ADDITIONS AND CORRECTIONS

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Yan Zhao, Núria González-García, and Donald G. Truhlar*: Benchmark Database of Barrier Heights for Heavy Atom Transfer, Nucleophilic Substitution, Association, and Unimolecular Reactions and its Use to Test Theoretical Methods

Pages 2015−2016. In Tables 4 and 5, when we calculated the total MSE and MUE for the NHTBH38/04 database, we accidentally excluded the barrier heights of the $CH_3 + FCl \rightarrow CH_3F + Cl$ reaction. In addition, footnote *a* was in the wrong place in Table 5. Here, we give the corrected columns of these tables.

TABLE 4: Mean Errors (kcal/mol) for the NHTBH38/04 Database

	total (38)	
methods	MSE	MUE
Pure DFT or Meta DFT		
VSXC	−4.82	5.21
mPWKCIS	−7.82	7.92
BB95	−7.91	7.95
TPSSKCIS	−8.11	8.22
MPWPW91	−8.29	8.41
PBE	−8.43	8.53
BP86	−8.71	8.83
TPSS	−8.90	8.95
BLYP	−9.06	9.09
mPWLYP	−9.36	9.40
LSDA	−12.35	12.55
Hybrid DFT		
MPW1K	0.46	1.77
BHandHLYP	0.62	2.07
B97-2	−1.43	2.23
mPW1PW91	−2.75	3.23
B98	−2.96	3.40
B97-1	−3.05	3.47
PBE1PBE	−3.03	3.52
X3LYP	−4.27	4.44
B3LYP	−4.42	4.58
O3LYP	−1.78	5.07
Hybrid Meta DFT		
BB1K	0.44	1.42
MPWB1K	0.35	1.46
MPWKCIS1K	0.38	1.66
B1B95	−2.05	2.27
MPW1B95	−1.94	2.31
MPW1KCIS	−4.54	4.74
TPSS1KCIS	−5.35	5.54
TPSSh	−6.84	6.92
Ab Initio WFT		
QCISD(T)	0.14	0.98
QCISD	1.89	1.92
MP4SDQ	4.12	4.14
MP2	5.27	5.46
MP3	5.96	5.96
HF	8.21	9.14

TABLE 5: Mean Errors (kcal/mol) for the NHTBH38/04 and HTBH38/04 Databases

	non-hydrogen transfer (38)		total (76)		weighted average[a]	
methods	MSE	MUE	MSE	MUE	MSE	MUE
Pure DFT or Meta DFT						
VSXC	−4.82	5.21	−4.84	5.04	−4.63	5.00
TPSSKCIS	−7.82	7.92	−7.41	7.47	−7.50	7.60
mPWKCIS	−7.91	7.95	−7.69	7.71	−7.73	7.78
BB95	−8.11	8.22	−8.13	8.18	−7.93	8.03
BLYP	−8.29	8.41	−7.91	7.96	−7.94	8.04
MPWPW91	−8.43	8.53	−8.43	8.48	−8.32	8.42
TPSS	−8.71	8.83	−8.21	8.27	−8.39	8.50
BP86	−8.90	8.95	−9.03	9.06	−8.85	8.90
PBE	−9.06	9.09	−9.19	9.20	−8.94	8.97
mPWLYP	−9.36	9.40	−8.96	8.98	−9.03	9.06
LSDA	−12.35	12.55	−15.04	15.13	−13.72	13.90
Hybrid DFT						
MPW1K	0.46	1.77	−0.07	1.55	0.16	1.73
BHandHLYP	0.62	2.07	0.79	2.40	0.68	2.28
B97-2	−1.43	2.23	−2.26	2.74	−1.76	2.54
mPW1PW91	−2.75	3.23	−3.15	3.39	−2.93	3.37
B98	−2.96	3.40	−3.56	3.78	−3.15	3.57
B97-1	−3.05	3.47	−3.72	3.93	−3.25	3.65
PBE1PBE	−3.03	3.52	−3.63	3.87	−3.33	3.76
X3LYP	−4.27	4.44	−4.12	4.26	−4.19	4.38
B3LYP	−4.42	4.58	−4.28	4.40	−4.32	4.50
O3LYP	−1.78	5.07	−2.88	4.57	−2.66	4.76
Hybrid Meta DFT						
BB1K	0.44	1.42	−0.06	1.29	0.13	1.37
MPWB1K	0.35	1.46	−0.25	1.37	0.00	1.45
MPWKCIS1K	0.38	1.66	0.26	1.68	0.30	1.73
B1B95	−2.05	2.27	−2.42	2.53	−2.27	2.45
MPW1B95	−1.94	2.31	−2.48	2.66	−2.24	2.54
MPW1KCIS	−4.54	4.74	−4.47	4.57	−4.45	4.64
TPSS1KCIS	−5.35	5.54	−5.02	5.11	−5.06	5.24
TPSSh	−6.84	6.92	−6.40	6.44	−6.55	6.62
Ab Initio WFT						
QCISD(T)	0.14	0.98	0.65	1.11	0.47	1.02
QCISD	1.89	1.92	2.31	2.36	2.11	2.16
MP4SDQ	4.12	4.14	4.01	4.02	4.25	4.26
MP2	5.27	5.46	4.48	4.80	5.23	5.52
MP3	5.96	5.96	5.20	5.20	5.70	5.70
HF	8.21	9.14	10.75	11.40	9.38	10.25

[a] This is calculated by using 1/4 times MSE (or MUE) for heavy-atom transfer reaction barrier heights plus 1/4 times MSE (or MUE) for S_N2 reaction barrier heights plus 1/4 times MSE (or MUE) for unimolecular and association reaction barrier heights plus 1/4 times MSE (or MUE) for hydrogen transfer reaction barrier heights.

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