Supporting Information for "Multi-Coefficient Density Functional Theory (MC-DFT)"

Jien-Lian Chen,Yi-Lun Sun, Kuo-Jui Wu, Wei-Ping Hu*
Department of Chemistry and Biochemistry, National Chung Cheng University
Chia-Yi, Taiwan 621

E-mail: chewph@ccu.edu.tw
Fax: 886-5-272-1040

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TABLE S1: Performance on 109 Atomization Energies and the Parameters of the Hybrid MC-DFT Methods

	MUE (kcal/mol)	X	c_1	c_2
B1B95-AE				
cc-pVTZ	3.13	26		
cc-pVDZ/cc-pVTZ	2.08	33	1.684	
cc-pVDZ/cc-pVTZ/aug-cc-pVDZ	1.93	33	1.476	0.284
MG3S	2.58	28		
6-31+G(d,p)/MG3S	2.58	28	1.065	
pc-2	2.69	27		
pc-1/pc-2	2.20	31	1.373	
pc-1/pc-2/aug-pc-1	2.14	34	1.247	0.506
MPW1B95-AE				
cc-pVTZ	3.10	33		
cc-pVDZ/cc-pVTZ	2.97	36	1.228	
cc-pVDZ/cc-pVTZ/aug-cc-pVDZ	2.30	36	1.085	0.715
MG3S	2.56	34		
6-31+G(d,p)/MG3S	2.54	34	1.057	
pc-2	2.79	33		
pc-1/pc-2	2.74	35	1.160	
pc-1/pc-2/aug-pc-1	2.51	37	0.835	0.831
MPW1PW91-AE				
cc-pVTZ	4.02	18		
cc-pVDZ/cc-pVTZ	3.24	26	1.595	
cc-pVDZ/cc-pVTZ/aug-cc-pVDZ	3.06	26	1.523	0.561
MG3S	3.45	20		
6-31+G(d,p)/MG3S	3.35	22	1.306	
TPSS1KCIS-AE				
cc-pVTZ	3.57	13		
cc-pVDZ/cc-pVTZ	3.55	13	1.046	
cc-pVDZ/cc-pVTZ/aug-cc-pVDZ	3.37	13	0.979	0.637
MG3S	3.17	13		
6-31+G(d,p)/MG3S	2.79	18	1.545	
B3LYP				
cc-pVTZ	4.83	20		
cc-pVDZ/cc-pVTZ	3.39	20	1.333	
cc-pVDZ/cc-pVTZ/aug-cc-pVDZ	3.35	20	1.370	-0.219
MG3S	4.28	20		

6-31+G(d,p)/MG3S	3.34	20	1.574	
pc-2	4.62	20		
pc-1/pc-2	3.22	20	1.439	
pc-1/pc-2/aug-pc-1	3.21	20	1.502	-0.253
B98				
cc-pVTZ	4.12	21.98		
cc-pVDZ/cc-pVTZ	2.05	21.98	1.399	
cc-pVDZ/cc-pVTZ/aug-cc-pVDZ	2.04	21.98	1.377	0.144
MG3S	3.02	21.98		
6-31+G(d,p)/MG3S	2.68	21.98	1.278	
pc-2	3.52	21.98		
pc-1/pc-2	2.06	21.98	1.459	
pc-1/pc-2/aug-pc-1	1.94	21.98	1.646	-0.492
BMK				
cc-pVTZ	3.08	42		
cc-pVDZ/cc-pVTZ	2.50	42	1.212	
cc-pVDZ/cc-pVTZ/aug-cc-pVDZ	2.38	42	1.123	0.450
MG3S	2.22	42		
6-31+G(d,p)/MG3S	2.20	42	1.058	

TABLE S2: Performance on the Barrier Heights and the Parameters of the Hybrid MC-DFT Methods

	MUE (kcal/mol)						
	HTBH	NHTBH	BH-average	AE	X	c_1	c_2
B1B95-BH							
cc-pVTZ	1.35	2.40	2.00	8.53	45		
cc-pVDZ/cc-pVTZ	0.91	1.10	0.98	3.46	39	1.981	
cc-pVDZ/cc-pVTZ/aug-cc-pVDZ	0.92	1.05	0.96	2.59	39	1.767	0.109
MG3S	1.16	1.44	1.29	6.31	42		
6-31+G(d,p)/MG3S	1.03	1.41	1.23	4.89	42	1.706	
MPW1B95-BH							
cc-pVTZ	1.42	2.49	2.08	6.99	48		
cc-pVDZ/cc-pVTZ	0.91	1.18	1.02	5.49	42	2.026	
cc-pVDZ/cc-pVTZ/aug-cc-pVDZ	0.92	1.17	1.01	5.07	42	1.954	0.037
MG3S	1.29	1.68	1.49	4.62	44		
6-31+G(d,p)/MG3S	1.31	1.42	1.35	3.79	43	1.291	
MPW1PW91-BH							
cc-pVTZ	1.40	2.79	2.19	13.36	46		
cc-pVDZ/cc-pVTZ	1.33	1.76	1.49	4.84	41	1.924	
cc-pVDZ/cc-pVTZ/aug-cc-pVDZ	1.27	1.70	1.43	8.39	41	1.315	0.325
MG3S	1.32	1.85	1.54	11.02	42.8		
6-31+G(d,p)/MG3S	1.32	1.85	1.54	11.02	42.8	1.000	
TPSS1KCIS-BH							
cc-pVTZ	1.90	2.92	2.53	11.30	43		
cc-pVDZ/cc-pVTZ	1.75	1.74	1.68	6.17	36	2.102	

cc-pVDZ/cc-pVTZ/aug-cc-pVDZ	1.62	1.68	1.59	6.06	36	1.562	0.287
MG3S	1.72	1.70	1.66	9.43	40		
6-31+G(d,p)/MG3S	1.73	1.53	1.60	6.00	38	1.905	
B3LYP							
cc-pVTZ	4.75	6.23	5.70	4.83	20		
cc-pVDZ/cc-pVTZ	3.04	3.70	3.35	11.57	20	2.540	
cc-pVDZ/cc-pVTZ/aug-cc-pVDZ	3.12	3.54	3.31	16.02	20	3.084	-0.255
MG3S	4.23	4.59	4.41	4.28	20		
6-31+G(d,p)/MG3S	3.50	4.28	3.87	11.30	20	3.961	
B98							
cc-pVTZ	4.49	4.91	4.93	4.12	21.98		
cc-pVDZ/cc-pVTZ	2.32	2.50	2.42	12.99	21.98	2.737	
cc-pVDZ/cc-pVTZ/aug-cc-pVDZ	2.25	2.30	2.27	18.49	21.98	3.355	-0.437
MG3S	4.16	3.38	3.78	3.02	21.98		
6-31+G(d,p)/MG3S	3.54	2.96	3.26	10.04	21.98	3.183	
BMK							
cc-pVTZ	1.62	2.75	2.34	3.08	42		
cc-pVDZ/cc-pVTZ	1.36	1.06	1.17	8.85	42	2.028	
cc-pVDZ/cc-pVTZ/aug-cc-pVDZ	1.31	1.08	1.16	6.56	42	1.769	0.132
MG3S	1.32	1.56	1.44	2.22	42		
6-31+G(d,p)/MG3S	1.32	1.22	1.25	3.96	42	1.608	