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Theoretical study of the borane and diborane positive ions

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Summary. We describe the geometric, electronic and energetic (ΔH_f) properties of $B_2H_6^+$ and BH_3^+. Comparisons with experimental measurements have also been made with borane, diborane, BH, BH^+ and BH_2^+. All the theoretical calculations have been performed with various basis sets: 6-31G, 6-31G** and 6-31$^+$G**(2*d*, *f*). The geometry optimizations are done at the SCF (RHF or UHF), MP2 and MP4 levels.

Key words: Boranes — Diboranes — Related positive ions — Electronic structures — Thermochemical properties — Appearance potential

1. Introduction

Although boranes have been known for a long time [1], there is still a lot of interest in them [2]. During the fifties and the sixties many experimental appearance potential measurements for the fragmentations of borane and diborane into ions such as $B_2H_n^+$ and BH_m^+ with $n = 0$ to 6 and $m = 0$ to 3 were reported. Even if appearance potentials can be measured within an accuracy of $\pm 10^{-2}$ eV and even if the simplest set of assumptions suffice for interpreting the data, the heats of formation of those ions remain uncertain. Indeed, the chemical processes which produce fragments are not always known and activation energies can alter the thermochemical values deduced from the appearance potentials. Moreover, ΔH_f determination for the ions requires accurate values for the heats of formation of borane and diborane. Efforts have been made during the last ten years to evaluate those quantities. From the experimental point of view, the short

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lifetime of BH_3 prevents the direct determination of its energy. From the theoretical point of view, the most accurate quantum chemical methods and the largest basis sets are needed to reach sufficiency accurate energies. At least polarized basis set are required [3] to get reliable stationary points on potential energy hypersurfaces. For example, a transition state with a 6-31G basis may in fact correspond to equilibrium structures with larger basis sets [4]. For the simple boron hydrides, Pople [5] has pointed out that the empirically derived heats of formation have been overestimated. Similarly, only high level theoretical methods give agreement with experimental values for the binding energy of borane. Calculated values between 35 [6] and 40 [7] kcal mol^{-1} may be compared with 35.5 [8] from kinetic studies, 37 to 39 [9] from electron impact measurements and 39.3 ± 6 [10] from recommended heats of formation from the JANAF tables [18]. The understanding of the electronic structure of boron derivatives including positive and negative ions has also been a subject of extensive study. One finds that similarities exist between boron and the carbon chemistry when both neutral molecules and ions (positive or negative) [11] are considered. The X.H.X bridged bond appears to be like protonated single (e.g. $B_2H_7^-$ [12]), double (e.g. B_2H_6 or $C_2H_3^{++}$ [13]) or triple ($B_2H_5^+$ [11]) bonds. Usually, one has more electron pairs than hydrogen atoms at one's disposal to build the electron description. This is not the case with ions such as BH_3^+ and $B_2H_6^+$. The electronic description of such chemically electron deficient compounds is of interest. Also note that BH_3^+ is isoelectronic with CH_3^{++} [14].

2. Results and discussion

Table 1 gives the geometrical parameters for the stationary points (at various theoretical levels). For BH_3^+, we obtain three equilibrium structures. Two of them correspond to the association complexes $BH_2^+ \cdots H$ and $BH^+ \cdots H_2$. The first ($BH_2^+ \cdots H$) has already been mentioned in a recent paper [15] as an alternative ion structure; however, we prefer to consider these structures as molecular complexes than as simple ions. (The electron distributions confirm this opinion.) From a geometrical point of view, BH_3^+ and $B_2H_6^+$ show large basis set and correlation effects; the molecular complexes seem to be particularly sensitive. For these compounds, accurate prediction requires post SCF (self consistent field) calculations (at least MP2) and polarized basis set (such as 6-31G**). For more conventional molecules or ions (where all bonds are at least two electron bonds), a single SCF treatment with polarized basis gives quite acceptable structures [16].

Table 2 shows the total energies obtained at different levels. The "extrapolated" values are obtained assuming additivity in the basis set expansion when one adds diffuse functions such as a second set of *d* or *f* functions to the polarized basis set. Some authors [17] use this procedure to obtain energies as accurately as possible; one of them [17b] writes:

$$\begin{aligned} E_{MP4}(6\text{-}31G^{**}(2d,f)) &\approx E_{MP4}(\text{extrapolated}) \\ &= E_{MP4}(6\text{-}31+G^{**}) + E_{MP4}(6\text{-}31G^{**}(2d)) \\ &\quad + E_{MP4}(6\text{-}31G^{**}(f)) - 2E_{MP4}(6\text{-}31G^{**}). \end{aligned} \tag{1}$$

When we compare the values obtained by such additivity assumptions (using the SCF equilibrium geometry) with more accurate MP4/6-31 + G**2*df*/MP4/6-31G** energies, we observe quite negligible differences. This confirms that the procedure introduced by Pople is an economical way to obtain reliable energies. Finally, basis set and correlation effects are both important. Choosing the energy of $BH^+ + H_2$ as the zero of energy, we find at the MP4 level the following energies (assuming relation (1)):

$[BH \cdots H_2]^+$	-23.5 kcal mol^{-1}	$BH_2^+ + H$	-15.3 kcal mol^{-1}
BH_3^+	-32.0 kcal mol^{-1}	$[BH_2 \cdots H]^+$	-29.9 kcal mol^{-1}

The $[BH_2 \cdots H]^+$ molecular complex lies on the dissociation path of BH_3^+ into the BH_2^+ and H fragments. The second complex ($[H_2 \cdots BH]^+$) lies on the dissociation path into H_2 and BH^+. On the potential energy hypersurface, both complexes must be separated from the BH_3^+ ion by transition structures. Finally, let us note that other dissociation products such as $BH + H_2^+$ and $BH_2 + H^+$, are, respectively, 134 and 112 kcal mol^{-1} higher in energy than $BH^+ + H_2$ (at the MP4/6-31 + G**2*df*//MP4/6-31G** level).

It is now possible to evaluate the heats of formation of the compounds of interest, as long as we include the zero point energies. Assuming a quadratic approximation for the potential energy hypersurface (close to the equilibrium structure), we can determine the frequencies of vibration by solving the CPHF (coupled perturbed Hartree–Fock) equations. As the frequencies obtained at the single determinantal level are usually overestimated, we have scaled the single determinant values using a relation previously established [4]:

$$\text{Nu(adjusted)} = -65.238 + 0.9556\ \text{Nu(6-31G**)} \approx \text{Nu(Exp)}. \qquad (2)$$

Statistical thermodynamics then gives access to the thermal correction ($\Delta H(00 \rightarrow 298\text{K})$), the standard entropy and the heat capacity. Values for BH_3, B_2H_6, BH_2^+, BH, BH^+, H_2 and H have been reported [4]; for borane and diborane positive ions, we calculated the following frequencies (cm^{-1}) at the SCF/6-31G** level:

for $B_2H_6^+$	267	565	625	693	731	999	1007	1010	1094
	1221	1525	1593	1925	2337	2492	2513	2801	2951
for BH_3^+	484	936	1045	1788	2328	3005			
for $[BH_2 \cdots H]^+$	505	827	1023	1066	2775	3013			
for $[BH \cdots H_2]^+$	761	940	1162	1762	2934	3379			

After scaling, one finds the following thermodynamic properties:

	$\Delta H(00 \rightarrow 298\text{K})$ (kcal mol^{-1})	S° (cal mol^{-1} K^{-1})	C_p (cal mol^{-1} K^{-1})
$B_2H_6^+$	37.67	16.72	61.01
BH_3^+	15.18	10.54	49.57
$[BH_2 \cdots H]^+$	14.70	11.08	51.75
$[BH \cdots H_2]^+$	16.90	9.83	50.51

Table 1. Optimized structures for both non-polarized [16] and polarized [16] basis set at the Hartree–Fock (HF) SCF level and for polarized basis set at the Møller–Plesset levels [16]

Compounds	Geometrical parameters	HF/6-31G	HF/6-31G**	MP2[a]/6-31G**	MP4[b]/6-31G**	Other work
$H_2BH_2BH_2$	BB	1.797	1.778	1.752	1.759	1.775[c]
$(D_{2h}-{}^1Ag)$	BH(t)	1.180	1.185	1.182	1.185	1.196
	BH(b)	1.318	1.317	1.305	1.307	1.339
	BBH(t)	119.05	119.02	119.06	19.06	120.2
	BBH(b)	47.10	47.54	47.77	47.79	
	H2B/BH2B	perpendic.	perpendic.	perpendic.	perpendic.	
$H_2BH_2BH_2^+$	BB	1.775	1.751	1.696	1.711	
$(C_s-{}^2A'')$	B′H(t)	1.170	1.173	1.176	1.179	
	B″H(t)	1.259	1.253	1.247	1.251	
	B′H(b)	1.476	1.453	1.403	1.410	
	B″H(b)	1.224	1.235	1.240	1.246	
	B″B′H(t)	114.60	114.56	115.67	115.43	
	B′B″H(t)	143.50	146.14	146.80	147.07	
	B″B′H(b)	43.03	44.14	46.00	45.69	
	B′B″H(b)	55.38	54.98	54.53	53.78	
	H2B′/B′H2B″	perpendic.	perpendic.	perpendic.	perpendic.	
	B′H2B″/B″H2	perpendic.	perpendic.	perpendic.	perpendic.	
BH_3	BH	1.186	1.188	1.184	1.186	1.160[c]
$(D_{3h}-{}^1A')$	HBH	120.00	120.00	120.00	120.00	120.00
$BH_2^+ \cdots H$	BH (twice)	1.164	1.171	1.177		1.171[d]
complex	B·H (once)	2.059	1.564	1.462		1.574
$(C_{2v}-{}^2A_1)$	HBH (once)	171.37	162.09	161.31		162.6
	HB·H (twice)	94.31	98.96	98.97		98.7

BH_3^+	BH (once)	1.160	1.162	1.163	1.165	1.164[d]
$(C_{2v}$–$^2B_2)$	BH (twice)	1.274	1.263	1.256	1.259	1.266
	HBH (twice)	141.22	144.06	145.44	145.24	142.5
	HBH (once)	77.56	71.89	69.12	69.53	75.0
$BH^+ \cdots H_2$	BH	1.168	1.168	1.169	1.171	
Complex	HH	0.794	0.818	0.858	0.865	
$(C_s$–$^2A')$	B···H	1.486	1.431	1.383	1.387	
	HB···H	98.89	99.37	102.36	103.01	
	HH···B	68.66	68.93	67.12	66.66	
BH_2^+	BH	1.164	1.1658	1.1671	1.169	
$(D_{\infty h}$–$^1\Sigma_g)$	HBH	180.00	180.00	180.00	180.00	
BH	BH	1.231	1.227	1.227	1.233	1.232[e]
$(C_{\infty v}$–$^1\Sigma^+)$						
BH^+	BH	1.184	1.184	1.188	1.195	1.215[e]
$(C_{\infty v}$–$^2\Sigma)$						
H_2	HH	0.730	0.733	0.734	0.737	
$(C_{\infty h}$–$^1\Sigma_g^+)$						

H(t) and H(b) stand respectively for terminal and bridged hydrogen atoms; all BH_3 and BH_3^+ structures are planar

[a] Second-order Møller–Plesset perturbation

[b] Fourth-order Møller–Plesset perturbation with single, double, triple and quadruple replacements

[c] JANAF85 [18]; [d] Pop88 [15]; [e] Lov83 [19]

Table 2. Total energies (a.u.) for the compounds of interest

Basis set level optimization level	E(HF/ 6-31G// HF/ 6-31G)	E(HF/ 6-31G**// Hf/ 6-31G**)	E(MP4/ Extrap[a]// HF/ 6-31G**)	E(MP2/ 6-31G**// MP2/ 6-31G**)	E(MP4/ 6-31G**// MP4/ 6-31G**)	E(MP4/ 6-31 + G**2df// MP4/ 6-31G**)
B_2H_6	−52.77544	−52.81986	−53.11433	−53.04890	−53.08049	−53.11346
$B_2H_6^+$	−52.37917	−52.42956	−52.69480	−52.63408	−52.66360	−52.69445
BH_3	−26.37679	−26.39287	−26.08014	−26.49090	−26.50755	−26.52253
BH_3^+	−25.95593	−25.97818	−26.08014	−26.05328	−26.06715	−26.08005
$[BH_2 \cdots H]^+$	−25.96234	−25.97889	−26.07331	−26.04858		
$[BH \cdots H_2]^+$	−25.93950	−25.96749	−26.06657	−26.04258	−26.05659	−26.06777
BH_2^+	−25.46111	−25.47339	−25.55531	−25.53536	−25.54675	−25.55535
BH	−25.10897	−25.11922	−25.22099	−25.18366	−25.20170	−25.21749
BH^+	−24.80906	−24.81644	−24.86458	−24.85282	−24.85986	−24.86482
B	−24.51949	−24.52204	−24.58907	−24.56246	−24.57594	−24.58909
B^+	−24.23404	−24.23406	−24.28855	−24.27150	−24.28779	−24.28855
H_2	−1.12683	−1.13133	−1.16453	−1.15766	−1.16457	−1.16457
H_2^+	−0.58408	−0.59450	−0.59450	−0.59450	−0.59450	−0.59450
H	−0.49823	−0.49823	−0.49823	−0.49823	−0.49823	−0.49823

[a] Extrapolated energies according to relation (1)

Table 3. Heats of formations of the boron derivatives (kcal mol^{-1})

Compound	Isogyric reaction	ΔH_f(Th.) (a)	ΔH_f(Th.) (b)	ΔH_f(Ref.)	References [22]
B_2H_6	$B_2H_6 + 2H \rightarrow 2B + 4H^2$	1.03	1.70	8.51	NBS82 (6.5 to 17.3)
$B_2H_6^+$	$B_2H_6^+ + H \rightarrow 2B + 3H_2 + H^+$	265.83	266.15	272.39	NBS82
				275.	Ross77
BH_3	$BH_3 + H \rightarrow B + 2H_2$	20.15	20.17	23.90	NBS82 (18 to 41.70)
$H_2 \cdots BH^+$	$BH_3^+ \rightarrow B + H_2 + H^+$	309.66	308.94	—	None
BH_3^+	$BH_3^+ \rightarrow B + H_2 + H^+$	299.43	299.52	308.00	±2.3 Wil67
$H \cdots BH_2^+$	$BH_3^+ \rightarrow B + H_2 + H^+$	305.43	—	—	None
BH_2^+	$BH_2^+ + H \rightarrow B + H_2 + H^+$	263.06	263.07	270.43	Wil67
BH	$BH + H \rightarrow B + H_2$	101.20	103.43	107.46	NBS82
BH^+	$BH^+ \rightarrow B + H^+$	330.17	330.03	334.20	NBS82
				332.	Ros77 from Bau64
B^+	$B^+ + H \rightarrow B + H^+$	324.06	324.07	326.65	±4 JANAF85
				324.60	Ros77 & NBS82 (ED177)

ΔH_f(H), ΔH_f(B), ΔH_f(H^+) used are 52.1 [23]; 134.49 [10]; 365.70 [24] kcal mol^{-1}

(a) With MP4/Extrap.//HF/6-31G** energies

(b) With MP4/6-31 + G**(2*d*,*f*)//MP4/6-31G** energies

Using the so-called "isogyric" approach of Pople [17], we have deduced the heats of formation reported in Table 3. Comparison with recommended experimental heats of formation shows the theoretical set of values are underestimated. Nevertheless, both sets of values correlate nicely (ΔH_f(reference) $= 6.266 + 0.995$ ΔH_f(Theoretical) with a correlation coefficient close to one). In terms of observables (see Table 4), one finds that the experimental measurements neither correlate better nor worse with values deduced from theory than with those deduced from reference heats of formation:

$$\text{Observable(Experiment)} = 7.881 + 0956\ \text{Observable(Theoretical)} \qquad (r = 1.00)$$

$$\text{Observable(Experiment)} = 3.515 + 0.973\ \text{Observable}(\Delta H_f(\text{Reference}))\ (r = 1.00)$$

Techniques such as those here used are known [20] to be accurate within ±2–3 kcal mol^{-1}. Hence the reliability of theory compared to experiments on transient species can be trusted. In addition the experimental determinations on the boron derivatives are difficult. Thus we conclude that our theoretical predictions are reliable.

Finally, we describe the electronic distribution in BH_3^+ and $B_2H_6^+$. Boy's localization of the UHF (Unrestricted Hartree–Fock) (6-31G**) wave function produces a map of centroids (for both alpha and beta localized orbitals) which can be associated with a molecular graph [21]. Figure 1 shows representations of the electronic structures. The BH_3^+ complexes correspond well, from the electronic point of view, with our description: $H_2 \cdots BH^+$ has an unshared electron on the boron atom and a pair of electrons binding the two hydrogen atoms; in

Table 4. Comparison between observables calculated from the theoretical ΔH_f, from the recommended ΔH_f with the measured values[b] (kcal mol^{-1})

Observable	Prediction[a]	From ΔH_f(Ref.)	Measurement	References [25]
$A''(B_2H_6^+)$	264.45	262.43	262.43	±0.2 Bru70
$A''(BH_3^+)$	318.00	323.39	343.14	±1.1 Wil67
$A'(BH_3^+)$	279.35	284.10	284.10	±2.3 Wil67
			282.26	±2.3 Gan69
$A'(BH_2^+)$	295.00	298.63	298.63	±2.3 Wil67
$A'(BH^+)$	309.86	310.30	315.00	±0.5 Wil67
$A'(B^+)$	356.00	351.10	365.05	Wil67
I(BH)	226.59	226.74	225.30	±1.15 Bau64
I(B)	189.59	188.41	191.35	Wil67
$BDE(H\text{–}B_2^+)$[c]	15.65	14.53	14.53	Wil67
$BDE(H\text{–}BH^+)$[c]	119.05	115.87	99.16	Wil67
$BDE(B\text{–}H)$[c]	83.16	79.13	83.94	Wil67
$BDE(H\text{–}B^+)$[c]	46.15	40.80	50.04	Wil67
$BDE(BH_3\text{–}BH_3)$[c]	38.65	39.29	34–40	[26]

Remarks: A' stands for the appearance potential from BH_3 and A'' from B_2H_6; BDE are bond dissociation energy and I means ionization potential

[a] with MP4/6-31 + G**(2*d*,*f*)//MP2/6-31G** energies

[b] Experimental values have been selected according to the best accuracy of measurement

[c] Calculated values

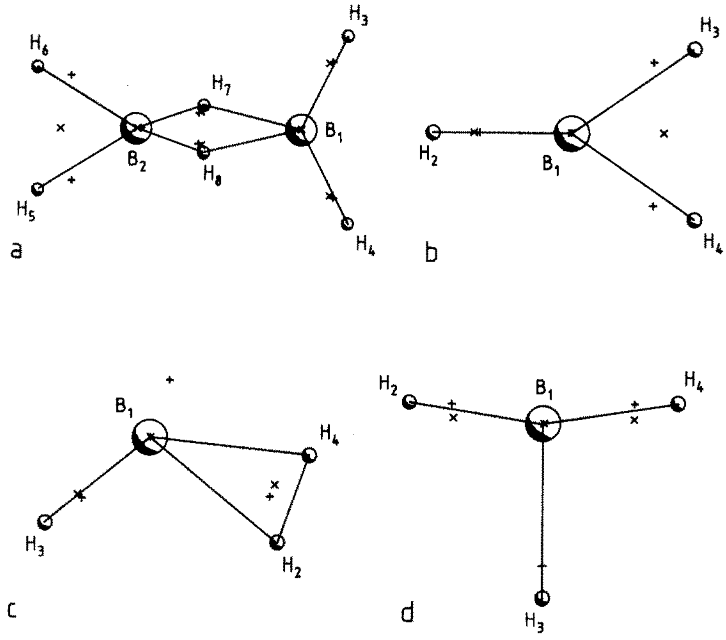

Fig. 1. Map of charge centroids for BH_3^+ and $B_2H_6^+$. The "*plus*" *sign* indicates the position of a centroids of charge corresponding to an alpha localized orbital and the "*cross*" *sign* stands for the corresponding beta centroid. **a** $B_2H_6^+$; **b** BH_3^+; **c** complex $H_2 \cdots BH^+$; **d** complex $H \cdots BH_2^+$

$H \cdots BH_2^+$, a hydrogen is bound to a quasi-linear BH_2^+ ion. BH_3^+ is distorted from the D_{3h} symmetry of the neutral borane. This geometrical distortion results in lengthening two B–H bonds. From the electronic point of view, these two hydrogens together with the boron form a three electron-three center bond: one finds one alpha centroid of charge on each B(1)–H(3) and B(1)–H(4) bond; the corresponding beta electron lies in a localized orbital formed by atomic functions lying on the three centers (chiefly 2*s* and 2*p* boron orbitals and 1*s* hydrogen atomic function). The $B_2H_6^+$ ion shows a similar geometrical distortion and electronic features for one of its two BH_2 terminal groups.

Finally, comparing BH_3^+ with the isoelectronic ion CH_3^{++} [12], one observes that BH_3^+ has two large BH bonds (1.26 Å) forming a relatively small angle (70°), whereas CH_3^{++} has one large CH bond (1.56 Å) and one large HCH angle (155°) between the other two CHs. Thus BH_3^+ has a nuclear structure close to the $H_2 \cdots BH^+$ complex and CH_3^{++} resembles the $H \cdots BH_2^+$ complex.

3. Conclusions

Large basis sets and calculations beyond the SCF level are required to give reliable descriptions of ions such as BH_3^+ and $B_2H_6^+$. This is true both for geometries and energies, due to the unusual three electron-three center bonds encountered in such species (see Fig. 1). We have characterized three minima for BH_3^+. Discarding possible molecular complexes, we find only one minimum on the $B_2H_6^+$ potential energy hypersurface. The heats of formation we determine seem to be several kcal mol^{-1} (up to 9 kcal mol^{-1}) lower than the accepted values (this has already been mentioned by other authors [5–7] for borane and diborane). Nevertheless, the appearance potentials deduced from our theoretical heats of formation compare well with the corresponding experimental values. Moreover, the type of calculation performed here is expected to be accurate to within 2–3 kcal mol^{-1}.

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