

A Thorough Benchmark of Density Functional  
Methods for General Main Group Thermochemistry,  
Kinetics, and Noncovalent Interactions

**Supporting Information**

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This Supporting Information contains:

- The formula for calculating the weighted total mean absolute deviation (WTMAD)
- Parameters for the DFT-D3(BJ) correction with corresponding reference (Table S1)
- Information about the best functionals for each subset of GMTKN30 (Table S2)
- Results for GMTKN30 with (aug-)def2-QZVP (Tables S3-S49)
- WTMADs for various basis sets and functionals (Table S50)
- Results for GMTKN30 for HF and the MP2 methods (Tables S51-S55)

**Table S1** – Parameters for the DFT-D3(BJ) correction with corresponding reference.

functional	$s_6$	$a_1$	$s_8$	$a_2$	Ref.
B97-D3	1.0	0.5545	2.2609	3.2297	<sup>a</sup>
BP86	1.0	0.3946	3.2822	4.8516	<sup>a</sup>
BOP	1.0	0.4870	3.2950	3.5043	this work
BLYP	1.0	0.4298	2.6996	4.2359	<sup>a</sup>
mPWLYP	1.0	0.4831	2.0077	4.5323	this work
OLYP	1.0	0.5299	2.6205	2.8065	this work
PBE	1.0	0.4289	0.7875	4.4407	<sup>a</sup>
PBEsol	1.0	0.4466	2.9491	6.1742	this work
revPBE	1.0	0.5238	2.3550	3.5016	<sup>a</sup>
BPBE	1.0	0.4567	4.0728	4.3908	this work
OPBE	1.0	0.5512	3.3816	2.9444	this work
rPW86PBE	1.0	0.4613	1.3845	4.5062	<sup>a</sup>
SSB	1.0	-0.0952	-0.1744	5.2170	this work
revSSB	1.0	0.4720	0.4389	4.0986	this work
TPSS	1.0	0.4535	1.9435	4.4752	<sup>a</sup>
oTPSS	1.0	0.4634	2.7495	4.3153	this work
B3LYP	1.0	0.3981	1.9889	4.4211	<sup>a</sup>
B3PW91	1.0	0.4312	2.8524	4.4693	this work
BHLYP	1.0	0.2793	1.0354	4.9615	this work
PBE0	1.0	0.4145	1.2177	4.8593	<sup>a</sup>
revPBE0	1.0	0.4679	1.7588	3.7619	this work
PBE38	1.0	0.3995	1.4623	5.1405	this work
revPBE38	1.0	0.4309	1.4760	3.9446	this work
TPSSh	1.0	0.00	0.4243	5.5253	this work
TPSS0	1.0	0.3768	1.2576	4.5865	<sup>a</sup>
PW6B95	1.0	0.2076	0.7257	6.3750	<sup>a</sup>
MPW1B95	1.0	0.1955	1.0508	6.4177	this work
PWB6K	1.0	0.1805	0.9383	7.7627	this work
MPWB1K	1.0	0.1474	0.9499	6.6223	this work
B1B95	1.0	0.2092	1.4507	5.5545	this work
BMK	1.0	0.1940	2.0860	5.9197	this work
CAM-B3LYP	1.0	0.3708	2.0674	5.4743	this work
LC- $\omega$ PBE	1.0	0.3919	1.8541	5.0897	this work
B2PLYP	0.64	0.3065	0.9147	5.0570	this work
B2GPPLYP	0.56	0.00	0.2597	6.3332	this work
PWPB95	0.82	0.00	0.2904	7.3141	this work
DSD-BLYP	0.50	0.00	0.2130	6.0519	this work

<sup>a</sup>*J. Comput. Chem.* 2011, in press.

**Table S2** – Best method on each rung of Jacob’s ladder and of all density functionals for all 30 subsets of GMTKN30.

set	GGA	meta-GGA	conventional hybrid	all hybrids	DHDF	best of all
MB08-165	rPW86PBE-D3	oTPSS-D3	PW6B95-D3	PW6B95-D3	PWPB95-D3	PWPB95-D3
W4-08	B97-D3	oTPSS-D3	PW6B95-D3	M062X-D3 PW6B95-D3	PWPB95-D3	PWPB95-D3
G21IP	B97-D3 <sup>a</sup>	TPSS-D3	PW6B95-D3 MPW1B95-D3	M062X-D3	XYG3	XYG3
G21EA	B97-D3	TPSS-D3	PW6B95-D3	PW6B95-D3	XYG3	XYG3 PW6B95-D3
PA	PBEsol-D3 <sup>a</sup>	oTPSS-D3	MPW1B95-D3	M062X-D3	DSD-BLYP-D3	M062X-D3
SIE11	OPBE-D3 revPBE-D3	M06L-D3	PWB6K-D3 revPBE38-D3 BHLYP-D3	M062X-D3	DSD-BLYP-D3 XYG3	DSD-BLYP-D3 XYG3
BHPERI	B97-D3	oTPSS-D3	B3PW91-D3 TPSS0-D3	B3PW91-D3 BHLYP-D3	DSD-BLYP-D3	DSD-BLYP-D3
BH76	OPBE-D3	M06L-D3	PWB6K-D3	M062X-D3	XYG3	XYG3
BH76RC	OLYP-D3 <sup>a</sup>	oTPSS-D3 M06L-D3	PW6B95-D3	M062X-D3	DSD-BLYP-D3	DSD-BLYP-D3
RSE43	OPBE-D3	oTPSS-D3 TPSS-D3	BHLYP-D3 revPBE38-D3	BHLYP-D3 revPBE38-D3	XYG3	XYG3 BHLYP-D3 revPBE39-D3
O3ADD6	OPBE-D3	M06L-D3	B3LYP-D3	M05-D3	PWPB95-D3 B2GPPLYP-D3	M05-D3
G2RC	rPW86PBE-D3	oTPSS-D3	B3LYP-D3	M062X-D3 B3LYP-D3	B2PLYP-D3	B2PLYP-D3
AL2X	BP86-D3	M06L-D3	PW6B95-D3	PW6B95-D3	XYG3	XYG3
NBPRC	BPBE-D3 <sup>a</sup>	TPSS-D3	B3PW91-D3	M062X-D3	DSD-BLYP-D3 XYG3	DSD-BLYP-D3 XYG3
ISO34	BP86-D3 <sup>a</sup>	oTPSS-D3	PW6B95-D3 B3PW91-D3 BMK-D3	CAM-B3LYP-D3	PWPB95-D3	PWPB95-D3
ISOL22	OPBE-D3 <sup>a</sup>	oTPSS-D3	revPBE38-D3	revPBE38-D3	PWPB95-D3	revPBE38-D3
DC9	BP86-D3 <sup>a</sup>	TPSS-D3	B3PW91-D3	$\omega$ B97X-D	DSD-BLYP-D3	DSD-BLYP-D3
DARC	BPBE-D3 <sup>a</sup> SSB-D3 <sup>a</sup>	TPSS-D3	B1B95-D3	M052X-D3	PWPB95-D3	M052X-D3
ALK6	BP86-D3 <sup>a</sup>	TPSS-D3	revPBE38-D3	M062X-D3	DSD-BLYP-D3	DSD-BLYP-D3 M062X-D3
BSR36	PBEsol-D3 <sup>a</sup>	oTPSS-D3	BMK-D3	M052X-D3 M06-D3	DSD-BLYP-D3	DSD-BLYP-D3
IDISP	PBEsol-D3	TPSS-D3	MPWB1K-D3	M052X-D3	PWPB95-D3	PBEsol-D3
WATER27	BPBE-D3	M06L-D3	PW6B95-D3	$\omega$ B97X-D	XYG3	$\omega$ B97X-D
S22	BLYP-D3 <sup>a</sup>	oTPSS-D3	MPW1B95-D3	$\omega$ B97X-D	B2PLYP-D3	$\omega$ B97X-D
ADIM6	OLYP-D3 <sup>a</sup>	oTPSS-D3	PBE38-D3	PBE38-D3 LC- $\omega$ PBE-D3	B2PLYP-D3	B2PLYP-D3
RG6	PBEsol-D3 <sup>a</sup>	TPSS-D3	PW6B95-D3 PBE0-D3 revPBE0-D3 revPBE38-D3	PW6B95-D3 PBE0-D3 revPBE0-D3 revPBE38-D3	PWPB95-D3 B2GPPLYP-D3	PBEsol-D3
HEAVY28	revPBE-D3 <sup>a</sup>	TPSS-D3	PW6B95-D3 MPW1B95-D3	PW6B95-D3 MPW1B95-D3 LC- $\omega$ PBE-D3	B2PLYP-D3 B2GPPLYP-D3	B2PLYP-D3 B2GPPLYP-D3
PCONF	BLYP-D3 <sup>a</sup>	TPSS-D3	B3LYP-D3 BHLYP-D3	M052X-D3	B2GPPLYP-D3	B2GPPLYP-D3
ACONF	OPBE-D3	TPSS-D3	B3PW91-D3 TPSSh-D3	B3PW91-D3 TPSSh-D3	DSD-BLYP-D3	B3PW91-D3 TPSSh-D3
SCONF	mPWLYP-D3	M06L-D3	MPW1B95-D3	M052X-D3	B2PLYP-D3 B2GPPLYP-D3	M052X-D3
CYCONF	B97-D3 <sup>a</sup>	M06L-D3	B3LYP-D3	M052X-D3	B2GPPLYP-D3	B2GPPLYP-D3

<sup>a</sup> Better than best meta-GGA.

**Table S3** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for SPW92. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD	RMSD
MB08-165	20.3	26.7
W4-08	47.4	54.1
G21IP	5.2	6.2
G21EA	7.5	8.5
PA	4.5	4.9
SIE11	17.9	20.6
BHPERI	11.0	11.7
BH76	15.3	17.5
BH76RC	8.5	11.0
RSE43	5.5	6.2
O3ADD6	12.1	13.9
G2RC	13.0	16.8
AL2X	6.9	7.3
NBPRC	10	11.6
ISO34	2.3	3.1
ISOL	5.1	7.0
DC9	24.3	30.1
DARC	11.7	12.6
ALK6	6.9	9.3
BSR36	1.8	2.2
IDISP	2.4	2.8
WATER27	39.3	53.4
S22	2.20	3.24
ADIM6	1.05	1.09
RG6	0.23	0.23
HEAVY28	1.05	1.22
PCONF	2.16	2.82
ACONF	0.40	0.44
SCONF	2.82	3.11
CYCONF	2.16	2.52

**Table S4** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for SVWN. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD	RMSD
MB08-165	20.3	26.8
W4-08	47.3	53.9
G21IP	5.2	6.3
G21EA	7.5	8.5
PA	4.5	4.9
SIE11	17.9	20.6
BHPERI	11.0	11.7
BH76	15.3	17.5
BH76RC	8.5	11.0
RSE43	5.4	6.1
O3ADD6	12.1	14.0
G2RC	13.1	16.8
AL2X	6.9	7.4
NBPRC	10.0	11.7
ISO34	2.3	3.1
ISOL	5.1	7.1
DC9	24.4	30.1
DARC	11.8	12.7
ALK6	6.9	9.4
BSR36	1.8	2.2
IDISP	2.4	2.8
WATER27	39.3	53.4
S22	2.20	3.25
ADIM6	1.04	1.08
RG6	0.23	0.23
HEAVY28	1.05	1.22
PCONF	2.16	2.83
ACONF	0.40	0.44
SCONF	2.82	3.11
CYCONF	2.17	2.53

**Table S5** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for B97-D3 without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	B97 <sup>a</sup>	B97-D3	B97 <sup>a</sup>	B97-D3
MB08-165	12.8	10.6	16.5	13.8
W4-08	4.0	3.9	6.2	6.1
G21IP	3.5	3.5	4.5	4.5
G21EA	2.4	2.4	3.0	3.0
PA	4.7	5.1	5.5	6.0
SIE11	10.0	11.6	14.5	15.0
BHPERI	6.4	2.2	7.2	2.8
BH76	6.2	7.2	7.1	8.1
BH76RC	3.2	3.0	4.2	4.1
RSE43	3.8	3.1	4.3	3.6
O3ADD6	5.7	6.2	8.2	7.5
G2RC	5.2	4.6	6.4	6.0
AL2X	11.8	6.4	12.3	7.0
NBPRC	7.4	3.9	9.9	5.0
ISO34	2.8	2.1	4.1	3.0
ISOL	12.2	9.1	16.4	12.1
DC9	20.2	15.1	23.3	16.7
DARC	21.9	13.4	22.4	13.7
ALK6	10.7	5.6	12.9	6.5
BSR36	12.8	6.2	14.5	7.5
IDISP	21.5	5.9	24.6	9.5
WATER27	18.1	2.8	28.3	5.1
S22	5.25	0.38	6.43	0.49
ADIM6	6.32	0.41	6.94	0.43
RG6	0.78	0.08	0.86	0.10
HEAVY28	1.47	0.16	1.54	0.19
PCONF	5.41	0.94	5.72	1.03
ACONF	1.30	0.07	1.45	0.07
SCONF	1.61	0.48	1.85	0.65
CYCONF	0.72	0.35	0.79	0.43

<sup>a</sup>The B97-D3 GGA-functional without DFT-D3 correction.

**Table S6** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for BP86 without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	BP86	BP86-D3	BP86	bBP86-D3
MB08-165	9.0	8.8	11.7	11.2
W4-08	11.0	11.2	13.8	14.0
G21IP	4.1	4.1	5.0	5.0
G21EA	6.7	6.7	10.6	10.6
PA	2.4	2.5	3.3	3.4
SIE11	11.6	12.5	15.0	15.5
BHPERI	3.1	4.5	3.7	4.9
BH76	9.2	9.9	10.3	10.9
BH76RC	3.7	3.6	5.2	5.2
RSE43	3.3	2.9	3.9	3.4
O3ADD6	4.6	5.2	5.6	6.5
G2RC	4.8	5.3	6.4	6.8
AL2X	6.2	2.0	6.8	3.2
NBPRC	3.1	1.5	4.3	1.9
ISO34	1.9	1.4	2.7	1.9
ISOL	8.2	5.7	11.2	7.7
DC9	12.3	8.5	14.1	11.1
DARC	10.6	4.7	11.6	5.3
ALK6	4.7	1.8	6.0	2.0
BSR36	9	3.0	10.1	3.8
IDISP	14.2	3.1	16.2	4.4
WATER27	6.9	6.3	11.5	7.7
S22	4.00	0.66	5.06	0.83
ADIM6	5.70	0.78	6.16	0.93
RG6	1.00	0.19	1.05	0.22
HEAVY28	1.34	0.22	1.41	0.28
PCONF	4.64	0.98	4.81	1.06
ACONF	0.77	0.18	0.86	0.22
SCONF	0.37	0.93	0.46	1.34
CYCONF	0.86	0.83	0.95	1.03

**Table S7** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for BOP without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	BOP	BOP-D3	BOP	BOP-D3
MB08-165	15.2	12.2	19.2	15.7
W4-08	5.7	5.7	8.4	8.4
G21IP	4.9	4.9	5.8	5.8
G21EA	2.7	2.7	3.1	3.2
PA	4.0	4.4	5.2	5.6
SIE11	11.2	12.2	15.2	15.6
BHPERI	7.9	2.6	9.0	3.2
BH76	7.1	8.3	8.2	9.2
BH76RC	3.5	3.2	4.4	4.2
RSE43	3.7	2.8	4.2	3.4
O3ADD6	6.7	7.1	9.7	8.8
G2RC	7.1	6.2	8.4	7.5
AL2X	14.0	6.8	14.5	7.4
NBPRC	9.3	4.7	12.1	6.2
ISO34	3.4	2.6	4.8	3.6
ISOL	13.5	9.7	18.2	12.9
DC9	21.9	15.5	26.6	18.7
DARC	26.3	16.3	26.7	16.4
ALK6	11.7	4.6	14.0	5.3
BSR36	14.2	5.5	15.9	6.7
IDISP	24.3	5.8	27.9	9.7
WATER27	24.2	6.0	37.0	9.3
S22	6.67	0.52	7.95	0.68
ADIM6	8.15	0.50	8.86	0.61
RG6	1.32	0.20	1.42	0.22
HEAVY28	2.29	0.29	2.37	0.34
PCONF	5.91	0.55	6.34	0.62
ACONF	1.46	0.09	1.62	0.13
SCONF	1.73	0.58	1.98	0.85
CYCONF	0.80	0.36	0.95	0.50

**Table S8** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for BLYP without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	BLYP	BLYP-D3	BLYP	BLYP-D3
MB08-165	11.1	9.4	14.4	12.3
W4-08	7.0	7.0	10.1	10.1
G21IP	4.7	4.7	5.6	5.6
G21EA	3.3	3.3	3.9	4.0
PA	2.5	2.6	3.4	3.6
SIE11	11.7	12.4	15.6	16
BHPERI	5.8	3.0	6.8	3.6
BH76	8.4	9.1	9.6	10.2
BH76RC	3.3	3.2	4.5	4.4
RSE43	3.5	3.0	4.1	3.5
O3ADD6	6.0	6.8	7.7	7.7
G2RC	5.5	5.2	6.8	6.4
AL2X	11.4	6.3	12.0	6.7
NBPRC	6.9	4.2	9.5	5.8
ISO34	3.2	2.7	4.4	3.7
ISOL	12.6	10.0	17.1	13.2
DC9	20.3	16.6	24.5	19.7
DARC	22.9	16.4	23.3	16.5
ALK6	10.9	6.0	14.3	7.9
BSR36	12.1	5.9	13.8	7.2
IDISP	20.2	7.0	23.7	10.8
WATER27	9.9	3.1	16.0	3.9
S22	4.77	0.24	5.93	0.34
ADIM6	6.04	0.85	6.59	0.94
RG6	0.99	0.08	1.09	0.08
HEAVY28	1.62	0.22	1.71	0.29
PCONF	4.84	0.52	5.15	0.55
ACONF	1.08	0.11	1.20	0.14
SCONF	0.89	0.56	1.08	0.85
CYCONF	0.65	0.43	0.72	0.49

**Table S9** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for mPWLYP without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	mPWLYP	mPWLYP-D3	mPWLYP	mPWLYP-D3
MB08-165	8.9	8.0	11.7	10.6
W4-08	8.8	8.8	12.0	12.1
G21IP	4.4	4.4	5.4	5.4
G21EA	3.6	3.6	4.5	4.5
PA	2.5	2.5	3.1	3.2
SIE11	12.4	12.8	16.2	16.4
BHPERI	4.7	3.2	5.6	3.9
BH76	9.3	9.7	10.5	10.9
BH76RC	3.4	3.3	4.7	4.6
RSE43	3.6	3.3	4.1	3.8
O3ADD6	5.9	6.6	7.1	7.4
G2RC	4.8	4.7	6.1	6.0
AL2X	9.5	6.5	10.1	6.9
NBPRC	5.7	4.2	8.0	5.9
ISO34	3.1	2.8	4.2	3.9
ISOL	12.1	10.5	16.4	14.1
DC9	19.3	17.2	22.9	20.3
DARC	20.7	16.8	21.1	17.1
ALK6	8.9	6.1	12.6	8.5
BSR36	11.4	7.3	13.3	8.9
IDISP	18.0	9.6	21.4	13.0
WATER27	3.0	7.4	4.7	9.7
S22	3.37	0.55	4.50	0.79
ADIM6	4.12	0.35	4.60	0.36
RG6	0.52	0.10	0.60	0.14
HEAVY28	0.88	0.22	1.00	0.28
PCONF	4.20	1.31	4.45	1.38
ACONF	0.88	0.25	0.99	0.30
SCONF	0.67	0.43	0.84	0.62
CYCONF	0.59	0.45	0.63	0.48

**Table S10** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for OLYP without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	OLYP	OLYP-D3	OLYP	OLYP-D3
MB08-165	13.9	11.1	18.0	14.3
W4-08	5.3	5.9	7.9	8.2
G21IP	4.2	4.2	5.2	5.2
G21EA	2.5	2.5	3.0	3.1
PA	4.5	5.3	5.4	6.3
SIE11	10.4	12.4	14.4	15.3
BHPERI	7.7	2.6	8.6	3.4
BH76	5.9	7.8	7.1	8.7
BH76RC	3.2	2.9	4.5	4.5
RSE43	3.6	2.5	4.1	3.1
O3ADD6	5.6	5.0	8.1	5.9
G2RC	4.9	5.6	6.7	7.3
AL2X	13.7	6.0	14.3	7.0
NBPRC	7.7	1.7	9.9	2.1
ISO34	2.5	1.7	4.0	2.3
ISOL	10.2	5.5	13.7	7.4
DC9	15.3	8.8	18.7	10.4
DARC	17.6	3.8	18.3	4.4
ALK6	10.9	1.9	14.7	2.8
BSR36	13.9	5.4	15.7	6.3
IDISP	25.7	4.5	28.3	5.5
WATER27	30.9	7.2	47.1	11.4
S22	7.33	0.71	8.83	0.93
ADIM6	8.52	0.08	9.39	0.09
RG6	1.13	0.12	1.31	0.13
HEAVY28	2.53	0.26	2.66	0.34
PCONF	6.92	1.34	7.45	1.39
ACONF	1.96	0.09	2.17	0.11
SCONF	2.78	0.45	3.19	0.55
CYCONF	0.88	0.41	1.03	0.54

**Table S11** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for PBE without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	PBE	PBE-D3	PBE	PBE-D3
MB08-165	9.0	9.2	11.5	11.6
W4-08	13.0	13.0	16.8	16.8
G21IP	3.9	3.9	4.8	4.8
G21EA	3.4	3.4	4.1	4.1
PA	2.1	2.2	2.8	2.9
SIE11	12.0	12.4	14.9	15.1
BHPERI	2.9	4.2	3.7	4.7
BH76	9.2	9.5	10.5	10.8
BH76RC	4.3	4.4	6.3	6.3
RSE43	3.5	3.3	4.0	3.8
O3ADD6	4.4	5.0	5.7	6.3
G2RC	6.2	6.5	7.7	8.0
AL2X	4.2	2.3	4.7	3.3
NBPRC	2.7	2.3	3.3	2.9
ISO34	1.8	1.6	2.5	2.1
ISOL	6.9	5.6	9.5	7.7
DC9	10.8	10.1	15.1	14.3
DARC	6.8	4.3	7.9	4.8
ALK6	2.8	3.6	4.5	5.4
BSR36	8.2	4.8	9.5	5.8
IDISP	11.8	4.8	13.3	6.1
WATER27	3.2	8.6	4.0	10.9
S22	2.57	0.48	3.58	0.63
ADIM6	3.34	0.58	3.73	0.60
RG6	0.38	0.05	0.43	0.07
HEAVY28	0.50	0.24	0.62	0.32
PCONF	3.94	1.51	4.05	1.64
ACONF	0.61	0.09	0.68	0.13
SCONF	0.36	0.44	0.44	0.70
CYCONF	0.86	0.84	0.97	1.01

**Table S12** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for PBEsol without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	PBEsol	PBEsol-D3	PBEsol	PBEsol-D3
MB08-165	12.8	13.2	17.0	17.6
W4-08	24.6	24.7	29.7	29.7
G21IP	3.7	3.7	4.9	4.9
G21EA	3.3	3.3	3.9	3.9
PA	1.5	1.5	2.1	2.1
SIE11	13.5	13.9	16.4	16.7
BHPERI	6.9	8.2	7.4	8.7
BH76	11.6	11.8	13.2	13.4
BH76RC	6.3	6.3	8.5	8.5
RSE43	4.1	4.0	4.7	4.5
O3ADD6	6.3	7.1	8.3	8.9
G2RC	9.7	9.9	12.1	12.4
AL2X	2.8	4.4	3.5	4.7
NBPRC	5.0	5.9	6.3	7.1
ISO34	2.1	2.0	2.7	2.6
ISOL	4.7	4.0	6.6	5.8
DC9	17.6	17.7	21.8	22.2
DARC	4.4	6.2	6.1	7.3
ALK6	4.2	5.7	6.4	7.8
BSR36	4.2	1.6	5.0	2.3
IDISP	5.4	0.5	6.0	0.6
WATER27	14.3	19.2	17.7	25.2
S22	1.81	1.01	2.50	1.45
ADIM6	2.49	0.31	2.75	0.33
RG6	0.31	0.03	0.35	0.04
HEAVY28	0.40	0.42	0.47	0.57
PCONF	3.59	1.92	3.75	2.33
ACONF	0.23	0.15	0.26	0.17
SCONF	1.34	1.65	1.51	1.87
CYCONF	1.46	1.49	1.81	1.82

**Table S13** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for revPBE without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	revPBE	revPBE-D3	revPBE	revPBE-D3
MB08-165	10.9	10.1	14.5	13.1
W4-08	7.1	7.0	9.6	9.5
G21IP	4.1	4.2	5.1	5.1
G21EA	2.8	2.8	3.3	3.3
PA	3.8	4.1	4.7	5.0
SIE11	10.4	11.5	13.5	14.1
BHPERI	4.2	3.4	4.7	3.9
BH76	7.1	8.0	8.1	9.0
BH76RC	3.1	3.0	4.8	4.8
RSE43	3.1	2.4	3.6	3.0
O3ADD6	5.3	5.8	6.8	6.8
G2RC	4.8	5.3	6.7	7.0
AL2X	8.5	3.4	9.3	4.9
NBPRC	5.0	1.8	6.6	2.3
ISO34	2.2	1.6	3.2	2.2
ISOL	9.1	6.2	12.3	8.2
DC9	14.2	9.6	16.1	11.5
DARC	13.9	6.1	14.7	6.6
ALK6	4.2	2.3	5.1	3.1
BSR36	11.4	4.8	12.9	5.8
IDISP	18.7	4.1	20.9	5.9
WATER27	17.6	3.2	27.6	5.6
S22	5.21	0.41	6.39	0.55
ADIM6	6.26	0.54	6.89	0.57
RG6	0.82	0.05	0.92	0.06
HEAVY28	1.53	0.15	1.61	0.19
PCONF	5.38	0.81	5.66	0.96
ACONF	1.20	0.07	1.34	0.07
SCONF	1.32	0.49	1.55	0.68
CYCONF	0.72	0.50	0.79	0.62

**Table S14** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for OPBE without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	OPBE	OPBE-D3	OPBE	OPBE-D3
MB08-165	13.7	13.1	18.2	17.4
W4-08	7.8	8.1	10.5	10.9
G21IP	4.5	4.6	5.3	5.3
G21EA	3.1	3.1	3.8	3.8
PA	6.6	7.2	7.0	7.8
SIE11	9.7	11.5	12.5	13.7
BHPERI	5.3	6.1	5.7	6.8
BH76	5.2	6.9	6.7	8.1
BH76RC	3.6	3.7	5.8	5.9
RSE43	3.4	2.3	3.9	2.9
O3ADD6	4.3	3.4	5.5	4.3
G2RC	7.4	8.7	9.7	11.5
AL2X	9.0	3.6	10.1	5.6
NBPRC	4.9	4.2	6.6	4.8
ISO34	3.3	2.9	4.7	4.0
ISOL	6.6	3.9	8.9	4.7
DC9	20.2	19.4	24.1	24.7
DARC	6.7	8.0	7.6	8.4
ALK6	4.3	7.3	4.9	9.8
BSR36	12.0	2.7	13.5	3.1
IDISP	22.3	3.6	24.3	4.2
WATER27	35.7	12.8	54.7	20.1
S22	7.73	0.83	9.23	1.08
ADIM6	9.37	0.31	10.26	0.34
RG6	1.27	0.15	1.41	0.19
HEAVY28	2.67	0.33	2.79	0.41
PCONF	7.62	1.46	8.04	2.20
ACONF	1.96	0.06	2.18	0.07
SCONF	2.50	0.52	2.95	0.63
CYCONF	1.01	0.90	1.13	1.15

**Table S15** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for BPBE without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	BPBE	BPBE-D3	BPBE	BPBE-D3
MB08-165	9.7	9.4	12.8	11.9
W4-08	8.7	8.7	11.8	11.8
G21IP	4.0	4.1	4.9	5.0
G21EA	2.7	2.7	3.3	3.3
PA	3.4	3.6	4.2	4.5
SIE11	10.8	11.7	13.8	14.3
BHPERI	3.4	4.3	3.9	4.8
BH76	7.6	8.4	8.8	9.5
BH76RC	3.5	3.5	5.4	5.4
RSE43	3.3	2.7	3.8	3.2
O3ADD6	4.8	5.1	5.5	6.1
G2RC	4.9	5.5	6.6	7.1
AL2X	6.9	2.3	7.6	3.8
NBPRC	3.7	1.3	5.1	1.9
ISO34	2.0	1.5	2.9	1.9
ISOL	8.0	5.0	11.0	6.7
DC9	12.3	8.8	15.0	11.7
DARC	10.9	3.7	11.9	4.3
ALK6	4.0	4.1	4.4	5.2
BSR36	9.9	2.9	11.1	3.5
IDISP	16.4	3.0	18.4	3.8
WATER27	14.9	2.1	23.8	3.3
S22	5.19	0.49	6.34	0.66
ADIM6	7.14	0.50	7.74	0.62
RG6	1.19	0.21	1.27	0.23
HEAVY28	1.80	0.26	1.87	0.30
PCONF	5.46	0.92	5.69	1.05
ACONF	1.03	0.12	1.15	0.16
SCONF	0.53	0.76	0.70	1.20
CYCONF	0.91	0.87	0.99	1.07

**Table S16** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for rPW86PBE without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	rPW86PBE	rPW86PBE-D3	rPW86PBE	rPW86PBE-D3
MB08-165	8.0	7.5	10.7	10.0
W4-08	8.4	8.4	11.4	11.4
G21IP	4.5	4.5	6.1	6.1
G21EA	5.4	5.4	6.3	6.3
PA	2.8	2.9	3.9	4.0
SIE11	11.4	11.8	15.0	15.2
BHPERI	3.5	2.7	4.1	3.2
BH76	8.3	8.7	9.6	9.9
BH76RC	3.3	3.2	5.0	5.0
RSE43	3.1	2.9	3.7	3.4
O3ADD6	6.1	6.8	7.5	7.7
G2RC	4.1	4.2	5.9	5.9
AL2X	6.7	4.1	7.4	4.7
NBPRC	4.3	3.3	6.2	4.4
ISO34	2.6	2.3	3.6	3.2
ISOL	10.7	9.3	14.3	12.3
DC9	18.1	16.1	20.1	18.1
DARC	16.5	13.0	17.1	13.4
ALK6	3.8	2.2	4.4	3.4
BSR36	10.4	6.6	12.1	8.1
IDISP	14.6	6.9	17.6	10.1
WATER27	2.3	7.2	3.8	9.4
S22	2.82	0.35	3.75	0.44
ADIM6	3.53	0.67	3.90	0.72
RG6	0.47	0.04	0.52	0.05
HEAVY28	0.58	0.25	0.68	0.32
PCONF	3.51	0.85	3.66	0.99
ACONF	0.57	0.09	0.65	0.13
SCONF	0.42	0.44	0.54	0.73
CYCONF	0.52	0.44	0.57	0.51

**Table S17** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for SSB-D3 without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	SSB	SSB-D3	SSB	SSB-D3
MB08-165	11.3	11.3	15.2	15.2
W4-08	12.0	12.1	14.9	15.0
G21IP	4.4	4.4	5.1	5.1
G21EA	4.4	4.4	5.0	5.0
PA	5.5	5.6	6.2	6.3
SIE11	11.7	12.0	14.5	14.7
BHPERI	2.8	2.4	3.4	3.3
BH76	6.8	7.0	8.0	8.2
BH76RC	3.6	3.6	5.6	5.6
RSE43	3.3	3.1	3.8	3.6
O3ADD6	3.6	4.2	4.7	4.8
G2RC	8.7	8.9	11	11.3
AL2X	5.4	3.3	6.2	4.6
NBPRC	3.6	3.4	4.2	4.0
ISO34	3.0	2.8	4.1	3.8
ISOL	5.5	4.4	7.1	5.6
DC9	19.8	19.5	25.3	25.3
DARC	4.5	3.7	4.9	5.0
ALK6	4.5	6.1	8.1	9.3
BSR36	9.4	6.1	11.0	7.5
IDISP	12.9	6.2	13.9	7.0
WATER27	8.6	2.2	14.1	3.9
S22	2.98	0.63	3.91	0.84
ADIM6	3.13	0.70	3.52	0.72
RG6	0.32	0.09	0.38	0.11
HEAVY28	0.55	0.21	0.65	0.25
PCONF	3.51	1.17	3.71	1.21
ACONF	0.83	0.33	0.92	0.37
SCONF	1.44	1.07	1.67	1.24
CYCONF	0.54	0.46	0.58	0.52

**Table S18** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for revSSB-D3 without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	revSSB	revSSB-D3	revSSB	revSSB-D3
MB08-165	11.3	11.4	14.8	15.1
W4-08	15.9	16.0	19.6	19.7
G21IP	5.3	5.3	6.2	6.2
G21EA	5.2	5.2	5.9	5.9
PA	5.0	5.1	5.6	5.6
SIE11	12.2	12.5	15.1	15.4
BHPERI	2.5	3.2	3.4	3.9
BH76	7.5	7.7	8.8	9.0
BH76RC	4.3	4.3	6.3	6.4
RSE43	3.5	3.4	4.1	3.9
O3ADD6	3.2	3.6	4.1	4.5
G2RC	9.2	9.5	11.9	12.2
AL2X	4.1	3.0	4.7	3.8
NBPRC	3.8	4.1	4.4	4.7
ISO34	2.9	2.8	4.0	3.7
ISOL	5.3	4.3	6.7	5.4
DC9	21.0	20.7	26.5	26.6
DARC	4.3	4.7	5.5	6.4
ALK6	5.1	6.6	8.8	9.9
BSR36	8.5	5.5	9.9	6.7
IDISP	11.3	5.2	12.2	5.8
WATER27	3.7	3.0	7.0	3.7
S22	2.45	0.49	3.43	0.68
ADIM6	2.91	0.67	3.28	0.68
RG6	0.30	0.07	0.35	0.09
HEAVY28	0.44	0.23	0.55	0.30
PCONF	3.55	1.39	3.68	1.42
ACONF	0.72	0.26	0.80	0.30
SCONF	0.90	0.60	1.11	0.77
CYCONF	0.63	0.62	0.72	0.73

**Table S19** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for TPSS without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	TPSS	TPSS-D3	TPSS	TPSS-D3
MB08-165	10.0	9.5	13.7	12.8
W4-08	5.2	5.3	6.8	7.0
G21IP	4.0	4.0	4.8	4.8
G21EA	2.2	2.2	2.7	2.7
PA	4.6	4.7	5.4	5.5
SIE11	10.7	11.6	14.0	14.4
BHPERI	2.7	3.1	3.1	3.6
BH76	8.6	9.0	9.6	10.0
BH76RC	3.8	3.7	5.0	5.0
RSE43	2.6	2.2	3.1	2.8
O3ADD6	3.7	4.4	5.1	6.1
G2RC	6.4	6.8	8.5	8.7
AL2X	3.9	2.2	4.3	2.9
NBPRC	2.6	1.7	3.6	2.1
ISO34	2.4	2.1	3.3	2.9
ISOL	8.8	7.0	11.6	8.9
DC9	12.3	9.7	14.3	11.8
DARC	11.1	6.6	11.9	7.2
ALK6	2.3	3.3	2.7	4.2
BSR36	10.7	6.2	12.1	7.2
IDISP	13.8	4.5	16.0	6.5
WATER27	5.6	4.9	9.8	5.9
S22	3.45	0.32	4.56	0.45
ADIM6	4.72	0.40	5.21	0.41
RG6	0.59	0.04	0.68	0.05
HEAVY28	0.93	0.20	1.03	0.26
PCONF	4.41	1.10	4.57	1.26
ACONF	0.71	0.05	0.79	0.06
SCONF	0.36	0.68	0.43	1.07
CYCONF	0.83	0.82	0.93	0.99

**Table S20** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for  $\sigma$ TPSS without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	$\sigma$ TPSS	$\sigma$ TPSS-D3	$\sigma$ TPSS	$\sigma$ TPSS-D3
MB08-165	6.5	6.5	8.8	8.5
W4-08	3.2	3.3	4.4	4.4
G21IP	4.5	4.5	5.3	5.3
G21EA	3.0	3.0	3.8	3.8
PA	3.4	3.6	4.4	4.6
SIE11	9.8	10.8	14.6	14.9
BHPERI	4.6	2.1	5.3	2.6
BH76	7.3	7.9	8.1	8.6
BH76RC	3.2	3.1	4.1	4.0
RSE43	2.6	2.2	3.2	2.8
O3ADD6	4.4	4.7	5.1	5.4
G2RC	3.5	3.5	5.2	5.2
AL2X	5.9	2.7	6.4	3.5
NBPRC	4.2	2.3	5.9	3.0
ISO34	2.0	1.6	2.8	2.1
ISOL	9.1	6.8	12.5	9.0
DC9	16.3	12.8	18.7	15.1
DARC	14.4	8.7	14.9	9.0
ALK6	3.1	5.0	4.1	6.4
BSR36	9.2	3.6	10.3	4.1
IDISP	16.8	5.1	19.1	6.9
WATER27	11.4	2.1	18.8	3.0
S22	4.48	0.31	5.73	0.40
ADIM6	5.85	0.37	6.43	0.39
RG6	0.80	0.05	0.92	0.06
HEAVY28	1.43	0.25	1.52	0.31
PCONF	5.29	1.14	5.50	1.29
ACONF	0.97	0.08	1.08	0.08
SCONF	0.55	0.50	0.70	0.78
CYCONF	0.92	0.90	1.02	1.10

**Table S21** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for M06L without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	M06L	M06L-D3	M06L	M06L-D3
MB08-165	13.3	13.2	17.4	17.4
W4-08	4.6	4.6	5.9	5.9
G21IP	4.5	4.5	5.5	5.5
G21EA	4.0	4.0	4.8	4.8
PA	4.6	4.6	5.8	5.8
SIE11	10.1	10.1	13.6	13.6
BHPERI	3.5	3.4	4.0	3.9
BH76	3.8	3.8	4.9	4.9
BH76RC	3.1	3.1	4.3	4.3
RSE43	3.1	3.1	3.7	3.6
O3ADD6	3.4	3.4	4.1	4.1
G2RC	5.9	5.9	7.8	7.8
AL2X	1.4	1.5	1.8	1.8
NBPRC	3.9	3.9	4.8	4.8
ISO34	2.2	2.2	2.8	2.8
ISOL	7.4	7.3	9.4	9.3
DC9	11.5	11.5	15.3	15.3
DARC	8.0	7.8	8.9	8.6
ALK6	8.1	8.2	10.3	10.4
BSR36	6.0	5.5	7.0	6.3
IDISP	6.6	6.4	10.3	9.6
WATER27	2.8	1.9	5.1	3.4
S22	0.80	0.44	0.91	0.52
ADIM6	0.28	1.03	0.33	1.20
RG6	0.43	0.43	0.49	0.48
HEAVY28	0.65	0.61	0.70	0.66
PCONF	0.97	1.17	1.07	1.27
ACONF	0.46	0.50	0.51	0.55
SCONF	0.39	0.40	0.59	0.60
CYCONF	0.40	0.38	0.47	0.45

**Table S22** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for B3LYP without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	B3LYP	B3LYP-D3	B3LYP	B3LYP-D3
MB08-165	8.2	6.4	10.6	8.5
W4-08	4.3	4.2	6.8	6.7
G21IP	3.6	3.6	4.4	4.4
G21EA	1.8	1.8	2.3	2.4
PA	2.3	2.4	3.4	3.6
SIE11	7.6	8.7	10.4	10.8
BHPERI	5.8	2.8	7.1	3.5
BH76	4.7	5.2	5.4	5.9
BH76RC	2.3	2.3	2.9	2.8
RSE43	2.4	2.0	2.9	2.5
O3ADD6	2.0	2.7	2.3	3.6
G2RC	2.6	2.7	3.2	3.2
AL2X	8.5	4.3	9.0	4.5
NBPRC	4.8	3.0	6.8	4.1
ISO34	2.3	1.9	3.3	2.6
ISOL	9.1	7.0	12.4	9.4
DC9	15.1	12.0	18.3	14.2
DARC	15.4	10.2	15.9	10.5
ALK6	9.1	4.7	12.3	6.4
BSR36	11.3	5.9	12.9	7.2
IDISP	17.5	6.6	19.8	8.7
WATER27	6.5	4.2	11.2	5.4
S22	3.77	0.36	4.90	0.44
ADIM6	5.02	0.43	5.50	0.47
RG6	0.81	0.07	0.90	0.09
HEAVY28	1.37	0.16	1.44	0.21
PCONF	3.97	0.34	4.27	0.39
ACONF	0.96	0.14	1.07	0.15
SCONF	1.03	0.45	1.18	0.56
CYCONF	0.45	0.24	0.55	0.31

**Table S23** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for B3PW91 without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	B3PW91	B3PW91-D3	B3PW91	B3PW91-D3
MB08-165	7.1	6.4	9.3	8.2
W4-08	3.2	3.2	4.8	4.7
G21IP	3.6	3.6	4.4	4.4
G21EA	2.2	2.2	2.7	2.7
PA	3.6	3.7	4.3	4.5
SIE11	7.9	9.0	10.2	10.8
BHPERI	3.8	1.4	4.4	2.0
BH76	4.1	4.7	4.7	5.2
BH76RC	2.1	2.2	3.0	3.1
RSE43	2.3	1.8	2.8	2.3
O3ADD6	2.9	3.9	3.2	4.7
G2RC	4.4	4.9	5.5	6.2
AL2X	5.3	1.6	5.8	2.4
NBPRC	2.8	1.6	3.7	1.9
ISO34	1.6	1.2	2.5	1.7
ISOL	5.9	2.6	8.1	3.7
DC9	9.7	6.9	12.3	9.5
DARC	6.9	2.3	7.8	2.6
ALK6	3.2	2.6	4.1	3.5
BSR36	9.7	3.8	10.9	4.4
IDISP	14.7	2.5	16.0	3.2
WATER27	10.6	2.0	17.7	2.3
S22	4.13	0.45	5.22	0.55
ADIM6	5.91	0.41	6.42	0.50
RG6	0.96	0.15	1.03	0.16
HEAVY28	1.50	0.20	1.56	0.22
PCONF	4.43	0.59	4.64	0.69
ACONF	0.93	0.03	1.04	0.05
SCONF	0.73	0.40	0.90	0.65
CYCONF	0.60	0.57	0.66	0.69

**Table S24** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for BHLYP without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	BHLYP	BHLYP-D3	BHLYP	BHLYP-D3
MB08-165	11.7	10.8	16.0	14.9
W4-08	19.3	19.1	24.1	24
G21IP	4.5	4.5	5.5	5.5
G21EA	5.3	5.3	6.2	6.2
PA	3.3	3.4	4.4	4.6
SIE11	5.0	5.3	6.6	7.0
BHPERI	9.3	6.8	10.1	7.3
BH76	2.4	2.3	3.0	2.9
BH76RC	3.9	3.9	4.8	4.8
RSE43	0.9	0.7	1.6	1.4
O3ADD6	5.4	6.2	8.7	9.4
G2RC	4.7	4.9	5.8	6.0
AL2X	6.0	2.7	6.6	2.9
NBPRC	4.3	3.1	5.3	3.7
ISO34	1.7	1.4	2.7	2.1
ISOL	6.0	4.4	7.8	5.5
DC9	10.7	8.2	14.7	11.5
DARC	8.1	4.2	8.7	4.5
ALK6	9.7	6.4	13.0	8.2
BSR36	10.8	6.5	12.4	7.9
IDISP	15.1	6.4	16.6	7.7
WATER27	4.0	4.7	7.5	5.8
S22	2.85	0.66	3.96	0.87
ADIM6	4.02	0.25	4.42	0.27
RG6	0.65	0.04	0.75	0.05
HEAVY28	1.19	0.18	1.26	0.23
PCONF	2.79	0.34	3.20	0.40
ACONF	0.87	0.23	0.97	0.24
SCONF	1.36	0.72	1.51	0.78
CYCONF	0.62	0.47	0.66	0.54

**Table S25** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for PBE0 without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	PBE0	PBE0-D3	PBE0	PBE0-D3
MB08-165	8.6	8.6	11.1	11.1
W4-08	4.0	4.0	6.2	6.1
G21IP	3.7	3.7	4.4	4.4
G21EA	2.5	2.5	2.9	2.9
PA	2.7	2.8	3.5	3.6
SIE11	7.1	7.8	8.3	8.7
BHPERI	2.4	1.6	2.7	2.2
BH76	4.1	4.4	4.6	4.9
BH76RC	2.5	2.5	3.4	3.4
RSE43	2.0	1.8	2.5	2.3
O3ADD6	4.8	5.7	5.9	6.7
G2RC	6.5	6.8	8.2	8.6
AL2X	2.7	1.9	2.9	2.3
NBPRC	2.6	3.3	3.1	3.6
ISO34	1.8	1.6	2.4	2.1
ISOL	4.2	2.9	5.6	3.9
DC9	10.3	9.2	13.1	12.7
DARC	3.5	3.1	4.0	4.3
ALK6	2.3	3.6	3.2	4.6
BSR36	8.1	4.6	9.3	5.5
IDISP	10.6	3.5	11.3	3.9
WATER27	2.8	6.4	4.8	7.9
S22	2.36	0.57	3.36	0.70
ADIM6	3.41	0.36	3.77	0.38
RG6	0.43	0.03	0.50	0.04
HEAVY28	0.65	0.17	0.74	0.23
PCONF	3.33	0.94	3.47	1.02
ACONF	0.63	0.10	0.70	0.11
SCONF	0.52	0.25	0.65	0.36
CYCONF	0.58	0.55	0.66	0.67

**Table S26** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for PBE38 without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	PBE38	PBE38-D3	PBE38	PBE38-D3
MB08-165	10.2	10.2	13.5	13.5
W4-08	8.6	8.5	11.0	10.9
G21IP	4.0	4.0	4.8	4.8
G21EA	3.6	3.6	4.3	4.4
PA	3.3	3.4	4.0	4.1
SIE11	5.5	6.1	6.3	6.9
BHPERI	3.2	1.8	3.7	2.4
BH76	2.2	2.4	2.5	2.8
BH76RC	2.5	2.6	3.1	3.2
RSE43	1.4	1.2	1.9	1.7
O3ADD6	6.5	7.1	8.9	9.5
G2RC	7.6	7.8	9.6	10.0
AL2X	2.0	2.1	2.2	2.3
NBPRC	2.9	3.9	3.4	4.3
ISO34	2.0	1.9	2.8	2.5
ISOL	3.5	2.5	4.3	3.3
DC9	10.8	10.1	13.5	13.4
DARC	3.3	6.3	4.9	6.9
ALK6	2.2	3.5	2.7	4.3
BSR36	8.1	4.6	9.2	5.4
IDISP	9.9	3.1	10.6	3.9
WATER27	3.1	5.6	5.4	6.7
S22	2.27	0.63	3.24	0.80
ADIM6	3.42	0.19	3.78	0.20
RG6	0.46	0.04	0.52	0.05
HEAVY28	0.71	0.15	0.79	0.21
PCONF	3.04	0.73	3.19	0.80
ACONF	0.64	0.12	0.71	0.13
SCONF	0.70	0.29	0.81	0.34
CYCONF	0.45	0.43	0.52	0.52

**Table S27** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for revPBE0 without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	revPBE0	revPBE0-D3	revPBE0	revPBE0-D3
MB08-165	7.7	6.7	10.5	9.1
W4-08	9.8	9.5	11.4	11.1
G21IP	4.0	4.0	4.6	4.6
G21EA	3.1	3.1	3.5	3.5
PA	4.3	4.5	5.0	5.3
SIE11	5.7	7.0	7.2	7.9
BHPERI	4.8	1.5	5.4	1.9
BH76	2.6	3.2	3.0	3.6
BH76RC	2.0	2.1	2.6	2.7
RSE43	1.7	1.1	2.2	1.7
O3ADD6	2.2	3.5	2.4	4.1
G2RC	4.5	5.0	5.7	6.5
AL2X	5.7	1.9	6.3	2.7
NBPRC	3.1	1.7	4.1	2.1
ISO34	1.8	1.4	2.7	1.9
ISOL	5.4	2.8	7.3	3.8
DC9	10.3	7.9	12.9	10.4
DARC	6.1	1.9	7.0	2.5
ALK6	3.2	1.9	3.9	2.4
BSR36	10.6	4.7	11.9	5.7
IDISP	15.7	2.7	16.9	3.2
WATER27	14.4	2.1	23.2	4.1
S22	4.30	0.32	5.39	0.41
ADIM6	5.53	0.73	6.08	0.78
RG6	0.76	0.03	0.85	0.03
HEAVY28	1.41	0.14	1.48	0.20
PCONF	4.41	0.42	4.70	0.57
ACONF	1.07	0.05	1.19	0.06
SCONF	1.45	0.48	1.66	0.59
CYCONF	0.47	0.35	0.53	0.43

**Table S28** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for revPBE38 without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	revPBE38	revPBE38-D3	revPBE38	revPBE38-D3
MB08-165	8.9	8.1	11.9	11.0
W4-08	14.7	14.5	17.3	17.1
G21IP	4.3	4.3	5.0	5.0
G21EA	4.0	4.0	5.0	5.1
PA	4.6	4.8	5.3	5.5
SIE11	4.6	5.3	5.6	6.2
BHPERI	5.5	2.4	6.2	2.9
BH76	1.4	1.6	1.8	2
BH76RC	2.4	2.5	2.9	3.0
RSE43	1.2	0.7	1.8	1.4
O3ADD6	4.3	5.1	6.2	7.1
G2RC	5.7	6.2	7.2	7.9
AL2X	4.5	1.6	4.8	2.1
NBPRC	2.5	2.3	3.3	2.7
ISO34	1.9	1.7	2.8	2.3
ISOL	4.0	2.1	5.3	2.8
DC9	10.4	9.1	12.7	11.4
DARC	3.7	4.1	4.1	4.7
ALK6	2.8	1.7	3.5	2.0
BSR36	10.1	5.0	11.3	5.9
IDISP	14.1	3.0	15.1	3.9
WATER27	12.5	2.3	20.7	4.5
S22	3.83	0.39	4.89	0.46
ADIM6	5.16	0.76	5.67	0.81
RG6	0.72	0.03	0.81	0.04
HEAVY28	1.34	0.21	1.40	0.28
PCONF	3.94	0.48	4.23	0.53
ACONF	1.01	0.15	1.12	0.17
SCONF	1.47	0.68	1.67	0.80
CYCONF	0.37	0.33	0.42	0.38

**Table S29** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for TPSSh without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	TPSSh	TPSSh-D3	TPSSh	TPSSh-D3
MB08-165	8.6	8.0	11.8	10.7
W4-08	4.9	4.9	7.2	7.3
G21IP	3.9	3.9	4.7	4.7
G21EA	2.6	2.6	2.9	3.0
PA	4.6	4.7	5.4	5.5
SIE11	8.6	9.5	10.8	11.3
BHPERI	2.4	1.9	2.9	2.4
BH76	6.6	7.1	7.5	7.9
BH76RC	3.5	3.5	4.4	4.4
RSE43	2.1	1.8	2.6	2.3
O3ADD6	3.2	4.3	4.3	5.5
G2RC	5.6	6.0	7.0	7.4
AL2X	3.4	2.2	3.7	2.6
NBPRC	2.4	1.9	3.1	2.2
ISO34	2.2	1.9	2.9	2.5
ISOL	7.3	5.5	9.7	7.1
DC9	10.4	7.9	12.9	10.7
DARC	8.2	4.1	9.1	4.8
ALK6	2.1	3.4	2.3	4.3
BSR36	10.5	6.0	11.8	7.0
IDISP	13.3	4.2	14.9	5.4
WATER27	5.7	4.3	10.0	5.1
S22	3.28	0.38	4.38	0.51
ADIM6	4.61	0.22	5.09	0.23
RG6	0.60	0.04	0.68	0.06
HEAVY28	0.96	0.17	1.05	0.23
PCONF	4.12	0.95	4.29	1.08
ACONF	0.71	0.03	0.80	0.04
SCONF	0.32	0.47	0.41	0.80
CYCONF	0.71	0.68	0.79	0.82

**Table S30** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for TPSS0 without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	TPSS0	TPSS0-D3	TPSS0	TPSS0-D3
MB08-165	8.6	7.8	11.4	10.4
W4-08	9.8	9.7	12.4	12.4
G21IP	4.1	4.1	4.9	4.9
G21EA	3.6	3.6	4.4	4.4
PA	4.8	4.9	5.5	5.7
SIE11	6.7	7.5	8.3	8.8
BHPERI	3.2	1.4	3.8	1.8
BH76	4.0	4.4	4.9	5.2
BH76RC	3.5	3.5	4.3	4.4
RSE43	1.5	1.2	2.0	1.8
O3ADD6	5.0	5.8	6.1	7.1
G2RC	5.1	5.4	6.4	6.9
AL2X	2.7	2.4	2.9	2.5
NBPRC	2.3	2.7	2.8	2.9
ISO34	2.1	1.8	2.6	2.1
ISOL	5.3	3.6	7.0	4.5
DC9	9.5	8.0	12.0	10.4
DARC	4.7	2.1	5.4	2.5
ALK6	2	3.3	2.1	4.1
BSR36	10.0	5.7	11.3	6.5
IDISP	12.3	3.4	13.4	3.9
WATER27	6.0	3.5	10.5	4.1
S22	3.04	0.44	4.11	0.58
ADIM6	4.44	0.20	4.89	0.20
RG6	0.59	0.05	0.68	0.06
HEAVY28	0.99	0.15	1.06	0.20
PCONF	3.68	0.65	3.86	0.73
ACONF	0.72	0.05	0.80	0.06
SCONF	0.50	0.29	0.61	0.48
CYCONF	0.54	0.51	0.60	0.62

**Table S31** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for PW6B95 without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	PW6B95	PW6B95-D3	PW6B95	PW6B95-D3
MB08-165	4.8	4.7	6.1	5.9
W4-08	2.4	2.4	4.1	4.1
G21IP	2.8	2.8	3.5	3.5
G21EA	1.2	1.3	1.6	1.6
PA	2.5	2.5	3.3	3.3
SIE11	7.0	7.5	8.6	8.9
BHPERI	3.5	2.3	4.0	2.6
BH76	3.2	3.5	3.7	4.0
BH76RC	1.5	1.6	2.1	2.1
RSE43	2.6	2.4	3.1	2.9
O3ADD6	3.5	4.3	4.4	5.1
G2RC	3.2	3.4	4.0	4.2
AL2X	2.3	1.3	2.5	1.7
NBPRC	2.1	1.8	2.7	2.0
ISO34	1.4	1.2	1.9	1.6
ISOL	5.5	4.6	7.1	5.8
DC9	8.4	7.0	10.4	9.3
DARC	5.8	3.6	6.6	4.2
ALK6	2.8	4.7	3.8	5.9
BSR36	6.6	4.1	7.4	4.6
IDISP	8.2	3.5	9.7	4.9
WATER27	5.9	1.7	10.7	3.5
S22	1.95	0.34	2.48	0.44
ADIM6	2.01	0.58	2.26	0.62
RG6	0.39	0.03	0.45	0.05
HEAVY28	0.68	0.13	0.73	0.17
PCONF	1.24	0.51	1.38	0.60
ACONF	0.21	0.15	0.23	0.19
SCONF	0.51	0.31	0.58	0.39
CYCONF	0.31	0.31	0.36	0.37

**Table S32** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for MPW1B95 without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	MPW1B95	MPW1B95-D3	MPW1B95	MPW1B95-D3
MB08-165	5.6	5.7	7.1	7.2
W4-08	2.6	2.6	4.5	4.5
G21IP	2.8	2.8	3.4	3.4
G21EA	2.2	2.2	2.6	2.6
PA	2.2	2.2	2.9	3.0
SIE11	6.7	7.3	7.9	8.3
BHPERI	3.3	2.0	3.7	2.3
BH76	2.9	3.2	3.4	3.6
BH76RC	1.8	1.9	2.5	2.5
RSE43	2.6	2.4	3.1	2.9
O3ADD6	4.5	5.3	5.8	6.5
G2RC	4.4	4.6	5.5	5.9
AL2X	1.6	2.3	2.0	2.5
NBPRC	2.0	2.4	2.3	2.6
ISO34	1.6	1.5	2.2	1.9
ISOL	4.4	3.3	5.5	4.1
DC9	9.5	8.3	12.0	11.7
DARC	3.5	2.1	3.9	2.6
ALK6	3.5	6.1	4.5	7.6
BSR36	5.8	2.8	6.4	3.2
IDISP	7.2	2.1	8.1	2.6
WATER27	6.7	1.9	11.9	3.8
S22	2.12	0.29	2.65	0.37
ADIM6	2.51	0.37	2.77	0.41
RG6	0.51	0.05	0.58	0.05
HEAVY28	0.85	0.13	0.89	0.15
PCONF	1.41	0.65	1.54	0.76
ACONF	0.23	0.19	0.25	0.24
SCONF	0.39	0.22	0.45	0.42
CYCONF	0.45	0.54	0.56	0.61

**Table S33** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for PWB6K without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	PWB6K	PWB6K-D3	PWB6K	PWB6K-D3
MB08-165	7.2	7.3	9.4	9.5
W4-08	8.8	8.7	11.7	11.7
G21IP	3.0	3.0	3.9	3.9
G21EA	3.2	3.2	4.0	4.0
PA	2.7	2.8	3.5	3.5
SIE11	5.0	5.3	6.0	6.3
BHPERI	4.8	3.9	5.3	4.4
BH76	1.4	1.4	1.7	1.8
BH76RC	2.4	2.4	2.8	2.8
RSE43	1.8	1.7	2.3	2.2
O3ADD6	6.4	6.9	9.7	10.0
G2RC	5.8	5.9	7.1	7.3
AL2X	1.0	1.8	1.5	2.2
NBPRC	2.5	2.8	2.8	3.1
ISO34	1.8	1.7	2.2	2.1
ISOL	3.5	3.0	4.2	3.6
DC9	8.4	7.9	11.3	11.1
DARC	2.4	2.6	3.0	3.4
ALK6	3.9	5.3	4.8	6.2
BSR36	6.1	4.5	6.9	5.1
IDISP	6.1	3.1	7.0	4.1
WATER27	2.8	2.0	5.8	2.3
S22	1.20	0.44	1.69	0.54
ADIM6	1.26	0.42	1.47	0.43
RG6	0.26	0.06	0.31	0.07
HEAVY28	0.48	0.15	0.53	0.20
PCONF	0.75	0.42	0.91	0.58
ACONF	0.16	0.05	0.18	0.09
SCONF	0.63	0.45	0.71	0.50
CYCONF	0.22	0.26	0.28	0.31

**Table S34** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for MPWB1K without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	MPWB1K	MPWB1K-D3	MPWB1K	MPWB1K-D3
MB08-165	6.7	6.7	8.7	8.8
W4-08	7.1	7.0	10.0	9.9
G21IP	3.1	3.1	3.9	3.9
G21EA	3.7	3.7	4.5	4.5
PA	2.6	2.7	3.4	3.4
SIE11	5.1	5.7	6.0	6.6
BHPERI	4.4	2.9	5.0	3.5
BH76	1.4	1.5	1.7	1.8
BH76RC	2.3	2.4	2.7	2.8
RSE43	2	1.7	2.4	2.2
O3ADD6	6.3	6.9	9.3	9.8
G2RC	5.8	6.1	7.2	7.5
AL2X	1.1	2.7	1.6	3.0
NBPRC	2.4	3.1	2.7	3.4
ISO34	1.9	1.8	2.5	2.4
ISOL	3.4	2.6	4.1	3.3
DC9	9.7	9.5	12.9	13.0
DARC	2.6	4.3	3.4	4.8
ALK6	3.7	6.2	4.5	7.5
BSR36	5.6	2.9	6.1	3.2
IDISP	6.1	1.5	6.8	2.3
WATER27	6.1	2.1	11.2	3.8
S22	1.81	0.32	2.32	0.43
ADIM6	2.29	0.35	2.52	0.39
RG6	0.49	0.04	0.56	0.05
HEAVY28	0.83	0.15	0.87	0.17
PCONF	1.03	0.80	1.21	0.98
ACONF	0.21	0.17	0.23	0.23
SCONF	0.52	0.24	0.59	0.34
CYCONF	0.35	0.47	0.44	0.51

**Table S35** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for B1B95 without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	B1B95	B1B95-D3	B1B95	B1B95-D3
MB08-165	5.8	5.6	7.6	7.2
W4-08	2.8	2.8	4.5	4.4
G21IP	2.9	2.9	3.6	3.6
G21EA	2.4	2.4	2.8	2.8
PA	2.5	2.7	3.3	3.4
SIE11	6.6	7.5	8.0	8.6
BHPERI	4.1	1.8	4.5	2.1
BH76	2.7	3.2	3.3	3.7
BH76RC	1.6	1.7	2.3	2.4
RSE43	2.7	2.4	3.2	2.9
O3ADD6	3.4	4.3	4.0	5.1
G2RC	3.6	4.0	4.6	5.2
AL2X	2.9	2.5	3.1	2.7
NBPRC	1.9	1.7	2.7	2.0
ISO34	1.6	1.4	2.2	1.8
ISOL	5.1	3.3	6.4	4.0
DC9	10.1	8.4	12.1	11.2
DARC	4.9	1.8	5.7	2.1
ALK6	2.5	6.5	3.3	8.7
BSR36	6.4	1.8	7.0	2.0
IDISP	9.1	1.6	10.2	2.3
WATER27	12.9	4.5	21.1	8.1
S22	3.26	0.43	3.84	0.59
ADIM6	4.02	0.35	4.35	0.43
RG6	0.89	0.18	0.95	0.20
HEAVY28	1.40	0.18	1.43	0.23
PCONF	2.01	1.11	2.19	1.32
ACONF	0.39	0.29	0.42	0.36
SCONF	0.52	0.37	0.59	0.63
CYCONF	0.47	0.57	0.55	0.63

**Table S36** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for BMK without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	BMK	BMK-D3	BMK	BMK-D3
MB08-165	5.5	5.8	7.2	7.6
W4-08	3.4	3.4	5.6	5.6
G21IP	3.3	3.3	4.5	4.5
G21EA	1.9	1.9	2.3	2.3
PA	2.3	2.3	3.0	3.1
SIE11	6.6	7.7	8.0	9.0
BHPERI	5.1	2.0	5.7	2.3
BH76	1.3	1.7	1.6	2.0
BH76RC	1.6	1.7	2	2.1
RSE43	1.5	1.1	2.1	1.7
O3ADD6	5.5	6.7	7.5	8.7
G2RC	4.2	4.6	5.6	6.2
AL2X	3.3	1.7	3.6	2.1
NBPRC	1.6	2.1	2.1	2.4
ISO34	1.3	1.2	1.8	1.6
ISOL	4.0	2.9	5.2	4.4
DC9	6.6	9.1	8.0	10.3
DARC	2.3	4.2	2.8	4.5
ALK6	2.5	6.5	2.8	9.9
BSR36	6.4	1.6	7.3	2.4
IDISP	7.7	2.3	8.5	3.5
WATER27	6.9	2.6	11.8	3.6
S22	2.61	0.98	3.05	1.45
ADIM6	3.83	0.83	4.00	1.04
RG6	1.15	0.40	1.18	0.45
HEAVY28	1.33	0.33	1.37	0.43
PCONF	0.73	2.71	1.08	2.87
ACONF	0.26	0.49	0.29	0.58
SCONF	0.49	0.49	0.54	0.78
CYCONF	0.23	0.26	0.26	0.31

**Table S37** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for M05 without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	M05	M05-D3	M05	M05-D3
MB08-165	7.0	6.7	8.9	8.7
W4-08	3.2	3.2	4.8	4.8
G21IP	3.4	3.4	4.2	4.3
G21EA	2.9	2.9	3.4	3.4
PA	3.7	3.8	4.9	4.9
SIE11	6.9	7.3	10.6	10.7
BHPERI	6.5	5.3	7.2	5.9
BH76	1.9	2.0	2.8	2.9
BH76RC	2.4	2.4	3.6	3.7
RSE43	2.4	2.2	2.9	2.8
O3ADD6	0.9	1.2	1.4	1.4
G2RC	4.5	4.6	6.1	6.2
AL2X	7.1	5.5	7.3	5.7
NBPRC	4.2	3.3	5.6	4.5
ISO34	2.4	2.2	3.5	3.3
ISOL	6.4	5.6	8.1	7.2
DC9	10.4	9.5	15.0	14.4
DARC	5.4	3.7	6.1	4.1
ALK6	1.8	3.3	2.6	4.0
BSR36	10.3	7.8	12.1	9.5
IDISP	13.0	8.1	14.1	9.2
WATER27	2.8	2.5	5.3	3.2
S22	2.07	0.52	2.81	0.71
ADIM6	1.84	0.78	2.12	0.81
RG6	0.25	0.06	0.31	0.09
HEAVY28	0.49	0.23	0.55	0.35
PCONF	2.08	0.60	2.36	0.77
ACONF	0.71	0.36	0.78	0.40
SCONF	1.64	1.35	1.81	1.47
CYCONF	0.39	0.34	0.49	0.41

**Table S38** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for M052X without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	M052X	M052X-D3	M052X	M052X-D3
MB08-165	6.8	6.8	9.8	9.9
W4-08	4.5	4.5	7.1	7.1
G21IP	3.2	3.2	4.3	4.3
G21EA	1.8	1.8	2.5	2.5
PA	1.5	1.5	1.8	1.8
SIE11	6.0	6.1	7.9	8.0
BHPERI	1.8	1.7	2.2	2.0
BH76	1.6	1.6	2.0	2.0
BH76RC	1.5	1.5	2.0	2.0
RSE43	1.2	1.2	1.9	1.8
O3ADD6	7.0	7.1	9.3	9.4
G2RC	4.4	4.4	5.6	5.6
AL2X	1.2	1.6	1.5	1.8
NBPRC	1.4	1.4	1.9	1.8
ISO34	1.4	1.3	1.8	1.8
ISOL	3.1	3.3	4.7	4.6
DC9	6.2	6.0	8.6	8.7
DARC	1.7	1.4	2.0	1.9
ALK6	1.8	1.7	2.3	2.2
BSR36	2.5	1.5	3.0	1.9
IDISP	3.0	1.1	3.6	2.0
WATER27	2.9	4.5	3.2	5.1
S22	0.79	0.35	1.04	0.47
ADIM6	0.89	0.40	1.05	0.42
RG6	0.26	0.25	0.31	0.30
HEAVY28	0.43	0.37	0.46	0.40
PCONF	0.62	0.26	0.71	0.31
ACONF	0.12	0.07	0.15	0.09
SCONF	0.20	0.20	0.24	0.25
CYCONF	0.09	0.10	0.11	0.12

**Table S39** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for M06 without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	M06	M06-D3	M06	M06-D3
MB08-165	6.1	6.0	7.9	7.8
W4-08	3.0	3.0	4.4	4.4
G21IP	3.1	3.1	3.9	3.9
G21EA	2.4	2.4	2.6	2.6
PA	3.0	3.0	4.0	4.0
SIE11	5.9	6.0	7.2	7.2
BHPERI	3.9	3.5	4.4	4.0
BH76	2	2.0	2.7	2.7
BH76RC	1.7	1.7	2.7	2.7
RSE43	2.0	2.0	2.6	2.6
O3ADD6	2.5	2.6	2.9	3.1
G2RC	4.3	4.3	5.8	5.8
AL2X	2.2	2.0	2.6	2.4
NBPRC	2.9	2.6	3.4	3.0
ISO34	1.3	1.3	1.8	1.8
ISOL	4.7	4.3	6.7	6.3
DC9	7.6	7.4	9.7	9.6
DARC	4.4	3.7	4.9	4.1
ALK6	3.6	3.7	3.9	4.0
BSR36	2.9	1.5	3.6	2.2
IDISP	3.8	3.8	6.1	4.6
WATER27	3.4	1.8	6.4	2.9
S22	1.06	0.26	1.28	0.35
ADIM6	0.35	1.95	0.44	2.28
RG6	0.39	0.36	0.42	0.39
HEAVY28	0.43	0.39	0.49	0.47
PCONF	0.49	1.08	0.56	1.18
ACONF	0.34	0.51	0.38	0.57
SCONF	0.56	0.55	0.67	0.68
CYCONF	0.13	0.13	0.15	0.15

**Table S40** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for M062X without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	M062X	M062X-D3	M062X	M062X-D3
MB08-165	4.6	4.7	6.3	6.4
W4-08	3.4	3.4	5.7	5.7
G21IP	2.5	2.5	3.5	3.5
G21EA	1.9	1.9	2.1	2.1
PA	1.1	1.1	1.5	1.5
SIE11	4.0	4.0	5.6	5.6
BHPERI	2.8	2.8	3.3	3.3
BH76	1.2	1.2	1.5	1.5
BH76RC	1.1	1.1	1.7	1.7
RSE43	1.0	1.0	1.7	1.7
O3ADD6	6.4	6.4	8.8	8.8
G2RC	2.7	2.7	3.2	3.2
AL2X	1.5	1.6	1.8	1.9
NBPRC	1.1	1.1	1.3	1.3
ISO34	1.2	1.2	1.7	1.7
ISOL	3.4	3.3	5.1	5.1
DC9	5.7	5.7	8.7	8.8
DARC	2.5	2.3	2.7	2.5
ALK6	1.1	1.2	1.5	1.5
BSR36	3.3	2.8	4.2	3.7
IDISP	1.9	1.7	2.8	2.3
WATER27	2.8	3.1	3.1	3.5
S22	0.40	0.36	0.56	0.51
ADIM6	0.41	0.30	0.43	0.40
RG6	0.30	0.30	0.33	0.33
HEAVY28	0.41	0.39	0.48	0.46
PCONF	0.89	1.05	1.05	1.20
ACONF	0.23	0.25	0.27	0.29
SCONF	0.33	0.35	0.41	0.42
CYCONF	0.20	0.22	0.26	0.28

**Table S41** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for M06HF without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	M06HF	M06HF-D3	M06HF	M06HF-D3
MB08-165	12.9	13.0	18.2	18.3
W4-08	7.4	7.4	12.3	12.3
G21IP	5.5	5.5	7.6	7.6
G21EA	3.1	3.1	4.4	4.4
PA	3.6	3.6	4.1	4.1
SIE11	4.2	4.2	5.9	5.9
BHPERI	2.3	2.4	2.7	2.9
BH76	2.4	2.4	3.1	3.1
BH76RC	2.5	2.5	3.6	3.6
RSE43	1.6	1.6	2.1	2.1
O3ADD6	11.2	11.3	16.7	16.7
G2RC	5.7	5.7	7.4	7.4
AL2X	5.7	6.1	5.8	6.1
NBPRC	2.6	2.8	3.5	3.6
ISO34	1.8	1.8	2.4	2.4
ISOL	2.8	2.9	4.4	4.4
DC9	8.2	8.5	12.6	12.9
DARC	1.7	2.2	2.2	2.6
ALK6	5.8	5.7	6.4	6.3
BSR36	4.7	3.8	5.5	4.5
IDISP	2.4	3.0	3.9	5.1
WATER27	5.8	7.5	6.6	8.5
S22	0.62	0.84	0.83	1.11
ADIM6	1.77	0.77	2.26	1.18
RG6	0.40	0.40	0.48	0.47
HEAVY28	0.66	0.60	0.73	0.66
PCONF	1.27	1.00	1.52	1.32
ACONF	0.47	0.40	0.48	0.42
SCONF	0.38	0.39	0.49	0.52
CYCONF	0.28	0.26	0.31	0.29

**Table S42** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for CAM-B3LYP without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	CAM-B3LYP	CAM-B3LYP-D3	CAM-B3LYP	CAM-B3LYP-D3
MB08-165	8.8	8.0	11.7	10.8
W4-08	4.3	4.3	7.1	7.0
G21IP	3.8	3.8	4.9	4.9
G21EA	2.3	2.3	3.0	3.0
PA	1.7	1.7	2.2	2.3
SIE11	7.1	7.8	9.6	10.0
BHPERI	6.2	4.1	7.2	4.8
BH76	3.2	3.6	3.8	4.1
BH76RC	1.9	2.0	2.5	2.5
RSE43	1.8	1.5	2.3	2.0
O3ADD6	4.1	5.0	5.2	6.1
G2RC	3.5	3.8	4.1	4.4
AL2X	5.4	2.5	5.8	2.7
NBPRC	3.0	2.4	4.1	2.9
ISO34	1.3	1.0	2.1	1.6
ISOL	5.4	4.0	6.9	4.9
DC9	9.0	6.9	12.3	9.6
DARC	7.2	3.9	7.8	4.2
ALK6	8.7	5.9	11.7	7.6
BSR36	8.6	4.8	9.9	5.9
IDISP	12.1	4.5	13.2	5.4
WATER27	2.8	9.4	3.3	12.5
S22	2.52	0.67	3.50	0.88
ADIM6	3.51	0.28	3.88	0.30
RG6	0.55	0.03	0.65	0.03
HEAVY28	1.00	0.15	1.08	0.22
PCONF	2.93	0.44	3.15	0.51
ACONF	0.69	0.13	0.77	0.14
SCONF	0.59	0.23	0.68	0.34
CYCONF	0.27	0.14	0.32	0.19

**Table S43** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for LC- $\omega$ PBE without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	LC- $\omega$ PBE	LC- $\omega$ PBE-D3	LC- $\omega$ PBE	LC- $\omega$ PBE-D3
MB08-165	10.3	10.1	14.2	13.8
W4-08	5.2	5.1	8.6	8.5
G21IP	4.5	4.5	5.5	5.5
G21EA	2.8	2.8	3.2	3.2
PA	2.8	2.9	3.2	3.3
SIE11	4.9	5.5	6.9	7.5
BHPERI	6.4	4.1	7.3	5.3
BH76	1.7	1.7	2.3	2.2
BH76RC	2.5	2.5	3.0	3.1
RSE43	1.1	0.9	1.6	1.4
O3ADD6	4.5	4.8	6.7	7.2
G2RC	6.2	6.5	7.7	8.1
AL2X	2.0	2.8	2.4	3.0
NBPRC	2.5	4.0	3.0	4.3
ISO34	2.3	2.1	3.3	3.1
ISOL	4.2	4.7	5.5	6.6
DC9	11.1	11.7	15.3	15.5
DARC	6.3	10.0	6.9	10.2
ALK6	1.7	3.3	1.9	4.2
BSR36	6.4	2.3	7.1	2.7
IDISP	8.0	4.1	9.0	6.9
WATER27	7.1	2.0	12.3	2.2
S22	2.81	0.28	3.59	0.37
ADIM6	3.84	0.19	4.21	0.23
RG6	0.60	0.07	0.66	0.09
HEAVY28	1.04	0.13	1.09	0.16
PCONF	2.81	0.37	2.97	0.49
ACONF	0.57	0.04	0.64	0.07
SCONF	0.71	0.24	0.82	0.30
CYCONF	0.48	0.49	0.55	0.58

**Table S44** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for  $\omega$ B97X-D. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD	RMSD
MB08-165	7.5	10
W4-08	3.2	5.6
G21IP	3.1	3.9
G21EA	1.6	1.9
PA	4.1	4.6
SIE11	7.1	8.4
BHPERI	3.7	4.3
BH76	2	2.4
BH76RC	1.7	2.1
RSE43	1.9	2.4
O3ADD6	2.7	3.6
G2RC	4.2	5.4
AL2X	2.5	3.1
NBPRC	1.6	2.1
ISO34	1.1	1.5
ISOL	2.5	3.2
DC9	4.4	6.1
DARC	2.0	2.4
ALK6	2.1	2.8
BSR36	3.4	4.2
IDISP	2.6	3.2
WATER27	1.3	1.7
S22	0.23	0.31
ADIM6	1.07	1.23
RG6	0.18	0.18
HEAVY28	0.25	0.27
PCONF	0.62	0.77
ACONF	0.26	0.31
SCONF	0.51	0.61
CYCONF	0.38	0.42

**Table S45** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for B2PLYP without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	B2PLYP	B2PLYP-D3	B2PLYP	B2PLYP-D3
MB08-165	5.1	3.9	6.6	5.3
W4-08	2.5	2.4	4.3	4.3
G21IP	2.3	2.3	2.8	2.8
G21EA	1.4	1.4	1.7	1.7
PA	1.4	1.5	2.3	2.4
SIE11	4.7	4.9	6.1	6.2
BHPERI	2.8	1.6	3.4	1.8
BH76	2.2	2.5	2.6	2.9
BH76RC	1.2	1.2	1.7	1.7
RSE43	1.2	1.0	1.9	1.7
O3ADD6	2.3	2.8	2.8	3.1
G2RC	1.7	1.8	2.2	2.3
AL2X	4.0	1.9	4.3	2.1
NBPRC	2.3	1.5	3.4	2
ISO34	1.4	1.2	2.0	1.7
ISOL	5.7	4.6	7.8	6.2
DC9	7.7	6.0	9.0	6.9
DARC	7.8	5.0	8.2	5.3
ALK6	4.2	1.8	5.7	2.2
BSR36	5.3	2.4	6.0	2.9
IDISP	8.7	3.0	9.7	3.7
WATER27	3.1	2.8	5.8	3.4
S22	1.79	0.27	2.31	0.33
ADIM6	2.76	0.04	3.02	0.05
RG6	0.47	0.06	0.52	0.07
HEAVY28	0.69	0.10	0.73	0.13
PCONF	1.99	0.17	2.14	0.22
ACONF	0.50	0.07	0.56	0.08
SCONF	0.59	0.23	0.67	0.28
CYCONF	0.22	0.12	0.27	0.14

**Table S46** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for XYG3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD	RMSD
MB08-165	5.2	6.5
W4-08	2.7	3.6
G21IP	1.4	1.8
G21EA	1.3	1.6
PA	1.4	2.1
SIE11	3.1	3.9
BHPERI	1.9	2.3
BH76	1.1	1.6
BH76RC	1.2	1.6
RSE43	0.7	1.4
O3ADD6	2.9	4.1
G2RC	1.9	2.3
AL2X	0.9	1.0
NBPRC	0.8	1.0
ISO34	1.1	1.5
ISOL	3.2	4.6
DC9	3.4	4.6
DARC	2.1	2.4
ALK6	1.6	1.9
BSR36	2.0	2.2
IDISP	3.1	3.3
WATER27	1.4	1.8
S22	0.45	0.60
ADIM6	1.06	1.16
RG6	0.20	0.23
HEAVY28	0.27	0.30
PCONF	0.51	0.63
ACONF	0.22	0.25
SCONF	0.35	0.39
CYCONF	0.16	0.18

**Table S47** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for B2GPPLYP without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	B2GPPLYP	B2GPPLYP-D3	B2GPPLYP	B2GPPLYP-D3
MB08-165	4.7	4.0	6.0	5.2
W4-08	3.1	3.0	5.2	5.2
G21IP	2.1	2.1	2.6	2.6
G21EA	1.9	1.9	2.1	2.1
PA	1.3	1.3	2.1	2.1
SIE11	3.1	3.4	4.3	4.5
BHPERI	2.1	1.3	2.6	1.5
BH76	1.2	1.3	1.6	1.7
BH76RC	1.0	1.1	1.5	1.5
RSE43	0.9	0.8	1.6	1.5
O3ADD6	1.3	1.7	1.7	2.3
G2RC	2.3	2.4	2.7	2.9
AL2X	2.5	1.1	2.7	1.2
NBPRC	1.5	1.0	2.1	1.3
ISO34	1.1	1.0	1.7	1.5
ISOL	4.1	3.3	5.6	4.5
DC9	4.8	3.5	5.8	4.4
DARC	4.1	2.4	4.6	2.7
ALK6	3.0	1.4	4.0	1.6
BSR36	3.6	1.7	4.1	2.0
IDISP	6.0	2.1	6.5	2.3
WATER27	2.0	2.6	3.8	3.1
S22	1.15	0.30	1.50	0.38
ADIM6	2.05	0.15	2.24	0.16
RG6	0.35	0.05	0.39	0.06
HEAVY28	0.47	0.10	0.51	0.14
PCONF	1.36	0.11	1.48	0.18
ACONF	0.37	0.08	0.41	0.09
SCONF	0.51	0.23	0.58	0.25
CYCONF	0.15	0.08	0.18	0.09

**Table S48** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for PWPB95 without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	PWPB95	PWPB95-D3	PWPB95	PWPB95-D3
MB08-165	2.8	2.5	3.8	3.4
W4-08	1.9	1.9	3.1	3.0
G21IP	2.0	2.0	2.4	2.4
G21EA	1.9	1.9	2.2	2.2
PA	2	2.0	2.5	2.6
SIE11	4.0	4.3	5.0	5.2
BHPERI	2.9	1.9	3.3	2.2
BH76	1.6	1.8	2	2.2
BH76RC	1.3	1.3	1.7	1.7
RSE43	1.6	1.4	2.1	2.0
O3ADD6	1.1	1.7	1.4	1.9
G2RC	2.4	2.5	2.9	3.1
AL2X	1.2	1.7	1.5	1.9
NBPRC	1.3	1.2	1.6	1.4
ISO34	1.0	0.9	1.3	1.2
ISOL	3.7	2.9	4.7	3.6
DC9	5.7	5.1	6.9	6.7
DARC	2.9	1.5	3.5	1.8
ALK6	2.9	4.6	3.5	5.6
BSR36	4.1	2.0	4.4	2.2
IDISP	4.7	1.2	5.3	1.5
WATER27	6.1	2.4	10.7	4.9
S22	1.50	0.32	1.82	0.46
ADIM6	1.69	0.36	1.86	0.40
RG6	0.36	0.05	0.41	0.06
HEAVY28	0.58	0.13	0.61	0.15
PCONF	0.69	0.62	0.84	0.74
ACONF	0.11	0.18	0.12	0.22
SCONF	0.40	0.24	0.46	0.32
CYCONF	0.20	0.24	0.25	0.27

**Table S49** – Mean absolute (MADs) and root mean square deviations (RMSDs) of the complete GMTKN30 database for DSD-BLYP without any London-dispersion corrections and with DFT-D3. All values are in kcal/mol and were obtained with the (aug-)def2-QZVP basis.

	MAD		RMSD	
	DSD-BLYP	DSD-BLYP-D3	DSD-BLYP	DSD-BLYP-D3
MB08-165	4.2	3.4	5.2	4.3
W4-08	2.5	2.5	3.4	3.4
G21IP	2.1	2.1	2.6	2.6
G21EA	2.0	2.0	2.2	2.2
PA	1.2	1.2	1.9	1.9
SIE11	3.0	3.1	3.9	4.0
BHPERI	1.9	1.2	2.3	1.4
BH76	1.2	1.2	1.8	1.8
BH76RC	1.0	1.0	1.4	1.4
RSE43	1	0.9	1.8	1.7
O3ADD6	2.0	2.4	2.5	2.7
G2RC	1.9	1.9	2.3	2.4
AL2X	2.3	1	2.4	1.2
NBPRC	1.3	0.8	1.9	1.0
ISO34	1.1	1.0	1.5	1.4
ISOL	3.9	3.1	5.2	4.2
DC9	4.0	3.0	5.0	3.8
DARC	4.0	2.2	4.4	2.6
ALK6	2.4	1.2	3.2	1.3
BSR36	2.9	1.1	3.2	1.3
IDISP	5.1	1.4	5.5	1.5
WATER27	2.5	1.5	4.9	1.9
S22	1.04	0.28	1.31	0.34
ADIM6	1.89	0.13	2.06	0.13
RG6	0.32	0.07	0.36	0.07
HEAVY28	0.42	0.11	0.45	0.14
PCONF	1.17	0.16	1.28	0.20
ACONF	0.32	0.06	0.36	0.07
SCONF	0.53	0.25	0.59	0.27
CYCONF	0.15	0.09	0.18	0.11

**Table S50** – Weighted total mean absolute (WTMADs) for the complete GMTKN30 set for various density functionals with three different basis sets. All values are in kcal/mol.

method	(aug-)def2-SV(P)	(aug-)def2-TZVPP	(aug-)def2-QZVP
B97-D	7.8	4.9	4.8
revPBE-D	7.6	4.6	4.5
TPSS-D	7.9	4.7	4.6
oTPSS-D3	6.9	3.7	3.7
B3LYP-D3	6.6	3.9	3.7
PW6B95-D3	5.9	2.6	2.5
MPW1B95-D3	6.0	2.7	2.6
B2PLYP-D3	6.4	2.4	2.0
XYG3	6.6	2.3	1.9
B2GPPLYP-D3	6.4	2.2	1.7
PWPB95-D3	5.6	1.8	1.6
DSD-BLYP-D3	6.5	2.0	1.5

**Table S51** – Mean absolute deviations (MADs) of the complete GMTKN30 database for HF. All values are in kcal/mol and were obtained with (aug-)def2-TZVPP (TZ) and (aug-)def2-QZVP (QZ). The last column shows the MADs at the CBS limit.

	TZ	QZ	CBS
MB08-165	25.8	25.3	25.
W4-08	97.3	96.1	95.9
G21IP	21.0	21.0	21.0
G21EA	26.6	26.7	26.7
PA	6.3	6.3	6.4
SIE11	13.6	13.4	13.4
BHPERI	23.1	23.2	23.3
BH76	11.0	11.3	11.4
BH76RC	8.4	8.2	8.2
RSE43	2.4	2.4	2.4
O3ADD6	14.1	14.1	14.1
G2RC	8.9	8.6	8.5
AL2X	11.1	10.9	10.9
NBPRC	9.2	9.4	9.4
ISO34	2.7	2.7	2.7
ISOL22	7.1	7.2	7.2
DC9	25.7	25.4	25.3
DARC	12.8	13.2	13.2
ALK6	17.4	17.3	17.2
BSR36	14.2	14.4	14.4
IDISP	21.7	21.9	21.9
WATER27	24.1	25.1	25.3
S22	4.78	4.98	5.03
ADIM6	5.68	5.74	5.76
RG6	0.87	0.90	0.91
HEAVY28	1.99	2.06	2.08
PCONF	2.80	2.87	2.89
ACONF	1.50	1.53	1.54
SCONF	3.41	3.58	3.62
CYCONF	1.98	2.00	2.01

**Table S52** – Mean absolute deviations (MADs) of the complete GMTKN30 database for MP2. All values are in kcal/mol and were obtained with (aug-)def2-TZVPP (TZ) and (aug-)def2-QZVP (QZ). The last column shows the MADs at the CBS limit.

	TZ	QZ	CBS
MB08-165	4.6	4.8	5.7
W4-08	6.6	7.2	8.7
G21IP	3.8	3.3	3.4
G21EA	4.4	3.2	2.3
PA	0.7	0.9	1.4
SIE11	5.8	5.0	4.6
BHPERI	6.1	6.1	6.2
BH76	4.8	4.5	4.4
BH76RC	3.4	3.4	3.7
RSE43	3.2	3.2	3.2
O3ADD6	5.1	5.4	5.7
G2RC	2.9	3.2	3.6
AL2X	1.8	2.4	2.9
NBPRC	1.4	1.4	1.5
ISO34	1.5	1.5	1.6
ISOL22	1.9	1.9	1.9
DC9	7.0	9.3	11.3
DARC	4.4	4.0	4.0
ALK6	2.0	5.2	8.2
BSR36	4.2	4.1	4.1
IDISP	5.5	4.9	4.6
WATER27	1.7	1.4	1.4
S22	1.17	1.02	0.98
ADIM6	0.37	0.29	0.27
RG6	0.14	0.11	0.19
HEAVY28	0.12	0.26	0.41
PCONF	0.85	0.73	0.68
ACONF	0.18	0.12	0.08
SCONF	0.27	0.12	0.16
CYCONF	0.30	0.24	0.22

**Table S53** – Mean absolute deviations (MADs) of the complete GMTKN30 database for SCS-MP2. All values are in kcal/mol and were obtained with (aug-)def2-TZVPP (TZ) and (aug-)def2-QZVP (QZ). The last column shows the MADs at the CBS limit.

	TZ	QZ	CBS
MB08-165	7.3	6.0	6.0
W4-08	6.6	3.9	6.2
G21IP	4.8	3.5	3.7
G21EA	5.6	3.8	3.5
PA	1.9	1.3	0.8
SIE11	6.5	5.6	4.9
BHPERI	1.3	1.4	1.4
BH76	5.8	5.5	5.4
BH76RC	2.0	1.8	1.9
RSE43	3.7	3.7	3.6
O3ADD6	3.0	3.1	3.3
G2RC	2.2	2.1	2.2
AL2X	1.7	1.2	1.1
NBPRC	1.3	1.2	1.1
ISO34	1.0	1.0	1.1
ISOL22	1.4	1.4	1.3
DC9	5.2	4.7	6.8
DARC	1.0	0.9	0.8
ALK6	2.6	2.4	4.5
BSR36	0.8	0.7	0.6
IDISP	2.1	2.4	2.5
WATER27	5.8	6.3	6.3
S22	0.64	0.65	0.66
ADIM6	0.85	0.99	1.05
RG6	0.30	0.19	0.09
HEAVY28	0.37	0.22	0.13
PCONF	0.31	0.36	0.41
ACONF	0.07	0.15	0.19
SCONF	0.51	0.77	0.87
CYCONF	0.27	0.30	0.31

**Table S54** – Mean absolute deviations (MADs) of the complete GMTKN30 database for S2-MP2. All values are in kcal/mol and were obtained with (aug-)def2-TZVPP (TZ) and (aug-)def2-QZVP (QZ). The last column shows the MADs at the CBS limit.

	TZ	QZ	CBS
MB08-165	5.2	5.2	6.1
W4-08	5.7	8.5	11.8
G21IP	3.7	3.5	4.0
G21EA	4.2	3.1	3.7
PA	0.9	0.7	1.1
SIE11	6.2	5.3	4.9
BHPERI	4.7	4.6	4.7
BH76	5.0	4.7	4.5
BH76RC	3.0	3.0	3.3
RSE43	3.5	3.5	3.5
O3ADD6	5.2	5.5	5.7
G2RC	2.5	2.7	3.0
AL2X	1.5	2.0	2.5
NBPRC	1.0	1.0	1.2
ISO34	1.3	1.3	1.4
ISOL22	1.5	1.4	1.4
DC9	6.3	8.5	10.6
DARC	3.4	3.1	3.0
ALK6	2.0	4.9	7.9
BSR36	3.2	3.1	3.0
IDISP	4.8	4.3	4.1
WATER27	1.6	1.8	1.6
S22	1.06	0.89	0.83
ADIM6	0.19	0.08	0.03
RG6	0.17	0.09	0.17
HEAVY28	0.11	0.18	0.32
PCONF	0.76	0.61	0.56
ACONF	0.16	0.09	0.06
SCONF	0.16	0.15	0.26
CYCONF	0.19	0.13	0.11

**Table S55** – Mean absolute deviations (MADs) of the complete GMTKN30 database for SOS-MP2. All values are in kcal/mol and were obtained with (aug-)def2-TZVPP (TZ) and (aug-)def2-QZVP (QZ). The last column shows the MADs at the CBS limit.

	TZ	QZ	CBS
MB08-165	9.7	8.4	8.0
W4-08	8.0	4.5	6.2
G21IP	5.3	4.0	4.1
G21EA	6.4	4.6	4.1
PA	2.8	2.2	1.8
SIE11	7.4	6.5	5.9
BHPERI	4.0	4.2	4.2
BH76	6.4	6.2	6.2
BH76RC	2.3	1.6	1.5
RSE43	4.0	3.9	3.9
O3ADD6	3.0	2.6	2.5
G2RC	2.9	2.5	2.5
AL2X	3.0	2.2	1.7
NBPRC	2.4	2.3	2.1
ISO34	1.0	1.0	1.0
ISOL22	2.2	2.2	2.1
DC9	5.6	5.1	5.7
DARC	2.0	2.4	2.5
ALK6	4.2	2.6	3.6
BSR36	2.5	2.7	2.8
IDISP	2.5	2.8	3.1
WATER27	9.0	9.6	9.5
S22	0.98	1.19	1.24
ADIM6	1.46	1.62	1.71
RG6	0.38	0.28	0.20
HEAVY28	0.56	0.46	0.36
PCONF	0.55	0.63	0.67
ACONF	0.20	0.28	0.32
SCONF	0.90	1.15	1.25
CYCONF	0.54	0.57	0.58