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**Supporting Information for:**  
**Tests of Second-Generation Density**  
**Functionals for Thermochemical Kinetics**

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Table S1. Mean errors (kcal/mol) for pure DFT methods

Method	BH4			BH6			AE3				AE6				HF%	cost(s)
	RMSE	MSE	MUE	RMSE	MSE	MUE	RMSE	MSE	MUE	MUE/ Bond	RMSE	MSE	MUE	MUE/ Bond		
BP86/6-31G(d)	11.2	-10.9	10.9	9.6	-8.8	8.8	27.0	26.2	26.2	3.4	19.2	13.6	14.2	2.9	0.00	19
BP86/6-31+G(d,p)	11.3	-11.3	11.3	9.9	-9.4	9.4	23.5	22.9	22.9	3.0	16.8	12.1	12.9	2.7	0.00	29
BP86/6-31+G(2d,p)	11.1	-11.1	11.1	9.7	-9.3	9.3	24.5	23.9	23.9	3.1	17.7	14.1	14.1	2.9	0.00	32
BP86/6-311G(3d,2pd)	11.7	-11.6	11.6	10.3	-10.0	10.0	28.5	28.0	28.0	3.7	20.6	16.8	16.8	3.5	0.00	67
BP86/6-311+G(2df,2p)	10.9	-10.8	10.8	9.6	-9.3	9.3	26.1	25.8	25.8	3.4	19.0	15.5	15.5	3.2	0.00	95
BP86/MG3S	10.9	-10.8	10.8	9.6	-9.3	9.3	26.1	25.8	25.8	3.4	19.1	16.0	16.0	3.3	0.00	97
BLYP/6-31G(d)	10.9	-10.3	10.3	9.2	-7.9	7.9	9.9	-3.9	9.5	1.2	7.9	-4.3	7.1	1.5	0.00	19
BLYP/6-31+G(d,p)	10.4	-10.3	10.3	8.9	-8.3	8.3	11.5	-8.4	9.3	1.2	8.7	-6.4	6.8	1.4	0.00	30
BLYP/6-31+G(2d,p)	10.1	-10.1	10.1	8.7	-8.1	8.1	11.6	-7.2	10.1	1.3	8.4	-4.4	6.2	1.3	0.00	33
BLYP/6-311G(3d,2pd)	10.7	-10.6	10.6	9.1	-8.6	8.6	10.7	-2.2	9.4	1.2	7.9	-1.2	6.3	1.3	0.00	66
BLYP/6-311+G(2df,2p)	9.7	-9.6	9.6	8.3	-7.8	7.8	11.7	-5.2	9.6	1.3	8.7	-2.9	6.5	1.3	0.00	93
BLYP/MG3S	9.7	-9.6	9.6	8.3	-7.8	7.8	11.7	-5.2	9.6	1.3	8.7	-2.4	6.7	1.4	0.00	96
PW91/6-31G(d)	11.8	-11.4	11.4	10.1	-9.2	9.2	25.8	24.8	24.8	3.2	18.7	11.6	14.8	3.1	0.00	22
PW91/6-31+G(d,p)	11.8	-11.7	11.7	10.3	-9.8	9.8	21.1	20.5	20.5	2.7	15.2	9.6	12.1	2.5	0.00	34
PW91/6-31+G(2d,p)	11.7	-11.5	11.5	10.2	-9.7	9.7	22.5	21.7	21.7	2.8	16.4	11.7	13.2	2.7	0.00	37
PW91/6-311G(3d,2pd)	12.4	-12.2	12.2	10.9	-10.4	10.4	26.4	25.5	25.5	3.3	19.4	14.0	16.4	3.4	0.00	69
PW91/6-311+G(2df,2p)	11.6	-11.3	11.3	10.2	-9.6	9.6	23.3	22.6	22.6	2.9	17.4	12.4	15.0	3.1	0.00	99
PW91/MG3S	11.6	-11.3	11.3	10.2	-9.6	9.6	23.3	22.6	22.6	2.9	17.5	12.9	15.2	3.1	0.00	98
BB95/6-31G(d)	10.8	-10.2	10.2	9.0	-8.0	8.0	19.1	17.0	17.0	2.2	14.2	9.2	11.4	2.4	0.00	19
BB95/6-31+G(d,p)	10.4	-10.4	10.4	8.8	-8.3	8.3	14.1	12.2	12.2	1.6	10.4	7.0	8.2	1.7	0.00	30
BB95/6-31+G(2d,p)	10.2	-10.2	10.2	8.8	-8.3	8.3	15.7	13.4	13.4	1.7	12.3	9.1	9.9	2.0	0.00	35
BB95/6-311G(3d,2pd)	10.9	-10.7	10.7	9.3	-8.7	8.7	19.3	16.7	16.7	2.2	15.1	10.9	12.8	2.6	0.00	68
BB95/6-311+G(2df,2p)	10.0	-9.8	9.8	8.6	-8.1	8.1	16.5	13.7	13.7	1.8	13.5	9.3	11.4	2.4	0.00	97
BB95/MG3S	10.0	-9.8	9.8	8.5	-8.0	8.0	16.5	13.7	13.7	1.8	13.7	9.7	11.6	2.4	0.00	99

Table S1. (Continued)

Method	BH4			BH6			AE3				AE6				HF%	cost(s)
	RMSE	MSE	MUE	RMSE	MSE	MUE	RMSE	MSE	MUE	MUE/ Bond	RMSE	MSE	MUE	MUE/ Bond		
G96LYP/6-31G(d)	9.2	-8.6	8.6	7.8	-6.4	6.7	17.3	-13.7	13.7	1.8	13.2	-10.1	10.1	2.1	0.00	19
G96LYP/6-31+G(d,p)	8.8	-8.8	8.8	7.6	-6.9	6.9	19.0	-16.5	16.5	2.2	14.1	-11.2	11.2	2.3	0.00	30
G96LYP/6-31+G(2d,p)	8.6	-8.6	8.6	7.4	-6.7	6.7	18.8	-15.4	15.4	2.0	13.6	-9.2	9.4	1.9	0.00	35
G96LYP/6-311G(3d,2pd)	9.0	-9.0	9.0	7.7	-7.3	7.3	15.6	-10.6	12.5	1.6	11.4	-6.1	7.7	1.6	0.00	68
G96LYP/6-311+G(2df,2p)	8.3	-8.2	8.2	7.1	-6.6	6.6	16.8	-12.3	12.4	1.6	12.3	-7.1	8.0	1.7	0.00	97
G96LYP/MG3S	8.3	-8.2	8.2	7.1	-6.6	6.6	16.8	-12.3	12.4	1.6	12.2	-6.5	8.0	1.7	0.00	99
PBE/6-31G(d)	11.5	-11.0	11.0	9.8	-8.9	8.9	24.2	23.2	23.2	3.0	17.8	10.2	14.5	3.0	0.00	20
PBE/6-31+G(d,p)	11.5	-11.3	11.3	10	-9.5	9.5	19.7	19.0	19.0	2.5	14.4	8.2	12.0	2.5	0.00	31
PBE/6-31+G(2d,p)	11.4	-11.1	11.1	9.9	-9.4	9.4	21	20.2	20.2	2.6	15.6	10.3	13.0	2.7	0.00	34
PBE/6-311G(3d,2pd)	12.1	-11.8	11.8	10.6	-10.1	10.1	25.1	24.1	24.1	3.1	18.6	12.7	15.9	3.3	0.00	65
PBE/6-311+G(2df,2p)	11.2	-10.9	10.9	9.9	-9.3	9.3	21.9	21.1	21.1	2.8	16.7	11.1	14.5	3.0	0.00	92
PBE/MG3S	11.2	-10.9	10.9	9.9	-9.3	9.3	21.9	21.1	21.1	2.8	16.7	11.6	14.7	3.0	0.00	95
mPWPW91/6-31G(d)	10.6	-10.1	10.1	8.9	-8.0	8.0	15.5	14.2	14.2	1.9	11.9	5.2	9.9	2.0	0.00	22
mPWPW91/6-31+G(d,p)	10.5	-10.4	10.4	9.0	-8.6	8.6	11.2	10.1	10.1	1.3	8.7	3.3	7.4	1.5	0.00	35
mPWPW91/6-31+G(2d,p)	10.4	-10.2	10.2	8.9	-8.5	8.5	12.6	11.3	11.3	1.5	9.8	5.4	8.3	1.7	0.00	38
mPWPW91/6-311G(3d,2pd)	11.1	-10.9	10.9	9.7	-9.2	9.2	16.8	15.3	15.3	2.0	12.9	7.9	10.8	2.2	0.00	72
mPWPW91/6-311+G(2df,2p)	10.2	-10.0	10.0	8.9	-8.5	8.5	14.1	12.6	12.6	1.6	11.4	6.4	9.6	2.0	0.00	102
mPWPW91/MG3S	10.2	-10.0	10.0	8.9	-8.5	8.5	14.1	12.6	12.6	1.6	11.4	6.8	9.8	2.0	0.00	101
VSXC/6-31G(d)	7.1	-6.3	6.3	5.8	-4.5	4.5	1.2	0.9	0.9	0.1	3.0	-0.6	2.0	0.4	0.00	28
VSXC/6-31+G(d,p)	6.6	-6.5	6.5	5.5	-5.1	5.1	2.2	-0.5	1.7	0.2	4.0	-1.2	3.2	0.7	0.00	41
VSXC/6-31+G(2d,p)	6.4	-6.3	6.3	5.3	-4.9	4.9	1.3	-1.2	1.2	0.2	3.6	-0.4	2.9	0.6	0.00	46
VSXC/6-311G(3d,2pd)	7.2	-7.1	7.1	6.2	-5.7	5.7	2.2	1.1	2.0	0.3	2.4	0.9	2.2	0.5	0.00	95
VSXC/6-311+G(2df,2p)	6.3	-6.2	6.2	5.4	-5.0	5.0	3.3	-1.6	2.3	0.3	3.5	-0.5	2.7	0.6	0.00	118
VSXC/MG3S	6.3	-6.2	6.2	5.4	-5.0	5.0	3.3	-1.6	2.3	0.3	3.4	-0.1	2.6	0.5	0.00	122

Table S1. (Continued)

Method	BH4			BH6			AE3				AE6				HF%	cost(s)
	RMSE	MSE	MUE	RMSE	MSE	MUE	RMSE	MSE	MUE	MUE/ Bond	RMSE	MSE	MUE	MUE/ Bond		
HCTH/6-31G(d)	7.9	-7.1	7.1	6.5	-4.8	5.3	3.8	1.9	2.7	0.4	7.3	-3.4	5.7	1.2	0.00	33
HCTH/6-31+G(d,p)	7.4	-7.4	7.4	6.2	-5.4	5.4	1.9	-1.4	1.7	0.2	6.7	-4.9	5.1	1.1	0.00	50
HCTH/6-31+G(2d,p)	7.3	-7.3	7.3	6.0	-5.3	5.3	2.7	-0.7	2.7	0.4	6.0	-3.4	4.7	1.0	0.00	54
HCTH/6-311G(3d,2pd)	8.0	-7.9	7.9	6.6	-6.0	6.0	5.3	1.9	4.1	0.5	5.7	-1.6	4.5	0.9	0.00	103
HCTH/6-311+G(2df,2p)	7.0	-7.0	7.0	5.8	-5.3	5.3	5.1	-1.2	4.1	0.5	6.6	-3.3	5.6	1.2	0.00	130
HCTH/MG3S	7.0	-7.0	7.0	5.8	-5.2	5.2	5.1	-1.2	4.1	0.5	6.0	-2.7	5.2	1.1	0.00	136
OLYP/6-31G(d)	8.6	-7.7	7.7	7.3	-5.7	6.0	5.6	4.3	4.6	0.6	6.0	-0.5	4.9	1.0	0.00	18
OLYP/6-31+G(d,p)	7.8	-7.6	7.6	6.7	-6.0	6.0	1.7	-0.6	1.3	0.2	5.1	-2.9	3.3	0.7	0.00	28
OLYP/6-31+G(2d,p)	7.6	-7.5	7.5	6.5	-5.9	5.9	2.1	0.7	1.9	0.3	5.3	-1.8	4.1	0.8	0.00	31
OLYP/6-311G(3d,2pd)	8.4	-8.4	8.4	7.2	-6.8	6.8	5.7	3.8	3.8	0.5	4.8	1.0	3.6	0.7	0.00	67
OLYP/6-311+G(2df,2p)	7.3	-7.2	7.2	6.3	-5.9	5.9	3.6	0.0	3.0	0.4	4.5	-1.0	4.1	0.9	0.00	97
OLYP/MG3S	7.3	-7.2	7.2	6.3	-5.9	5.9	3.6	0.0	3.0	0.4	4.1	-0.6	3.8	0.8	0.00	101
OPW91/6-31G(d)	7.0	-6.3	6.3	5.8	-4.8	4.8	14.3	13.2	13.2	1.7	11.9	3.4	10.5	2.2	0.00	21
OPW91/6-31+G(d,p)	6.6	-6.6	6.6	5.6	-5.4	5.4	11.0	9.7	9.7	1.3	9.9	1.7	8.3	1.7	0.00	31
OPW91/6-31+G(2d,p)	6.5	-6.5	6.5	5.6	-5.3	5.3	12.4	11.4	11.4	1.5	10.6	4.2	9.7	2.0	0.00	35
OPW91/6-311G(3d,2pd)	7.5	-7.5	7.5	6.6	-6.3	6.3	14.6	14.0	14.0	1.8	11.8	5.5	10.9	2.3	0.00	69
OPW91/6-311+G(2df,2p)	6.7	-6.7	6.7	5.9	-5.7	5.7	11.9	11.6	11.6	1.5	10.7	4.6	10.5	2.2	0.00	93
OPW91/MG3S	6.6	-6.5	6.5	5.8	-5.6	5.6	11.5	11.2	11.2	1.5	10.2	4.4	10.0	2.1	0.00	97

Table S2. Mean errors (kcal/mol) for hybrid DFT methods

Method	BH4			BH6			AE3				AE6				HF%	cost(s)
	RMSE	MSE	MUE	RMSE	MSE	MUE	RMSE	MSE	MUE	MUE/ Bond	RMSE	MSE	MUE	MUE/ Bond		
B3PW91/6-31G(d)	6.2	-5.1	5.1	5.2	-3.9	3.9	3.4	0.3	3.0	0.4	7.4	-4.3	6.0	1.2	20.00	26
B3PW91/6-31+G(d,p)	5.5	-5.4	5.4	4.7	-4.4	4.4	3.9	-1.6	3.8	0.5	7.3	-4.9	6.0	1.2	20.00	37
B3PW91/6-31+G(2d,p)	5.3	-5.2	5.2	4.5	-4.3	4.3	2.5	-0.7	2.5	0.3	5.4	-2.8	3.8	0.8	20.00	39
B3PW91/6-311G(3d,2pd)	5.9	-5.9	5.9	5.2	-5.1	5.1	2.9	2.6	2.6	0.3	4.4	-0.7	3.6	0.7	20.00	100
B3PW91/6-311+G(2df,2p)	5.2	-5.1	5.1	4.6	-4.4	4.4	1.4	1.2	1.2	0.2	4.5	-1.4	3.4	0.7	20.00	96
B3PW91/MG3S	5.2	-5.1	5.1	4.6	-4.4	4.4	1.4	1.2	1.2	0.2	3.9	-0.9	3.1	0.6	20.00	102
B3LYP/6-31G(d)	7.4	-6.3	6.3	6.3	-4.7	5.0	4.9	-4.8	4.8	0.6	6.9	-6.0	6.0	1.2	20.00	23
B3LYP/6-31+G(d,p)	6.4	-6.3	6.3	5.6	-5.0	5.0	7.5	-7.5	7.5	1.0	8.1	-7.0	7.3	1.5	20.00	36
B3LYP/6-31+G(2d,p)	6.2	-6.1	6.1	5.3	-4.8	4.8	6.4	-6.4	6.4	0.8	6.2	-5.0	5.7	1.2	20.00	38
B3LYP/6-311G(3d,2pd)	6.7	-6.6	6.6	5.8	-5.4	5.4	3.2	-2.7	2.7	0.4	3.3	-2.5	2.7	0.6	20.00	103
B3LYP/6-311+G(2df,2p)	5.8	-5.8	5.8	5.1	-4.7	4.7	5.1	-4.5	4.5	0.6	4.4	-3.4	3.4	0.7	20.00	98
B3LYP/MG3S	5.8	-5.8	5.8	5.1	-4.7	4.7	5.1	-4.5	4.5	0.6	4.1	-2.9	3.2	0.7	20.00	102
BH&HLYP/6-31G(d)	5.5	-0.5	5.4	4.7	0.1	4.4	33.4	-32.6	32.6	4.3	27.6	-25.0	25.0	5.2	50.00	23
BH&HLYP/6-31+G(d,p)	3.1	-0.3	3.0	3.0	0.0	2.9	34.4	-33.4	33.4	4.4	28.1	-24.7	24.7	5.1	50.00	38
BH&HLYP/6-31+G(2d,p)	2.7	-0.1	2.5	2.5	0.2	2.4	33.2	-32.5	32.5	4.2	26.3	-22.6	23.1	4.8	50.00	44
BH&HLYP/6-311G(3d,2pd)	3.0	-0.7	2.8	2.5	-0.6	2.3	30.6	-30.0	30.0	3.9	24.1	-20.8	20.9	4.3	50.00	137
BH&HLYP/6-311+G(2df,2p)	2.5	0.1	2.2	2.2	0.1	2.0	31.4	-30.7	30.7	4.0	24.5	-21.0	21.0	4.3	50.00	122
BH&HLYP/MG3S	2.5	0.1	2.2	2.2	0.1	2.0	31.4	-30.7	30.7	4.0	24.2	-20.5	20.7	4.3	50.00	126
B1B95/6-31G(d)	5.9	-4.1	4.1	4.8	-2.9	2.9	3.0	0.3	2.6	0.3	5.8	-3.0	4.4	0.9	28.00	38
B1B95/6-31+G(d,p)	4.4	-4.2	4.2	3.7	-3.2	3.2	3.7	-2.3	3.5	0.5	5.8	-4.0	4.5	0.9	28.00	54
B1B95/6-31+G(2d,p)	4.1	-4.0	4.0	3.4	-3.1	3.1	2.4	-1.3	2.3	0.3	4.4	-1.8	3.4	0.7	28.00	61
B1B95/6-311G(3d,2pd)	4.8	-4.6	4.6	4.2	-3.8	3.8	1.3	0.7	1.3	0.2	3.2	-0.5	2.7	0.6	28.00	132
B1B95/6-311+G(2df,2p)	3.9	-3.8	3.8	3.4	-3.2	3.2	1.0	-0.9	0.9	0.1	3.8	-1.2	3.0	0.6	28.00	158
B1B95/MG3S	3.9	-3.8	3.8	3.4	-3.1	3.1	1.0	-0.9	0.9	0.1	3.4	-0.8	2.7	0.6	28.00	126

Table S2. (Continued)

Method	BH4			BH6			AE3				AE6				HF%	cost(s)
	RMSE	MSE	MUE	RMSE	MSE	MUE	RMSE	MSE	MUE	MUE/ Bond	RMSE	MSE	MUE	MUE/ Bond		
PBE0/6-31G(d)	6.3	-5.2	5.2	5.3	-4.2	4.2	6.6	3.8	4.0	0.5	9.4	-3.3	7.2	1.5	25.00	23
PBE0/6-31+G(d,p)	5.5	-5.4	5.4	4.8	-4.6	4.6	5.8	1.8	4.5	0.6	8.8	-3.9	7.1	1.5	25.00	36
PBE0/6-31+G(2d,p)	5.3	-5.2	5.2	4.7	-4.5	4.5	5.3	2.8	3.3	0.4	7.3	-1.7	5.1	1.1	25.00	40
PBE0/6-311G(3d,2pd)	6.1	-5.9	5.9	5.6	-5.3	5.3	6.3	5.5	5.5	0.7	6.9	0.0	6.0	1.2	25.00	93
PBE0/6-311+G(2df,2p)	5.3	-5.1	5.1	4.8	-4.6	4.6	4.6	3.9	3.9	0.5	6.7	-0.8	5.7	1.2	25.00	89
PBE0/MG3S	5.3	-5.1	5.1	4.8	-4.6	4.6	4.6	3.9	3.9	0.5	6.1	-0.3	5.4	1.1	25.00	92
mPW1Pw91/6-31G(d)	5.7	-4.5	4.5	4.8	-3.5	3.5	5.1	-3.0	4.8	0.6	9.3	-7.1	8.0	1.7	25.00	26
mPW1Pw91/6-31+G(d,p)	4.8	-4.7	4.7	4.2	-3.9	3.9	6.7	-5.0	5.6	0.7	9.5	-7.7	8.0	1.7	25.00	39
mPW1Pw91/6-31+G(2d,p)	4.6	-4.5	4.5	4.0	-3.8	3.8	5.1	-4.0	4.3	0.6	7.5	-5.5	5.6	1.2	25.00	44
mPW1Pw91/6-311G(3d,2pd)	5.4	-5.3	5.3	4.8	-4.6	4.6	2.0	-1.2	1.9	0.2	5.7	-3.7	4.1	0.8	25.00	99
mPW1Pw91/6-311+G(2df,2p)	4.6	-4.5	4.5	4.1	-4.0	4.0	3.0	-2.6	2.6	0.3	6.3	-4.4	4.9	1.0	25.00	96
mPW1Pw91/MG3S	4.6	-4.5	4.5	4.1	-3.9	3.9	3.0	-2.6	2.6	0.3	5.6	-3.9	4.6	1.0	25.00	99
B97-1/6-31G(d)	7.1	-5.7	5.7	5.8	-3.8	3.9	5.2	-3.4	4.5	0.6	6.4	-5.1	5.6	1.2	21.00	28
B97-1/6-31+G(d,p)	6.1	-5.9	5.9	5.0	-4.2	4.2	6.0	-5.5	5.5	0.7	6.4	-5.8	5.8	1.2	21.00	40
B97-1/6-31+G(2d,p)	6.0	-5.7	5.7	4.9	-4.1	4.1	5.2	-4.0	4.5	0.6	5.0	-3.3	4.4	0.9	21.00	46
B97-1/6-311G(3d,2pd)	6.7	-6.3	6.3	5.6	-4.8	4.8	4.5	-0.6	4.3	0.6	4.2	-1.3	4.1	0.8	21.00	130
B97-1/6-311+G(2df,2p)	5.8	-5.5	5.5	4.8	-4.1	4.1	4.8	-2.3	4.5	0.6	4.9	-2.2	4.7	1.0	21.00	108
B97-1/MG3S	5.8	-5.5	5.5	4.9	-4.1	4.1	4.8	-2.3	4.5	0.6	4.6	-1.7	4.4	0.9	21.00	110
B98/6-31G(d)	6.7	-5.5	5.5	5.5	-3.6	4.0	5.6	-4.8	4.8	0.6	6.6	-5.7	5.7	1.2	21.98	29
B98/6-31+G(d,p)	5.8	-5.7	5.7	4.8	-4.1	4.1	7.0	-6.8	6.8	0.9	7.2	-6.3	6.3	1.3	21.98	43
B98/6-31+G(2d,p)	5.6	-5.5	5.5	4.6	-4.0	4.0	5.7	-5.2	5.2	0.7	5.3	-3.8	4.2	0.9	21.98	48
B98/6-311G(3d,2pd)	6.3	-6.1	6.1	5.2	-4.6	4.6	3.5	-1.9	3.4	0.4	3.2	-1.8	2.8	0.6	21.98	141
B98/6-311+G(2df,2p)	5.4	-5.3	5.3	4.5	-4.0	4.0	4.2	-3.3	3.4	0.4	3.9	-2.5	3.3	0.7	21.98	121
B98/MG3S	5.4	-5.3	5.3	4.5	-4.0	4.0	4.2	-3.3	3.4	0.4	3.6	-2.0	3.0	0.6	21.98	124

Table S2. (Continued)

Method	BH4			BH6			AE3				AE6				HF%	cost(s)
	RMSE	MSE	MUE	RMSE	MSE	MUE	RMSE	MSE	MUE	MUE/ Bond	RMSE	MSE	MUE	MUE/ Bond		
MPW1K/6-31G(d)	4.3	-1.0	3.8	3.5	-0.7	2.7	16.7	-14.3	14.3	1.9	17.3	-15.0	15.0	3.1	42.80	26
MPW1K/6-31+G(d,p)	2.0	-1.2	1.7	1.7	-1.0	1.4	17.7	-15.1	15.1	2.0	17.5	-14.9	14.9	3.1	42.80	41
MPW1K/6-31+G(2d,p)	1.6	-1.0	1.4	1.3	-0.9	1.2	16.1	-14.1	14.1	1.8	15.3	-12.6	12.6	2.6	42.80	46
MPW1K/6-311G(3d,2pd)	2.3	-1.7	1.8	2.2	-1.8	1.8	13.6	-11.9	11.9	1.6	13.1	-11.1	11.1	2.3	42.80	131
MPW1K/6-311+G(2df,2p)	1.5	-1.0	1.4	1.5	-1.2	1.4	14.2	-12.6	12.6	1.6	13.5	-11.4	11.4	2.4	42.80	122
MPW1K/MG3S	1.5	-1.0	1.4	1.5	-1.1	1.4	14.2	-12.6	12.6	1.6	13.0	-10.9	10.9	2.3	42.80	127
B97-2/6-31G(d)	5.9	-4.3	4.3	4.9	-2.4	3.3	2.3	-0.6	1.8	0.2	5.6	-3.6	4.2	0.9	21.00	38
B97-2/6-31+G(d,p)	4.7	-4.5	4.5	3.8	-2.9	3.1	2.7	-2.3	2.3	0.3	5.4	-4.1	4.1	0.8	21.00	57
B97-2/6-31+G(2d,p)	4.5	-4.4	4.4	3.7	-2.8	3.0	2.0	-1.2	1.4	0.2	4.1	-1.9	3.1	0.6	21.00	64
B97-2/6-311G(3d,2pd)	5.4	-5.0	5.0	4.5	-3.5	3.8	2.7	1.0	2.0	0.3	3.7	-0.6	3.2	0.7	21.00	143
B97-2/6-311+G(2df,2p)	4.5	-4.3	4.3	3.7	-2.9	3.2	2.5	-0.4	2.1	0.3	4.3	-1.2	3.8	0.8	21.00	154
B97-2/MG3S	4.5	-4.3	4.3	3.7	-2.9	3.2	2.5	-0.4	2.1	0.3	3.9	-0.7	3.5	0.7	21.00	167
O3LYP/6-31G(d)	7.2	-5.8	5.8	6.1	-4.2	4.8	5.9	3.9	3.9	0.5	7.4	-1.3	5.2	1.1	11.61	19
O3LYP/6-31+G(d,p)	6.1	-5.7	5.7	5.4	-4.6	4.7	4.6	0.1	4.2	0.5	7.4	-3.0	5.9	1.2	11.61	31
O3LYP/6-31+G(2d,p)	5.8	-5.6	5.6	5.1	-4.5	4.5	3.9	1.4	3.0	0.4	6.6	-1.9	4.2	0.9	11.61	35
O3LYP/6-311G(3d,2pd)	6.6	-6.4	6.4	5.7	-5.3	5.3	4.3	3.9	3.9	0.5	4.6	0.8	3.5	0.7	11.61	100
O3LYP/6-311+G(2df,2p)	5.6	-5.4	5.4	4.9	-4.5	4.5	1.4	1.1	1.1	0.1	4.1	-0.7	2.5	0.5	11.61	92
O3LYP/MG3S	5.6	-5.4	5.4	4.9	-4.4	4.4	1.4	1.1	1.1	0.1	3.6	-0.2	2.4	0.5	11.61	91
BB25/6-31G(d)	6.2	-4.7	4.7	5.1	-3.4	3.4	3.5	2.0	3.1	0.4	5.3	-1.7	4.3	0.9	25.00	40
BB25/6-31+G(d,p)	4.9	-4.8	4.8	4.1	-3.7	3.7	2.4	-0.8	2.4	0.3	4.8	-2.9	3.6	0.7	25.00	58
BB25/6-31+G(2d,p)	4.7	-4.6	4.6	3.9	-3.6	3.6	1.9	0.2	1.8	0.2	3.9	-0.7	3.0	0.6	25.00	62
BB25/6-311G(3d,2pd)	5.4	-5.2	5.2	4.6	-4.2	4.2	2.9	2.3	2.3	0.3	3.6	0.7	3.2	0.7	25.00	133
BB25/6-311+G(2df,2p)	4.5	-4.4	4.4	4.0	-3.7	3.7	1.5	0.6	1.1	0.1	3.8	-0.2	3.1	0.6	25.00	121
BB25/MG3S	4.7	-4.6	4.6	4.0	-3.7	3.7	1.8	1.0	1.3	0.2	3.8	0.9	2.9	0.6	25.00	139

Notes:

- 1 The geometries of all molecules were optimized at the QCISD level with the MG3 basis set. The QCISD/MG3 geometries for all molecules in BH6 and AE6 can be obtained from the Truhlar group database website: <http://comp.chem.umn.edu/database>
- 2 HF% denotes the fraction X of the Hartree-Fock exchange in each method; it is given as a percentage.
- 3 Cost is defined as the total computer time in seconds to run the BH6 test suite on a single processor of an IBM Regatta computer.
- 4 BH4 and AE4 are the subsets of BH6 and AE6 that contain no atom heavier than F.
- 5 To obtain MUE/bond from MUE, we divide MUE by the average number of bonds in the data set; this average number of bonds is 7.667 for AE3 and 4.833 for AE6.