25.1	−24.0

Table S21: PBE/def2-TZVP: uncorrected interaction energies (ΔE) and CP correction (ΔCP). All energies in kcal/mol.

	ΔE	ΔCP
2a	−1.5	1.5
2b	1.0	1.1
3a	−1.2	3.4
3b	−7.5	2.7
4a	11.0	2.2
4b	12.3	2.3
5a	−16.4	2.3
5b	−6.3	1.7
6a	−64.3	1.2
6b	−63.8	1.0
7a	−89.5	3.1
7b	−0.2	2.2

Table S22: PBE-TS-VDW/T2: uncorrected interaction energies (ΔE), CP correction (ΔCP), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$), and three body energy and CP corrected interaction energies ($\Delta(E+0.5CP+E^{ABC})$). Note that half the CP correction was used to obtain these values. All energies in kcal/mol.

	ΔE	ΔCP	$\Delta(E+E^{ABC})$	$\Delta(E+0.5CP+E^{ABC})$
2a	−36.2	0.3	−34.4	−34.2
2b	−23.8	0.3	−22.6	−22.5
3a	−30.8	0.8	−29.0	−28.6
3b	−22.7	0.6	−22.0	−21.7
4a	−42.9	0.5	−39.7	−39.5
4b	−45.4	0.5	−41.9	−41.7
5a	−35.9	0.4	−34.9	−34.7
5b	−24.6	0.3	−23.6	−23.4
6a	−87.5	0.5	−85.3	−85.1
6b	−82.5	0.4	−80.7	−80.5
7a	−142.3	0.9	−137.7	−137.3
7b	−37.3	0.6	−34.0	−33.8

Table S23: M06-2X/def2-TZVP: uncorrected interaction energies (ΔE), CP correction (ΔCP), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$), and three body energy and CP corrected interaction energies ($\Delta(E+0.5CP+E^{ABC})$). Note that half the CP correction was used to obtain these values. All energies in kcal/mol.

	ΔE	ΔCP	$\Delta(E+E^{ABC})$	$\Delta(E+0.5CP+E^{ABC})$
2a	−29.8	1.3	−28.0	−27.4
2b	−19.6	0.9	−18.4	−17.9
3a	−24.4	3.1	−22.6	−21.1
3b	−21.1	2.5	−20.4	−19.2
4a	−28.1	1.9	−25.0	−24.0
4b	−27.6	1.9	−24.1	−23.2
5a	−36.2	1.6	−35.2	−34.4
5b	−22.6	1.3	−21.7	−21.0
6a	−82.1	1.3	−79.9	−79.2
6b	−79.6	1.1	−77.7	−77.2
7a	−128.0	2.8	−123.4	−122.0
7b	−22.1	1.8	−18.9	−18.0

Table S24: M06-L/def2-TZVP: uncorrected interaction energies (ΔE), CP correction (ΔCP), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$), and three body energy and CP corrected interaction energies ($\Delta(E+0.5CP+E^{ABC})$). Note that half the CP correction was used to obtain these values. All energies in kcal/mol.

	ΔE	ΔCP	$\Delta(E+E^{ABC})$	$\Delta(E+0.5CP+E^{ABC})$
2a	−28.5	3.0	−26.7	−25.2
2b	−18.6	2.1	−17.3	−16.3
3a	−23.7	4.4	−21.9	−19.8
3b	−19.3	3.3	−18.6	−16.9
4a	−27.0	4.8	−23.9	−21.5
4b	−25.6	4.8	−22.2	−19.8
5a	−32.5	2.1	−31.4	−30.4
5b	−21.2	2.0	−20.3	−19.3
6a	−84.7	1.8	−82.5	−81.6
6b	−80.8	1.4	−78.9	−78.2
7a	−132.2	4.2	−127.6	−125.5
7b	−28.9	2.3	−25.6	−24.5

Table S25: PBE-NL/def2-TZVP: uncorrected interaction energies (ΔE), CP correction (ΔCP), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$), and three body energy and CP corrected interaction energies ($\Delta(E+0.5CP+E^{ABC})$). Note that half the CP correction was used to obtain these values. All energies in kcal/mol.

	ΔE	ΔCP	$\Delta(E+E^{ABC})$	$\Delta(E+0.5CP+E^{ABC})$
2a	−31.2	1.5	−29.4	−28.7
2b	−20.3	1.1	−19.1	−18.5
3a	−28.5	3.4	−26.6	−24.9
3b	−22.8	2.7	−22.1	−20.7
4a	−36.1	2.2	−32.9	−31.8
4b	−37.5	2.3	−34.0	−32.9
5a	−37.0	2.3	−35.9	−34.8
5b	−25.0	1.7	−24.0	−23.1
6a	−86.6	1.2	−84.4	−83.8
6b	−82.3	1.0	−80.4	−79.9
7a	−139.2	3.1	−134.6	−133.1
7b	−33.1	2.2	−29.8	−28.7

Table S26: PBE-XDM6/TZV: uncorrected interaction energies (ΔE), CP correction (ΔCP), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$), and three body energy and CP corrected interaction energies ($\Delta(E+0.5CP+E^{ABC})$). Note that half the CP correction was used to obtain these values. All energies in kcal/mol.

	ΔE	ΔCP	$\Delta(E+E^{ABC})$	$\Delta(E+0.5CP+E^{ABC})$
2a	−24.8	—	−23.1	−22.0
2b	−15.7	—	−14.5	−13.8
3a	−23.7	—	−21.9	−18.7
3b	−22.1	—	−21.4	−18.8
4a	−29.1	—	−25.9	−24.7
4b	−29.0	—	−25.5	−24.2
5a	−36.6	—	−35.6	−33.4
5b	−24.2	—	−23.2	−21.5
6a	−89.8	—	−87.6	−86.1
6b	−86.3	—	−84.4	−83.2
7a	−139.9	—	−135.3	−131.7
7b	−26.6	—	−23.3	−21.0

Table S27: PBE-XDM10/TZV: uncorrected interaction energies (ΔE), CP correction (ΔCP), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$), and three body energy and CP corrected interaction energies ($\Delta(E+0.5CP+E^{ABC})$). Note that half the CP correction was used to obtain these values. All energies in kcal/mol. CP correction energies are omitted because the PBE/def2-TZVP correction was substituted.

	ΔE	ΔCP	$\Delta(E+E^{ABC})$	$\Delta(E+0.5CP+E^{ABC})$
2a	−25.8	—	−24.0	−23.0
2b	−16.5	—	−15.3	−14.6
3a	−24.1	—	−22.3	−19.2
3b	−22.0	—	−21.3	−18.8
4a	−31.7	—	−28.6	−27.4
4b	−32.2	—	−28.8	−27.5
5a	−35.5	—	−34.4	−32.2
5b	−23.6	—	−22.6	−20.9
6a	−90.4	—	−88.2	−86.6
6b	−86.7	—	−84.9	−83.6
7a	−140.5	—	−135.9	−132.3
7b	−28.1	—	−24.8	−22.5

Table S28: PBE-XDM6/cc-pVTZ(seg-opt): uncorrected interaction energies (ΔE), CP correction (ΔCP), three body energy corrected interaction energies $\Delta(E+E^{ABC})$, and three body energy and CP corrected interaction energies ($\Delta(E+0.5CP+E^{ABC})$). Note that half the CP correction was used to obtain these values. All energies in kcal/mol. Energies for **7a** are omitted because the basis set is undefined for iron. In the paper, the values of PBE-XDM6/TZV have been substituted. CP correction energies are omitted because the PBE/def2-TZVP correction was substituted.

	ΔE	ΔCP	$\Delta(E+E^{ABC})$	$\Delta(E+0.5CP+E^{ABC})$
2a	−22.6	—	−20.9	−19.8
2b	−14.2	—	−13.0	−12.3
3a	−19.8	—	−18.0	−14.9
3b	−17.1	—	−16.4	−13.9
4a	−20.7	—	−17.5	−16.3
4b	−21.3	—	−17.8	−16.6
5a	−33.3	—	−32.3	−30.1
5b	−21.2	—	−20.2	−18.6
6a	−83.1	—	−80.9	−79.4
6b	−79.7	—	−77.9	−76.6
7a	—	—	—	—
7b	−26.3	—	−23.1	−20.7

Table S29: PBE-XDM10/cc-pVTZ(seg-opt): uncorrected interaction energies (ΔE), CP correction (ΔCP), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$), and three body energy and CP corrected interaction energies ($\Delta(E+0.5CP+E^{ABC})$). Note that half the CP correction was used to obtain these values. All energies in kcal/mol. Energies for **7a** are omitted because the basis set is undefined for iron. In the paper, the values of PBE-XDM10/TZV have been substituted. CP correction energies are omitted because the PBE/def2-TZVP correction was substituted.

	ΔE	ΔCP	$\Delta(E+E^{ABC})$	$\Delta(E+0.5CP+E^{ABC})$
2a	−23.8	—	−22.0	−20.9
2b	−15.1	—	−13.9	−13.2
3a	−20.3	—	−18.5	−15.3
3b	−17.1	—	−16.4	−13.9
4a	−23.6	—	−20.5	−19.3
4b	−24.8	—	−21.3	−20.1
5a	−32.2	—	−31.2	−29.0
5b	−20.7	—	−19.7	−18.1
6a	−83.7	—	−81.4	−79.9
6b	−80.1	—	−78.2	−77.0
7a	—	—	—	—
7b	−27.8	—	−24.6	−22.2

Table S30: VDW3: uncorrected interaction energies (ΔE), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$). Note that VDW3 is defined only together with the D3 dispersion correction. All energies in kcal/mol.

	ΔE	$\Delta(E+E^{ABC})$
2a	−30.4	−28.6
2b	−20.2	−19.0
3a	−32.0	−30.2
4a	−28.9	−25.7
4b	−31.3	−27.8
5a	−43.7	−42.7
5b	−25.3	−24.3
6a	−110.4	−108.2
6b	−107.1	−105.3
7b	−22.7	−19.4

Table S31: PM6: uncorrected interaction energies (ΔE). All energies in kcal/mol.

	ΔE
2a	−9.1
2b	−4.8
3a	−8.9
4a	−1.1
4b	−0.4
5a	−22.7
5b	−14.9
6a	−75.2
6b	−74.8
7b	−4.5

Table S32: PM6-DH2: interaction energies (ΔE), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$). Note that these interaction energies necessarily include the two-body dispersion correction. All energies in kcal/mol.

	ΔE	$\Delta(E+E^{ABC})$
2a	−31.5	−29.7
2b	−21.1	−19.9
3a	−28.8	−27.0
4a	−38.3	−35.1
4b	−40.1	−36.6
5a	−42.3	−41.3
5b	−31.1	−30.1
6a	−92.1	−89.9
6b	−89.6	−87.8
7b	−27.1	−23.8

Table S33: DFTB3-D3: interaction energies (ΔE), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$). All energies in kcal/mol.

	ΔE	$\Delta(E+E^{ABC})$
2a	−30.0	−28.2
2b	−21.0	−19.7
3a	−26.9	−25.1
4a	−40.4	−37.2
4b	−42.5	−39.1
5a	−31.2	−30.2
5b	−23.6	−22.6
6a	−97.1	−94.9
6b	−91.5	−89.6
7b	−31.3	−28.1

Table S34: DFTB3: interaction energies (ΔE), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$). All energies in kcal/mol.

	ΔE	$\Delta(E+E^{ABC})$
2a	−0.2	1.5
2b	0.7	1.9
3a	−2.5	−0.6
4a	3.9	7.1
4b	4.9	8.4
5a	−12.9	−11.9
5b	−6.2	−5.2
6a	−75.6	−73.4
6b	−73.5	−71.6
7b	−0.4	2.9

Table S35: OM2-D3: interaction energies (ΔE), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$). All energies in kcal/mol.

	ΔE	$\Delta(E+E^{ABC})$
2a	−32.3	−30.5
2b	−20.5	−19.2
3a	−27.2	−25.3
4a	−32.7	−29.5
4b	−33.7	−30.2
5a	−36.5	−35.5
5b	−26.7	−25.7
6a	−95.0	−92.8
6b	−91.2	−89.4
7b	−23.8	−20.6

Table S36: OM2: interaction energies (ΔE), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$). All energies in kcal/mol.

	ΔE	$\Delta(E+E^{ABC})$
2a	−8.1	−6.3
2b	−2.9	−1.7
3a	−7.2	−5.4
4a	1.9	5.0
4b	3.3	6.8
5a	−20.7	−19.7
5b	−12.1	−11.1
6a	−77.5	−75.3
6b	−76.5	−74.7
7b	1.0	4.3

Table S37: OM3-D3: interaction energies (ΔE), three body energy corrected interaction energies ($\Delta(E+E^{ABC})$). All energies in kcal/mol.

	ΔE	$\Delta(E+E^{ABC})$
2a	−32.3	−30.5
2b	−20.6	−19.4
3a	−31.8	−30.0
4a	−36.1	−32.9
4b	−37.3	−33.8
5a	−32.9	−31.9
5b	−24.5	−23.5
6a	−91.2	−89.0
6b	−86.9	−85.0
7b	−24.3	−21.0

Table S38: OM3: interaction energies (ΔE), three body energy corrected interaction energies ($\Delta(E + E^{ABC})$). All energies in kcal/mol.

	ΔE	$\Delta(E + E^{ABC})$
2a	−3.1	−1.3
2b	0.3	1.5
3a	−8.2	−6.4
4a	4.2	7.4
4b	5.7	9.2
5a	−13.7	−12.7
5b	−7.0	−6.0
6a	−71.1	−68.9
6b	−70.0	−68.1
7b	4.0	7.2

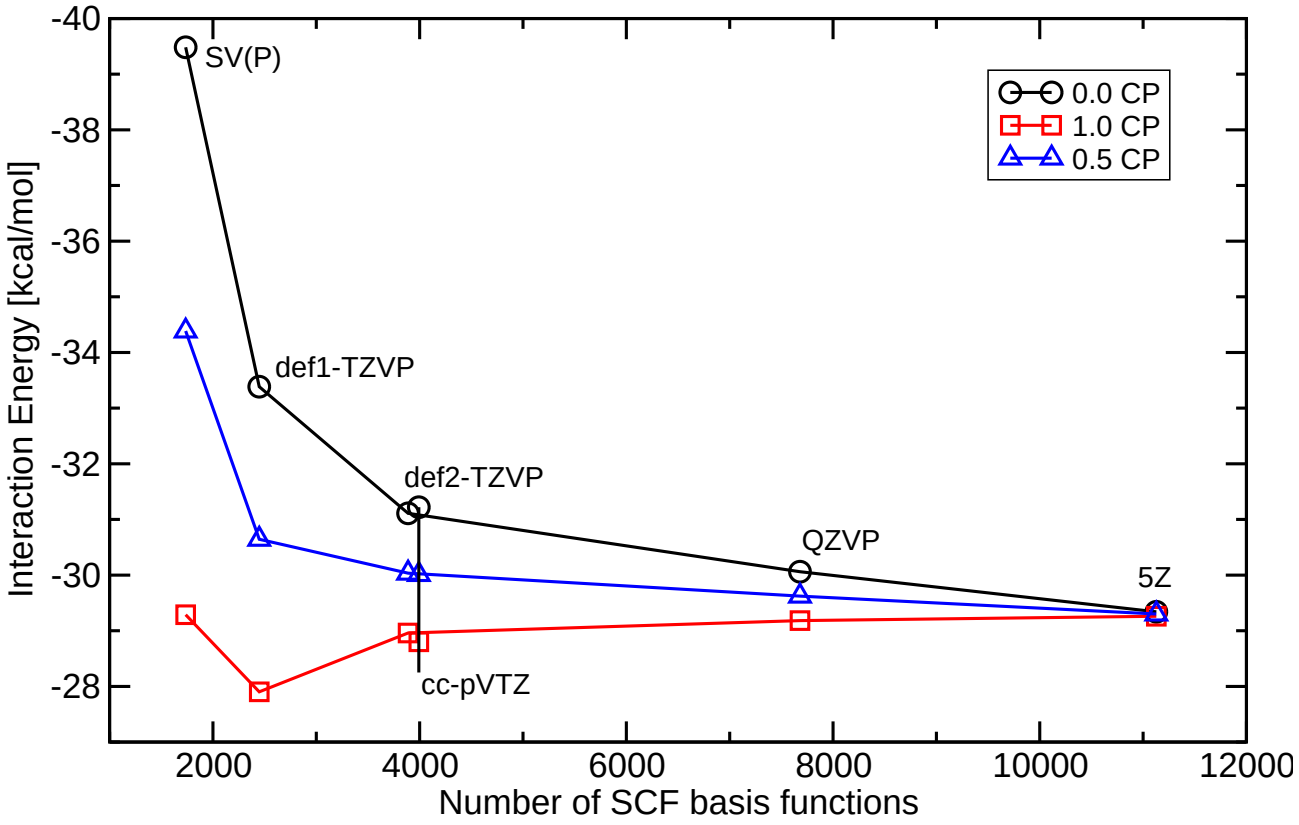

Figure S1: Interaction energies of **4a** calculated with different basis sets using the PBE-D3 functional. The connecting lines are drawn merely to guide the eye.

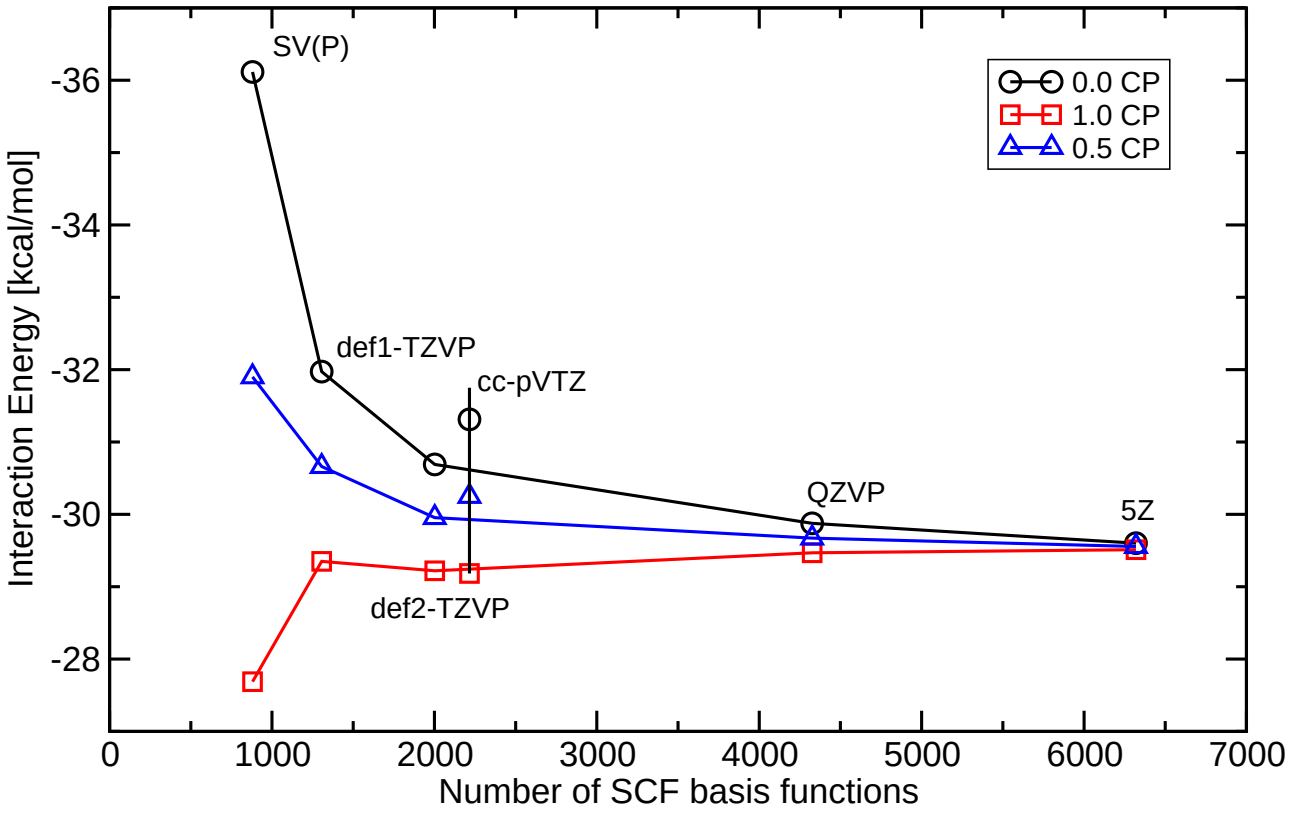

Figure S2: Interaction energies of **2a** calculated with different basis sets using the PBE-D3 functional. The connecting lines are drawn merely to guide the eye.

Table S39: The following tables contain all energies necessary for the MP2/CBS and related methods used in the paper. In the first line, the complex and the basis sets are indicated. The second line contains the column headings indicating Hartree–Fock energies (SCF), opposite spin MP2 contributions (OS) and same spin MP2 contributions (SS). All following lines correspond to a molecular structure and basis. Host, Guest and Complex are the indicated entities in their respective, relaxed structures (TPSS/def2-TZVP geometries from Grimme, S. *Chem.–Eur. J.*, **2012**, *18*, 9955–9964) and full basis. Hhg and Ghg are Host and Guest in the Complex structure and the full Complex basis, i.e. with ghost basis functions. Hh and Gg are Host and Guest in the Complex structure and the respective plain basis, i.e. without ghost basis functions.

2a	cc-pVDZ			cc-pVTZ		
	SCF	OS	SS	SCF	OS	SS
Host	-1608.01743574559	-4.0114092652	-1.5283758488	-1608.37664368020	-4.9228051690	-1.7560881599
Guest	-674.50632058106	-1.5501323124	-0.5885637724	-674.66427828206	-1.9048915650	-0.6798380907
Complex	-2282.51288830689	-5.6039853446	-2.1580561309	-2283.02285317821	-6.8783475814	-2.4831802381
Hhg	-1608.01786708814	-4.0186192214	-1.5311757401	-1608.37349590305	-4.9275468577	-1.7569658020
Ghg	-674.51065503072	-1.5544618900	-0.5909632660	-674.66576066235	-1.9084337619	-0.6813217257
Hh	-1608.01282098807	-4.0119293862	-1.5279842014	-1608.37190741707	-4.9229512493	-1.7555044995
Gg	-674.50577768430	-1.5496568009	-0.5887640333	-674.66414258689	-1.9047125545	-0.6801360769

2b	cc-pVDZ			cc-pVTZ		
	SCF	OS	SS	SCF	OS	SS
Host	-1608.01743574559	-4.0114092652	-1.5283758488	-1608.37664368020	-4.9228051690	-1.7560881599
Guest	-414.19622407585	-0.9602471175	-0.3625473202	-414.29425192803	-1.1825863636	-0.4185969159
Complex	-2022.20005058509	-5.0038173372	-1.9205219457	-2022.65279630493	-6.1435530883	-2.2088611424
Hhg	-1608.01907042576	-4.0167708597	-1.5304947090	-1608.37559374925	-4.9261016316	-1.7565905834
Ghg	-414.19864861214	-0.9623152899	-0.3635579129	-414.29552387799	-1.1846458236	-0.4192763181
Hh	-1608.01513297813	-4.0113923618	-1.5278936682	-1608.37430898553	-4.9225045681	-1.7554343441
Gg	-414.19633765140	-0.9597283522	-0.3624937129	-414.29464643725	-1.1822631309	-0.4185992821

3a	cc-pVDZ			cc-pVTZ		
	SCF	OS	SS	SCF	OS	SS
Host	-2622.39637367681	-5.9486335555	-2.2312921756	-2623.06758529976	-7.4274881662	-2.6258555799
Guest	-1182.29645812768	-2.4989199699	-0.9912833096	-1182.60953543426	-3.1174206304	-1.1624655619
Complex	-3804.68522516129	-8.4870616136	-3.2581009823	-3805.65928359807	-10.5920898886	-3.8297729191
Hhg	-2622.41401580901	-5.9349314503	-2.2165241284	-2623.08474249123	-7.4089303600	-2.6065790337
Ghg	-1182.30670754442	-2.5063035621	-0.9954457357	-1182.61191531269	-3.1236160656	-1.1651943789
Hh	-2622.40525389230	-5.9279542438	-2.2131953207	-2623.08086179135	-7.4024995905	-2.6043963243
Gg	-1182.29428292825	-2.4978895232	-0.9914329624	-1182.60727080549	-3.1168018655	-1.1628228829

3b	cc-pVDZ			cc-pVTZ		
	SCF	OS	SS	SCF	OS	SS
Host	-2622.39637367681	-5.9486335555	-2.2312921756	-2623.06758529976	-7.4274881662	-2.6258555799
Guest	-1075.58308164849	-1.4235080930	-0.5638738427	-1075.76374581653	-1.7859818797	-0.6645070536
Complex	-3697.98777352125	-7.3929602836	-2.8143009071	-3698.83380526077	-9.2386226053	-3.3131407326
Hhg	-2622.40958316689	-5.9340047508	-2.2167257573	-2623.08199050902	-7.4083031067	-2.6072810427
Ghg	-1075.59208138761	-1.4300580085	-0.5670976045	-1075.76666384163	-1.7912807396	-0.6665424333
Hh	-2622.40395482647	-5.9295382314	-2.2146188987	-2623.07927679892	-7.4041920945	-2.6058976452
Gg	-1075.58213155889	-1.4236077692	-0.5639861205	-1075.76292696173	-1.7862333984	-0.6646760442

4a	cc-pVDZ			cc-pVTZ		
	SCF	OS	SS	SCF	OS	SS
Host	-2288.63263262272	-5.5363208023	-2.2034210724	-2289.13706212382	-6.8005279641	-2.5277202921
Guest	-2271.95917483636	-5.3701761425	-2.3568475260	-2272.41217324227	-6.5562036682	-2.6847080541
Complex	-4560.55317083219	-10.9972845857	-4.6398589370	-4561.49658072619	-13.4597519567	-5.3007537610
Hhg	-2288.63919279774	-5.5453012156	-2.2075970146	-2289.13790094218	-6.8083297039	-2.5299196962
Ghg	-2271.96651286932	-5.3775042795	-2.3604902388	-2272.41418287543	-6.5627046408	-2.6869114645
Hh	-2288.63086226946	-5.5361445967	-2.2032174939	-2289.13545492183	-6.8003274457	-2.5275075770
Gg	-2271.95898633457	-5.3702791792	-2.3569528786	-2272.41197759718	-6.5563098767	-2.6848140208

4b	cc-pVDZ			cc-pVTZ		
	SCF	OS	SS	SCF	OS	SS
Host	-2288.63263262272	-5.5363208023	-2.2034210724	-2289.13706212382	-6.8005279641	-2.5277202921
Guest	-2650.71139691731	-6.2685683172	-2.7647215413	-2651.24182543570	-7.6540182705	-3.1483266446
Complex	-4939.29947223389	-11.9019240040	-5.0531146912	-4940.32066452417	-14.5646509761	-5.7704341802
Hhg	-2288.63592679626	-5.5462273103	-2.2081743431	-2289.13524835546	-6.8091515115	-2.5304772069
Ghg	-2650.71915728186	-6.2762699525	-2.7683554672	-2651.24409341631	-7.6609412461	-3.1504336168
Hh	-2288.62803734865	-5.5365583328	-2.2035940555	-2289.13272973419	-6.8007823628	-2.5279244731
Gg	-2650.71146776794	-6.2684717937	-2.7645366044	-2651.24187974206	-7.6538963752	-3.1481288413

5a	cc-pVDZ			cc-pVTZ		
	SCF	SS	OS	SCF	OS	SS
Host	-2858.96035135028	-6.9553834472	-2.5584754277	-2859.65429284572	-8.6076387258	-2.9787410796
Guest	-413.65083702752	-0.8881172924	-0.3233582298	-413.76730412161	-1.1193418203	-0.3851680071
Complex	-3272.63516022950	-7.8667652101	-2.9074023451	-3273.43448512670	-9.7555804591	-3.3935251454
Hhg	-2858.95955723297	-6.9587052535	-2.5581372319	-2859.65055589459	-8.6087311967	-2.9767413084
Ghg	-413.65914870577	-0.8953262005	-0.3270911548	-413.76742038189	-1.1242210348	-0.3874004619
Hh	-2858.95551951471	-6.9529903716	-2.5553870103	-2859.64940347603	-8.6050400059	-2.9755399215
Gg	-413.64679016156	-0.8884407505	-0.3238236636	-413.76361060238	-1.1200540116	-0.3858004338

5b	cc-pVDZ			cc-pVTZ		
	SCF	SS	OS	SCF	OS	SS
Host	-2858.96035135028	-6.9553834472	-2.5584754277	-2859.65429284572	-8.6076387258	-2.9787410796
Guest	-379.26106086638	-0.8201013001	-0.2985449838	-379.36123598374	-1.0246269277	-0.3515959402
Complex	-3238.22783231938	-7.7976434621	-2.8804945869	-3239.01325880917	-9.6593665312	-3.3576207077
Hhg	-2858.95949859775	-6.9573147859	-2.5576491719	-2859.65127567136	-8.6077569460	-2.9765557462
Ghg	-379.26777234082	-0.8265775995	-0.3017860083	-379.36185569928	-1.0292445315	-0.3536180310
Hh	-2858.95608236418	-6.9526276815	-2.5554218331	-2859.65028554689	-8.6047692527	-2.9755529610
Gg	-379.25847887696	-0.8211854292	-0.2992285588	-379.35882439174	-1.0258866880	-0.3523451437

6a	cc-pVDZ			cc-pVTZ		
	SCF	OS	SS	SCF	SS	OS
Host	-3589.97775765243	-7.7581098390	-2.9850810243	-3590.88541772189	-9.7305026081	-3.5320848914
Guest	-212.71023754994	-0.5809361244	-0.1706378426	-212.77182915658	-0.7181549368	-0.2011056807
Complex	-3802.80011665045	-8.3558007991	-3.1749510240	-3803.75721966215	-10.4707498430	-3.7563125203
Hhg	-3589.98111599377	-7.7662689833	-2.9893977119	-3590.88051314765	-9.7363334377	-3.5346186507
Ghg	-212.71051399975	-0.5824414328	-0.1714035767	-212.77147355276	-0.7193579320	-0.2015928717
Hh	-3589.96928974161	-7.7582306520	-2.9854265788	-3590.87719496159	-9.7314055405	-3.5327671492
Gg	-212.70963937044	-0.5809890410	-0.1708196628	-212.77111263014	-0.7182359667	-0.2013304697

6b	cc-pVDZ			cc-pVTZ		
	SCF	OS	SS	SCF	SS	OS
Host	-3589.97775765243	-7.7581098390	-2.9850810243	-3590.88541772189	-9.7305026081	-3.5320848914
Guest	-173.67178330716	-0.4713115466	-0.1370534968	-173.72307649052	-0.5832059102	-0.1617632163
Complex	-3763.76067475963	-8.2422977704	-3.1376669826	-3764.70922250548	-10.3315170185	-3.7128820282
Hhg	-3589.97722759012	-7.7654829585	-2.9889789287	-3590.87833884272	-9.7360756032	-3.5346027143
Ghg	-173.67186238438	-0.4725677557	-0.1376833674	-173.72259806497	-0.5842213006	-0.1621835398
Hh	-3589.96796569531	-7.7589020769	-2.9857495613	-3590.87563147103	-9.7320469440	-3.5330989917
Gg	-173.67112107485	-0.4714292655	-0.1372352765	-173.72228666301	-0.5833313223	-0.1619817123

7a	cc-pVDZ			cc-pVTZ		
	SCF	OS	SS	SCF	SS	OS
Host	-4188.31425407386	-9.0476895179	-3.4810573765	-4189.37481907332	-11.3481618900	-4.1186977596
Guest	-2069.84536001717	-2.4915997522	-0.9377232052	-2070.05567252730	-3.0849422335	-1.0977671807
Complex	-6258.31719377290	-11.6029741536	-4.4756905233	-6259.56260814882	-14.4988542595	-5.2763114697
Hhg	-4188.32740600986	-9.0711411541	-3.4922128624	-4189.36948954322	-11.3624686904	-4.1240741434
Ghg	-2069.83863393214	-2.5063427151	-0.9476870795	-2070.04787020050	-3.0969963268	-1.1058786527
Hh	-4188.30200091202	-9.0506065365	-3.4821298616	-4189.36279250859	-11.3518240538	-4.1200343803
Gg	-2069.83630563870	-2.4990071159	-0.9443778474	-2070.04702200630	-3.0924313909	-1.1045331831

7b	cc-pVDZ			cc-pVTZ		
	SCF	OS	SS	SCF	SS	OS
Host	-4188.31425407386	-9.0476895179	-3.4810573765	-4189.37481907332	-11.3481618900	-4.1186977596
Guest	-462.91824006608	-1.1879747981	-0.4003282713	-463.03674048731	-1.4703495290	-0.4694020585
Complex	-4651.23204505203	-10.2718081282	-3.9132977480	-4652.40085881518	-12.8578223257	-4.6230846307
Hhg	-4188.32792212894	-9.0570829100	-3.4862627785	-4189.37951372420	-11.3539067477	-4.1212127791
Ghg	-462.92032250289	-1.1902334126	-0.4015075944	-463.03793350378	-1.4723990431	-0.4701003040
Hh	-4188.31412073527	-9.0468472028	-3.4811043227	-4189.37486593438	-11.3475834317	-4.1188589358
Gg	-462.91825377156	-1.1875120699	-0.4002840574	-463.03695379236	-1.4699844241	-0.4693963982

The following is a listing of the D3(BJ) parameters for DFTB3, OM2, and OM3, as published in Grimme, S. *Angew. Chem. Int. Ed.*, (2013) submitted.

	DFTB3	OM2	OM3
a_1	0.746	0.690	0.613
a_2	4.191	3.446	3.258
s_6	1.000	1.000	1.000
s_8	3.209	0.531	0.501

The parameter file of the `dftd3` program by the Grimme group for DFTB3 may read:

```
1.0 0.746 3.209 4.191 0.0 4
```

The following is a listing of the 5Z basis in the Turbomole format, constructed from partial decontraction of the def2-QZVP basis set and some of the polarization functions of cc-pV5Z.

```
$basis
*
h 5Z
*
   3  s
  190.69169000      0.70815167000E-03
  28.605532000      0.54678827000E-02
  6.5095943000      0.27966605000E-01
   1  s
  1.8412455000      0.10764538000
   1  s
 0.59853725000       1.0000000000
   1  s
 0.21397624000       1.0000000000
   1  s
 0.80316286000E-01   1.0000000000
   1  p
  4.5160000000       1.0000000000
   1  p
  1.7120000000       1.0000000000
   1  p
 0.64900000000       1.0000000000
   1  p
 0.24600000000       1.0000000000
   1  d
  2.9500000000       1.0000000000
   1  d
  1.2060000000       1.0000000000
   1  d
 0.49300000000       1.0000000000
   1  f
  2.5060000000       1.0000000000
   1  f
 0.87500000000       1.0000000000
*
c 5Z
*
   8  s
  67025.071029      0.38736308501E-04
  10039.986538      0.30107917575E-03
  2284.9316911      0.15787918095E-02
  647.14122130      0.66087087195E-02
  211.09472335      0.23367123250E-01
  76.177643862      0.70420716898E-01
  29.633839163      0.17360344953
  12.187785081      0.32292305648
   1  s
  53.026006299      0.74897404492E-01
   1  s
```

```
  15.258502776       0.76136220983
   1  s
  5.2403957464        1.0000000000
   1  s
  2.2905022379        1.0000000000
   1  s
 0.69673283006        1.0000000000
   1  s
 0.27599337363        1.0000000000
   1  s
 0.10739884389        1.0000000000
   4  p
  105.12555082       0.84647553844E-03
  24.884461066       0.66274038534E-02
  7.8637230826       0.30120390419E-01
  2.8407001835       0.99951435476E-01
   1  p
  1.1227137335       0.23826299282
   1  p
 0.46050725555        1.0000000000
   1  p
 0.18937530913        1.0000000000
   1  p
 0.75983791611E-01    1.0000000000
   1  d
  3.1340000000        1.0000000000
   1  d
  1.2330000000        1.0000000000
   1  d
 0.48500000000        1.0000000000
   1  d
 0.19100000000        1.0000000000
   1  f
  2.0060000000        1.0000000000
   1  f
 0.83800000000        1.0000000000
   1  f
 0.35000000000        1.0000000000
   1  g
  1.7530000000        1.0000000000
   1  g
 0.67800000000        1.0000000000
*
n 5Z
*
   8  s
  90726.889210       0.39257887368E-04
  13590.528801       0.30513316455E-03
  3092.9883781       0.16000560446E-02
  875.99876362       0.66982937306E-02
  285.74469982       0.23690078765E-01
  103.11913417       0.71455405268E-01
  40.128556777       0.17632774876
  16.528095704       0.32677592815
   1  s
  69.390960983       0.80052094386E-01
   1  s
  20.428200596       0.78268063538
   1  s
  7.1292587972        1.0000000000
   1  s
  3.1324304893        1.0000000000
   1  s
```

```
 0.98755778723       1.0000000000
   1  s
 0.38765721307       1.0000000000
   1  s
 0.14909883075       1.0000000000
   4  p
  150.05742670     -0.86216165986E-03
  35.491599483     -0.68571273236E-02
  11.247864223     -0.31795688855E-01
  4.0900305195     -0.10537396822
   1  p
  1.6220573146     -0.24519708041
   1  p
 0.66442261530       1.0000000000
   1  p
 0.27099770070       1.0000000000
   1  p
 0.10688749984       1.0000000000
   1  d
  4.6470000000       1.0000000000
   1  d
  1.8130000000       1.0000000000
   1  d
 0.70700000000       1.0000000000
   1  d
 0.27600000000       1.0000000000
   1  f
  2.9420000000       1.0000000000
   1  f
  1.2040000000       1.0000000000
   1  f
 0.49300000000       1.0000000000
   1  g
  2.5110000000       1.0000000000
   1  g
 0.94200000000       1.0000000000
*
o 5Z
*
   8  s
  116506.46908      0.40383857939E-04
  17504.349724      0.31255139004E-03
  3993.4513230      0.16341473495E-02
  1133.0063186      0.68283224757E-02
  369.99569594      0.24124410221E-01
  133.62074349      0.72730206154E-01
  52.035643649      0.17934429892
  21.461939313      0.33059588895
   1  s
  89.835051252      0.96468652996E-01
   1  s
  26.428010844      0.94117481120
   1  s
  9.2822824649       1.0000000000
   1  s
  4.0947728533       1.0000000000
   1  s
  1.3255349078       1.0000000000
   1  s
 0.51877230787       1.0000000000
   1  s
 0.19772676454       1.0000000000
   4  p
```

```
  191.15255810       0.25115697705E-02
  45.233356739       0.20039240864E-01
  14.353465922       0.93609064762E-01
  5.2422371832       0.30618127124
    1   p
  2.0792418599       0.67810501439
    1   p
 0.84282371424        1.0000000000
    1   p
 0.33617694891        1.0000000000
    1   p
 0.12863997974        1.0000000000
    1   d
  5.8790000000        1.0000000000
    1   d
  2.3070000000        1.0000000000
    1   d
 0.90500000000        1.0000000000
    1   d
 0.35500000000        1.0000000000
    1   f
  4.0160000000        1.0000000000
    1   f
  1.5540000000        1.0000000000
    1   f
 0.60100000000        1.0000000000
    1   g
  3.3500000000        1.0000000000
    1   g
  1.1890000000        1.0000000000
*
$end
```