J Mol Model (2011) 17:1223–1226
DOI 10.1007/s00894-010-0813-6

ERRATUM

Erratum to: A UB3LYP and UMP2 theoretical investigation on unusual cation-π interaction between the triplet state HB=BH $\left(^3\Sigma_g^-\right)$ and H^+, Li^+, Na^+, Be^{2+} or Mg^{2+}

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Published online: 31 July 2010

Erratum to: J Mol Model (2010) 16:615–627
DOI: 10.1007/s00894-009-0575-1

Erratum to: J Mol Model (2010) 16:823
DOI: 10.1007/s00894-009-0588-9

Unfortunately, 147 erroneous values are found in Tables 2 and 7. The corrected data are given as following (see Tables 2 and 7 (in bold)). The author, *Wen-zheng Xu*, and the corresponding affiliation (*School of Automation Science and Electrical Engineering, Beijing University of Aeronautics and Astronautics, Beijing, 100191, China*) are deleted. Thus, the authors and the affiliations should be corrected as following:

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The online version of the original article can be found at http://dx.doi.org/10.1007/s00894-009-0575-1.

The online version of the original article can be found at http://dx.doi.org/10.1007/s00894-009-0588-9.

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Table 2 Binding energies of the cation-π complexes ($-D_e$ (kJ/mol))

	HB=BH$\left(^3\Sigma_g^-\right)$…$H^+$	HB=BH$\left(^3\Sigma_g^-\right)$…$Li^+$	HB=BH$\left(^3\Sigma_g^-\right)$…$Na^+$	HB=BH$\left(^3\Sigma_g^-\right)$…$Be^{2+}$	HB=BH$\left(^3\Sigma_g^-\right)$…$Mg^{2+}$
UMp2(full)/6-311++G**	**623.56 (617.11)**[a]	**51.77 (48.52)**	30.73 **(27.68)**	**497.66 (491.54)**	**243.28 (239.03)**
UMp2(full)/6-311++G(2df,2p)	**620.90 (617.45)**[a]	**53.75** (51.39)	**35.16** (32.80)	**497.53 (493.16)**	**248.98 (245.54)**
	597.57[b]	**49.60**	**31.75**	**493.98**	**245.71**
UMP2(full)/aug-cc-pVTZ	**624.34 (617.68)**	**58.05 (52.11)**	**40.89** (31.13)	**513.95 (491.84)**	**261.27 (245.72)**
	598.59	**50.55**	29.76	**493.47**	**246.14**
UB3LYP/6-311++G(2df,2p)	**620.63**	**57.08 (56.34)**	**37.68 (36.15)**	**530.92 (530.29)**	**284.51 (283.53)**
		54.54	35.00	**531.53**	**284.10**
UB3LYP/aug-cc-pVTZ	**621.29**	58.02 **(57.44)**	37.40 **(37.08)**	**532.61 (531.86)**	**286.84 (286.47)**
		55.66	**35.94**	**533.14**	**287.06**
	HB=BH($^1\Delta_g$)…H^+	HB=BH($^1\Delta_g$)…Li^+	HB=BH($^1\Delta_g$)…Na^+	HB=BH($^1\Delta_g$)…Be^{2+}	HB=BH($^1\Delta_g$)…Mg^{2+}
MP2(full)/6-311++G** [c]	857.88 (852.87)[a]	116.39 (111.78)	78.88 (74.64)	723.21 (716.60)	411.32 (405.84)
MP2(full)/6-311++G(2df,2p)[c]	851.12 (848.43)[a]	115.63 (112.43)	81.78 (77.26)	714.92 (710.37)	410.40 (406.32)
	832.31[b]	109.23	75.16	707.92	404.68
MP2(full)/aug-cc-pVTZ[c]	854.36 (849.32)	119.15 (112.88)	86.11 (75.84)	725.61 (708.08)	419.61 (405.45)
	834.26	110.07	73.54	706.13	404.20
B3LYP/6-311++G(2df,2p)[c]	849.65	120.34 (119.55)	88.08 (86.43)	744.54 (743.97)	453.35 (452.11)
		116.51	84.35	742.09	450.81
B3LYP/aug-cc-pVTZ[c]	849.82	120.97 (120.43)	87.33 (87.04)	745.85 (745.26)	455.02 (454.67)
		117.49	85.05	743.57	453.51
	H_2C=CH_2…H^+	H_2C=CH_2…Li^+	H_2C=CH_2…Na^+	H_2C=CH_2…Be^{2+}	H_2C=CH_2…Mg^{2+}
Mp2(full)/6-311++G**	**703.04 (693.86)**[a]	**88.40 (82.13)**	**57.02** (51.54)	**565.72 (554.86)**	**295.81 (287.63)**
Mp2(full)/6-311++G(2df,2p)	**695.08 (690.23)**[a]	**88.91** (84.72)	**60.72 (55.22)**	**564.11 (557.77)**	**302.43 (296.75)**
	662.54[b]	**79.87**	**51.64**	**554.82**	**293.07**
MP2(full)/aug-cc-pVTZ	**701.11 (691.98)**	**94.52 (86.29)**	**66.57** (54.65)	**585.79 (559.79)**	**319.69 (299.36)**
	663.84	**81.38**	**52.28**	**557.03**	**296.02**
B3LYP/6-311++G(2df,2p)	**703.51**	**91.77 (90.97)**	**62.46 (60.65)**	**593.51 (591.70)**	**331.53 (330.22)**
		86.35	**57.18**	**589.28**	**327.22**
B3LYP/aug-cc-pVTZ	**705.07**	**93.27 (92.60)**	**62.23** (61.81)	**596.52 (595.63)**	**334.91 (334.39)**
		87.93	58.25	**593.21**	**331.38**
	HC≡CH…H^+	HC≡CH…Li^+	HC≡CH…Na^+	HC≡CH…Be^{2+}	HC=CH…Mg^{2+}
Mp2(full)/6-311++G** [c]	652.92 (642.39)[a]	87.94 (80.26)	55.60 (49.09)	542.79 (530.34)	273.14 (263.69)
Mp2(full)/6-311++G(2df,2p)[c]	646.95 (641.79)[a]	87.43 (83.04)	58.42 (53.11)	541.08 (534.22)	280.75 (274.87)
	619.93[b]	79.53	50.93	531.78	272.83
MP2(full)/aug-cc-pVTZ[c]	653.11 (643.73)	91.64 (84.49)	63.51 (52.60)	561.41 (535.74)	295.98 (277.32)
	621.98	81.34	50.39	533.78	275.44

B3LYP/6-311++G(2df,2p)[c]	661.88	91.83 (91.00)	60.88 (59.25)	573.98 (573.20)	308.77 (307.48)
		87.67	57.17	572.76	306.37
B3LYP/aug-cc-pVTZ[c]	663.53	93.27 (92.62)	60.55 (60.15)	576.82 (575.89)	312.02 (311.51)
		89.37	58.15	575.66	310.61

[a] The value in the parenthesis is BSSE-corrected ($-D_{e(\mathrm{BSSE})}$).

[b] The binding energy is ΔE with BSSE and ZPE ($-D_{e(\mathrm{BSSE\text{-}ZPE})}$) correction.

[c] Calculated values from Ref. [1].

Table 7 Binding energies of the σ-binding 1:1 and 2:1 complexes between BH and the cations at B3LYP/6-311++G(2df,2p) level ($-D_e$ (kJ/mol))

HB…H^+		HB…Li^+		HB…Na^+		HB…Be^{2+}		HB…Mg^{2+}	
894.17[a]	**862.64**[c]	**152.42**[a] **(151.65)**[b]	**140.44**[c]	**112.02 (110.19)**	**100.81**	**703.92 (703.28)**	**688.94**	**427.58 (426.22)**	**414.07**
HBH^+…BH		$HBLi^+$…BH		$HBNa^+$…BH		$HBBe^{2+}$…BH		$HBMg^{2+}$…BH	
-50.96203[d]	-51.02393[e]	-57.98697	-58.09420	-212.76260	-212.88947	-64.71640	-64.64264	-250.12630	-250.13691
-51.07831[f]		-58.08541		-212.87577		-64.69116		-250.16835	
69.27 (68.09)	**51.01**	**126.26 (124.94)**	**100.32**	**94.95 (92.66)**	**70.06**	**525.82 (524.68)**	**493.98**	**333.88 (331.94)**	**304.73**

[a] The uncorrected binding energies.

[b] The BSSE-corrected binding energies ($-D_{e(\mathrm{BSSE})}$).

[c] The binding energies with BSSE and ZPE ($-D_{e(\mathrm{BSSE\text{-}ZPE})}$) correction.

[d] The total energies of HBM^+/M^{2+}…BH.

[e] The total energies of $HB{=}BH\left(^3\Sigma_g^-\right)\ldots M^+/M^{2+}$.

[f] The total energies of $HB{=}BH(^1\Delta_g)\ldots M^+/M^{2+}$.