ADDITIONS AND CORRECTIONS

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Ambili S. Menon, Geoffrey P. F. Wood, Damian Moran, and Leo Radom*: Bond Dissociation Energies and Radical Stabilization Energies: An Assessment of Contemporary Theoretical Procedures

Page 13638. As a consequence of using an incorrect value for the B3-LYP/6-31G(d) C−H bond length in methane, the bond dissociation energies (BDEs) for methane, and hence all the radical stabilization energies (RSEs), obtained with density functional theory (DFT) procedures and listed respectively in Tables 1 (page 13640) and 2 (page 13642), are incorrect. However, none of our qualitative conclusions are affected. The corrected BDEs for methane are presented in Table 1, and the corrected RSEs are compared with W1 and experimental values in Table 2.

TABLE 1: Bond Dissociation Energies of Methane (0 K, kJ mol^{-1})

method	BDE	method	BDE
UBMK	430.6	UM05−2X	427.8
RBMK	434.7	UB2-PLYP	423.3
UMPWB1K	430.4	RB2-PLYP	427.1
RMPWB1K	434.3	UMPW2-PLYP	423.8
UM05	425.4	RMPW2-PLYP	427.7

TABLE 2: Comparison of Calculated Radical Stabilization Energies with W1 and Experimental Values (0 K, kJ mol^{-1})

radical ($^{\bullet}\mathrm{CH_2X}$)	UBMK	RBMK	UMPWB1K	RMPWB1K	UM05	UM05-2X	UB2-PLYP	RB2-PLYP	UMPW2-PLYP	RMPW2-PLYP	W1	expt
$^{\bullet}\mathrm{CH_2NH_2}$	54.1	54.4	54.5	54.3	51.5	51.6	51.6	51.9	51.1	51.2	49.3	45.6 ± 8.4
$^{\bullet}\mathrm{CH_2OH}$	39.1	39.4	39.3	39.1	36.6	35.4	36.6	36.9	36.1	36.2	35.3	36.5 ± 0.63
$^{\bullet}\mathrm{CH_2OCH_3}$	39.4	39.8	37.4	38.8	36.6	35.0	36.9	37.3	36.2	36.4	35.2	36.6
$^{\bullet}\mathrm{CH_2F}$	16.4	16.8	17.5	17.7	14.9	13.5	15.6	15.8	15.1	15.3	14.8	15.0 ± 4.2
$^{\bullet}\mathrm{CH_2CH_3}$	17.5	17.1	19.1	18.8	22.5	17.5	17.4	17.2	17.2	17.0	15.8	19.3 ± 1.3
$^{\bullet}\mathrm{CH_2CH_2CH_3}$	14.5	14.2	15.1	15.2	19.0	14.2	14.2	14.2	13.9	13.8	12.7	17.6 ± 2.1
$^{\bullet}\mathrm{CH_2CF_3}$	−5.9	−6.1	−5.4	−4.4	−0.4	−5.6	−4.1	−4.1	−4.6	−4.7	−6.1	−6.9 ± 4.5
$^{\bullet}\mathrm{CH_2CF_2CF_3}$	−2.4	−2.6	−2.8	−1.2	2.6	−2.6	−1.2	−1.2	−1.7	−1.7		
$^{\bullet}\mathrm{CH_2PH_2}$	30.9	30.2	30.8	29.6	33.7	28.1	28.7	28.1	28.5	27.6	27.0	
$^{\bullet}\mathrm{CH_2SH}$	37.9	37.4	43.4	42.2	44.0	40.5	40.8	40.5	40.3	39.7	41.4	46.1 ± 8.4
$^{\bullet}\mathrm{CH_2Cl}$	20.7	20.2	26.4	25.6	27.1	22.9	23.2	22.9	22.8	22.4	23.0	20.5 ± 2.3
$^{\bullet}\mathrm{CH_2Br}$	17.8	17.2	20.5	19.7	22.8	13.9	17.0	16.8	16.6	16.3		22.1 ± 2.4
$^{\bullet}\mathrm{CH_2BH_2}$	47.8	48.8	44.3	45.7	43.7	42.8	42.8	43.9	42.7	43.8	40.9	
$^{\bullet}\mathrm{CH_2CH{=}CH_2}$	74.6	66.6	77.2	67.3	85.2	76.6	71.8	70.5	72.2	69.0	70.3	68.9 ± 3
$^{\bullet}\mathrm{CH_2C{\equiv}CH}$	59.2	53.0	61.8	54.3	67.7	58.9	55.9	56.5	55.9	55.0	53.6	54.7 ± 4.2
$^{\bullet}\mathrm{CH_2C_6H_5}$	62.3	56.8	63.5	57.0	72.1	62.0	54.5	58.3	55.1	57.1	59.1	61.6 ± 5.0
$^{\bullet}\mathrm{CH_2CHO}$	40.7	35.8	43.0	36.8	43.0	41.8	36.8	38.1	37.1	37.2	36.6	39.8
$^{\bullet}\mathrm{CH_2COOH}$	25.4	24.0	26.6	25.4	30.1	26.3	25.3	25.6	25.0	25.0	23.7	24.7 ± 3.3
$^{\bullet}\mathrm{CH_2COOCH_3}$	25.7	24.4	26.8	25.9	30.8	26.5	25.8	26.2	25.5	25.6	23.3	31.3 ± 10.5
$^{\bullet}\mathrm{CH_2OCOCH_3}$	25.4	25.7	25.4	25.7	26.6	21.1	23.1	23.4	22.5	22.6	17.5	34.0
$^{\bullet}\mathrm{CH_2CN}$	36.7	31.3	40.2	33.2	43.8	36.0	34.4	36.1	34.5	34.7	33.1	32.8 ± 4.2
$^{\bullet}\mathrm{CH_2NO_2}$	18.0	16.9	17.0	15.4	20.9	15.0	15.2	15.6	14.7	14.8	13.5	22.7
MD (W1)	3.0	1.5	4.1	2.3	6.5	1.9	1.4	1.8	1.1	1.0		
MAD (W1)	3.6	3.1	4.1	2.8	6.5	2.1	1.9	1.9	1.7	1.6		
LD (W1)	−3.5	−4.0	8.2	8.2	14.9	6.3	5.6	5.9	−4.1	5.2		
MD (expt)	0.8	−1.1	3.0	0.5	5.6	0.4	−0.3	0.1	−0.5	−0.7	−0.8	
MAD (expt)	3.3	3.2	4.0	2.7	5.9	3.5	3.0	2.8	2.9	2.6	2.1	
LD (expt)	−8.2	−8.7	8.9	8.7	16.3	−8.2	−7.1	6.3	−6.6	−5.8	−4.9	

Supporting Information Available: Table S1 contains the revised total energies that lead to the revised BDEs and RSEs given in Tables 1 and 2 above, and in more detail in Tables S2 and S3 of the Supporting Information. This material is available free of charge via the Internet at http://pubs.acs.org.

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