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# Structure and stability of $\text{BF}_3 \cdot \text{F}$ and $\text{AlF}_3 \cdot \text{F}$ superhalogens

Gennady L. Gutsev<sup>a,b,\*</sup>, Puru Jena<sup>a</sup>, Rodney J. Bartlett<sup>c</sup><sup>a</sup> *Physics Department, Virginia Commonwealth University, Richmond, VA 23284-2000, USA*<sup>b</sup> *Institute of Chemical Physics at Chernogolovka of the Russian Academy of Sciences, Chernogolovka, Moscow Region 142432, Russian Federation*<sup>c</sup> *Quantum Theory Project, University of Florida, P.O. Box 118435, Gainesville, FL 32611-8435, USA*

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## Abstract

Structure and stability of  $\text{BF}_4$ ,  $\text{AlF}_4$ ,  $\text{BF}_4^-$  and  $\text{AlF}_4^-$  are studied at the MBPT(4) and CCSD(T) levels of theory.  $\text{AlF}_4$  is confirmed to have a configuration of an adduct type, which is stable by 5.8 kcal/mol towards  $\text{AlF}_3 + \text{F}$ .  $\text{BF}_4$  has to be considered rather as a Van der Waals complex which is bound by 1.6 kcal/mol.  $\text{BF}_3 \cdot \text{F}$  and  $\text{AlF}_3 \cdot \text{F}$  possess very high adiabatic electron affinities of 6.75 and 7.93 eV, respectively, and are superhalogens. We computed the adiabatic electron affinities of  $\text{BF}_3$  and  $\text{AlF}_3$  to be  $-0.76$  and  $0.90$  eV, respectively, which indicates that  $\text{BF}_3^-$  is metastable. © 1998 Elsevier Science B.V. All rights reserved.

## 1. Introduction

The  $\text{BF}_4^-$  and  $\text{AlF}_4^-$  anions are known to be stable in the gas phase [1] and enter salts of the  $[\text{C}]^+[\text{A}]^-$  type [2,3]. An important property of these anions is their high vertical detachment energies (VDE) [4], which exceed significantly the electron affinities of the most electronegative atoms F and Cl. The corresponding neutral parents should be superhalogens of the  $\text{MX}_{k+1}$  type [5]. However, there are scarce data on the thermodynamical stability of  $\text{MX}_{k+1}$  systems.

Recently, we have found [6] using a rather high level of theory (namely, the infinite-order coupled-

cluster method with all singles and doubles and noniterative inclusion of triple excitations [CCSD(T)] that the superhalogens  $\text{LiF}_2$ ,  $\text{LiCl}_2$ ,  $\text{NaF}_2$  and  $\text{NaCl}_2$  are stable with respect to bond rupture by  $\approx 20$  kcal/mol.  $\text{AlF}_4$  has been found [7] to have a  $\text{C}_s$  equilibrium configuration which is stable towards dissociation to  $\text{AlF}_3 + \text{F}$  by 4.4 kcal/mol at the MBPT(2)/6-31 + G(d) level. To our knowledge, no data on the stability of  $\text{BF}_4$  have been reported.

This communication presents a study of the structure and thermodynamical stability of  $\text{BF}_4$ ,  $\text{AlF}_4$ ,  $\text{BF}_4^-$  and  $\text{AlF}_4^-$ , as well as an evaluation of the adiabatic electron affinities ( $A_{\text{ad}}$ ) of  $\text{BF}_4$  and  $\text{AlF}_4$  at rather reliable levels of theory with a reasonably large 6-311 + G(2d) basis set for all the atoms but Al, for which the 6-311 + G(3d) basis was chosen. As a corollary, we have calculated the structure of  $\text{BF}_3$ ,  $\text{AlF}_3$ ,  $\text{BF}_3^-$  and  $\text{AlF}_3^-$ , and evaluated the  $A_{\text{ad}}$ s of  $\text{BF}_3$  and  $\text{AlF}_3$ .

\* Corresponding author at address a. E-mail: [glgutsev@hsc.vcu.edu](mailto:glgutsev@hsc.vcu.edu)

## 2. Computational details

The present calculations have been performed with the ACESII suite of programs [8] at the MBPT(4) [9] and CCSD(T) [10,11] levels of theory. The 6-311 + G(2d) basis set [12,13] has been employed for F and B. An additional set of 3d-functions has been placed at Al (the 6-311 + G(3d) basis). Since the  $A_{\text{ad}}$  of  $\text{BF}_3$  was found to be negative at both MBPT(4) and CCSD(T) levels, it was interesting to check the performance of the HFDFPT approach in such a case. Therefore, the calculations for  $\text{BF}_3$  and  $\text{BF}_3^-$  have also been performed at the Hartree–Fock–density functional theory (HFDFPT) [14] level.

The adiabatic electron affinity measures the energy gain due to the attachment of an additional electron and is defined as the difference in the total energies of the anion and parent ground states. Within the Born–Oppenheimer approximation, one can define the  $A_{\text{ad}}$  as

$$A_{\text{ad}} = E_{\text{tot}}(N, R_e) + Z_N - E_{\text{tot}}(A, R_e^-) - Z_A \\ = \Delta E_{\text{el}} + \Delta E_{\text{nuc}} \quad (1)$$

where  $R_e$  and  $R_e^-$  denote the equilibrium geometrical configurations of the neutral molecule and the anion, respectively. The zero-point vibrational energies ( $Z$ ) are estimated within the harmonic approximation.

Bond rupture energies are calculated as the differences in the total energies of species formed in a

particular dissociation channel corrected for the corresponding  $Z$ s, namely

$$D_0(M - X) = E_{\text{tot}}(M) + Z_M + E_{\text{tot}}(X) \\ + Z_X - E_{\text{tot}}(MX) - Z_{MX} \\ = D_e(AB) + \Delta E_{\text{nuc}}. \quad (2)$$

## 3. Results and discussion

### 3.1. Geometries and vibrational frequencies

In order to estimate dissociation energies of the tetrafluorides, we have optimized the geometries of  $\text{BF}_3$ ,  $\text{AlF}_3$ ,  $\text{BF}_3^-$  and  $\text{AlF}_3^-$  and computed their harmonic vibrational frequencies. Comparison of the results of our calculations for  $\text{BF}_3$  and  $\text{AlF}_3$  with the experimental data presented in Table 1 shows that agreement is rather good at all the levels of theory used in the present work. As for the anions, there are no experimental data on their structures, except for an ESR spectrum of  $\text{BF}_3^-$  [21] obtained in tetramethylsilane matrix at 77°K. Based on the analysis of this spectrum, it has been concluded that ' $\text{BF}_3^-$  is appreciably nonplanar', which was later confirmed by the results of HF/STO-3G calculations [22]. The results of our calculations for  $\text{BF}_3^-$  and  $\text{AlF}_3^-$  are shown in Table 2 together with the results of a previous study [7] performed at the MBPT(2)/6-31 + G(d) level. Both anions have  $C_{3v}$  symmetry with nearly tetrahedral angles. Comparison of our results for  $\text{AlF}_3^-$  with

Table 1

Equilibrium geometries and vibrational frequencies of  $\text{BF}_3$  and  $\text{AlF}_3$  calculated at the HFDFPT (BLYP), MBPT(4) and CCSD(T) levels of theory with the 6-311 + G(2d) basis (the 6-311 + G(3d) basis is used for Al)

Property	$\text{BF}_3$				$\text{AlF}_3$		
	BLYP	MBPT(4)	CCSD(T)	Exp. <sup>a</sup>	MBPT(4)	CCSD(T)	Exp. <sup>b</sup>
$R_e(\text{M-F})$	1.321	1.314	1.313	1.314	1.638	1.635	1.631
$\omega(e')$	438	482	484	480	249	250	270
$\omega(a'')$	642	696	697	691	297	298	300
$\omega(a')$	865	884	887	888	687	692	672
$\omega(e')$	1387	1452	1460	1449	950	957	965
$Z$	7.37	7.79	7.82	7.77	4.83	4.87	4.92
$E_{\text{tot}}$	-324.60010	-324.17489	-324.16897	-	-541.57590	-541.56845	-

Bond lengths are in Å, vibrational frequencies are in  $\text{cm}^{-1}$ , zero-point energies are in kcal/mol and total energies are in hartrees.

<sup>a</sup> $R(\text{B-F})$  is from Ref. [15–17]; frequencies are from Ref. [18].

<sup>b</sup> $R(\text{Al-F})$  and  $\omega(a')$  are from Ref. [19]; all other frequencies are from Ref. [20].

Table 2

Equilibrium geometries and vibrational frequencies of  $\text{BF}_3^-$  and  $\text{AlF}_3^-$  calculated at the HFDF (BLYP), MBPT(4) and CCSD(T) levels of theory with the 6-311 + G(2d) basis (the 6-311 + G(3d) basis is used for Al)

Property	$\text{BF}_3^-$			$\text{AlF}_3^-$		
	BLYP	MBPT(4)	CCSD(T)	MBPT(4)	CCSD(T)	MBPT(2) <sup>a</sup>
$R_e(\text{M-F})$	1.398	1.401	1.398	1.713	1.707	1.734
$\angle \text{FMX}^\circ$	106.62	107.71	107.74	110.19	110.13	108.41
$\omega(e)$	291	414	417	226	228	223
$\omega(a_1)$	493	591	594	320	323	317
$\omega(a_1)$	688	760	776	619	627	622
$\omega(e)$	1034	1051	1064	736	746	731
$Z$	5.48	6.12	6.19	4.09	4.14	4.07
$E_{\text{tot}}$	-324.57840	-324.14654	-324.14094	-541.60862	-541.60164	-541.11497

Bond lengths are in Å, vibrational frequencies in  $\text{cm}^{-1}$ , zero-point energies are in kcal/mol and total energies are in hartrees.

<sup>a</sup>The basis is 6-31 + G(d); see Ref. [7].

those obtained at the MBPT(2)/6-31 + G(d) level shows a relatively small difference in vibrational frequencies, whereas the Al-F bond length is elongated by 0.027 Å at the MBPT(2)/6-31 + G(d) level compared to that obtained at the CCSD(T)/6-311 + G(2d) level.

Both anions  $\text{BF}_4^-$  and  $\text{AlF}_4^-$  have  $T_d$  symmetry. Their computed bond lengths and vibrational frequencies are presented in Table 3 and are in nice agreement with experimental data. The neutral  $\text{AlF}_4$  is confirmed to have a  $C_s$  configuration (Fig. 1) and optimizations at the MBPT(2)/6-311 + G(2d) level led to geometrical parameters and harmonic frequencies similar to those found [7] at the HF/6-31 + G(d) level.  $\text{BF}_4$  is found to have also a  $C_s$  equilibrium

configuration which is stable towards dissociation to  $\text{BF}_3 + \text{F}$  by 1.6 kcal/mol. The longest X-F bond lengths are 2.26 and 2.66 Å, and the first vibrational frequencies are 82 and 26  $\text{cm}^{-1}$  in  $\text{AlF}_4$  and  $\text{BF}_4$ , respectively, which allows a classification of  $\text{AlF}_4$  as an adduct and  $\text{BF}_4$  as a Van der Waals complex. No thermodynamically stable configurations either  $\text{BF}_4$  or  $\text{AlF}_4$  were found in optimizations subjected to  $C_{2v}$ ,  $C_{3v}$  and  $T_d$  constrains.

The triatomic superhalogens  $\text{MX}_2$  are stable towards dissociation to  $\text{MX} + \text{X}$  ( $\text{X} = \text{F}$  or  $\text{Cl}$ ) by about 20 kcal/mol [6], whereas a dissociative behavior has been found for a larger superhalogen  $\text{PF}_6$  [23,24]. The anion  $\text{PF}_6^-$  is rather stable with respect to  $\text{PF}_5 + \text{F}^-$  (by  $\approx 4$  eV) and possesses a high

Table 3

Equilibrium bond lengths and vibrational frequencies of  $\text{BF}_4^-$  and  $\text{AlF}_4^-$  calculated at the MBPT(4) and CCSD(T) levels of theory with the 6-311 + G(2d) basis (the 6-311 + G(3d) basis is used for Al)

Property	$\text{BF}_4^-$			$\text{AlF}_4^-$		
	MBPT(4)	CCSD(T)	Exp. <sup>a</sup>	MBPT(4)	CCSD(T)	Exp. <sup>b</sup>
$R_e(\text{M-F})$	1.410	1.407	1.38	1.700	1.696	1.69
$\omega(e)$	347	350	355	201	202	210
$\omega(t_2)$	513	518	530	306	308	322
$\omega(a_1)$	748	758	774	606	611	622
$\omega(t_2)$	1067	1082	1060	775	782	760
$Z$	8.84	8.95	8.94	6.08	6.13	6.13
$E_{\text{tot}}$	-424.03741	-424.02962	-	-641.49177	-641.48259	-

Bond lengths are in Å, vibrational frequencies are in  $\text{cm}^{-1}$ , zero-point energies are in kcal/mol and total energies are in hartrees.

<sup>a</sup> $R(\text{B-F})$  is from JANAF Thermochemical Data Tables and was obtained from the  $[\text{BF}_4]^-[\text{K}]^+$  salt; frequencies are from Ref. [2].

<sup>b</sup> $R(\text{Al-F})$  is from Ref. [28]; frequencies are from Ref. [29].

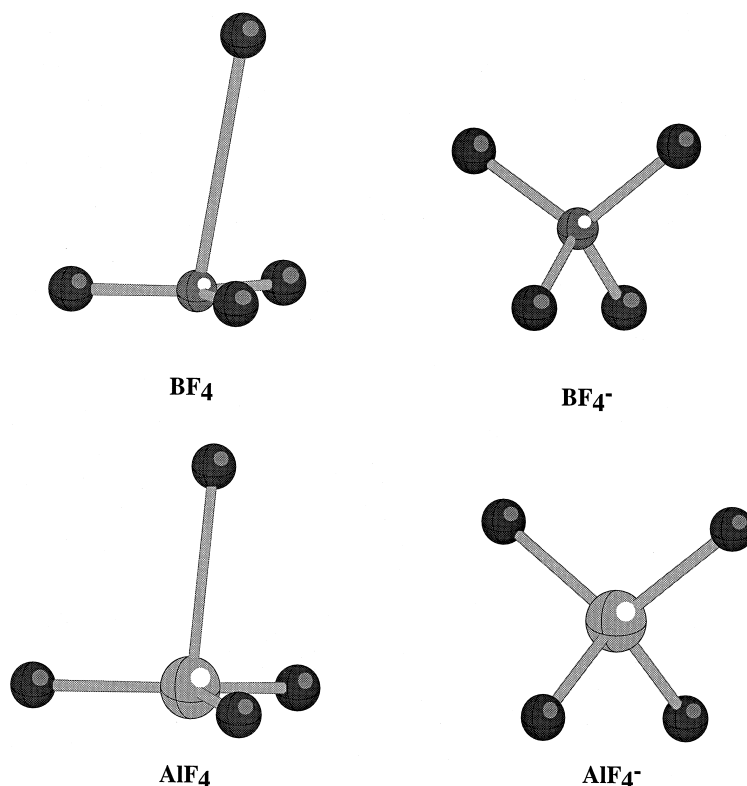


Fig. 1. Equilibrium configurations of  $\text{BF}_4$ ,  $\text{BF}_4^-$ ,  $\text{AlF}_4$  and  $\text{AlF}_4^-$ .

vertical detachment energy of 7.35 eV [25]. It appears that  $\text{MX}_4$  superhalogens have marginal thermodynamical stability, and superhalogen anions  $\text{MX}_{k+1}^-$  should dissociate to  $\text{MX}_k + \text{X}$  after the detachment of an extra electron for  $k > 3$ . The cases when an anion is rather stable but dissociates after the detachment of an extra electron seem to be not rare, e.g.  $\text{SF}_4\text{Cl}^-$  [26] and  $\text{SCl}_5^-$  [27].

### 3.2. Electron affinities and thermodynamical stability

The  $A_{\text{ad}}$  of  $\text{BF}_3$  was found to be negative at all the levels of theory (see Table 4). In order to confirm that the  $\text{BF}_3^-$  anion is stable with respect to the detachment of an extra electron, we have performed a CCSD(T) calculation of the total energy of the neutral parent  $\text{BF}_3$  at the equilibrium geometry of  $\text{BF}_3^-$ . The total energy of  $\text{BF}_3$  was found to be higher by 0.95 eV than that of  $\text{BF}_3^-$ . Thus,  $\text{BF}_3^-$  is metastable with respect to the decay channel  $\text{BF}_3 + e$ .

The results obtained at the LDA, BLYP and

B3LYP levels of the HF-DFT theory (at the geometries optimized at the HF-DFT(BLYP) level) show a similar behavior. The  $A_{\text{ad}}$  values obtained at these levels are slightly higher (by  $\approx 0.15$ – $0.20$  eV) than the values obtained at the levels from MBPT(2) to CCSD(T). Generally, the CCSD(T)/6-311 + G(2d) level should be expected to provide an accuracy of about 0.1–0.2 eV in the evaluation of adiabatic electron affinities [31]. The  $A_{\text{ad}}$  of  $\text{AlF}_3$  appears to be not very sensitive to the level of theory or the basis set, because the change in the values computed at the MBPT(2) through CCSD(T) levels (see Table 4) does not exceed 0.04 eV, and values computed at the MBPT(2), MBPT(3) and MBPT(4) levels with a smaller 6-31 + G(d) basis (0.91, 0.90 and 0.93 eV, respectively [7]) are close to the value of 0.90 eV obtained at the highest CCSD(T)/6-311 + G(2d) level. The  $A_{\text{ad}}$  of  $\text{AlF}_4$  is larger than the  $A_{\text{ad}}$  of  $\text{BF}_4$  by 1.2 eV, and both of them are in the range of valence ionization potentials of ordinary organic compounds.

Table 4

Adiabatic electron affinities of  $\text{BF}_3$ ,  $\text{AlF}_3$ ,  $\text{AlF}_4$  and  $\text{BF}_4$  computed according to Eq. (1)

Level	$\text{BF}_3$	$\text{AlF}_3$	$\text{BF}_4^a$	$\text{AlF}_4^a$	Level	$\text{BF}_3$
$A_{\text{ad}}$						
HF	-1.20	0.65	4.81	6.25	HF	-1.20
MBPT(2)	-0.80	0.87	6.98	8.21	$X_\alpha$	-1.32
MBPT(4)	-0.77	0.89	6.80	7.98	LDA	-0.57
CCSD	-0.79	0.89	6.63	8.01	BLYP	-0.59
CCSD + T <sup>b</sup>	-0.76	0.91	6.74	7.93	B3LYP	-0.60
CCSD(T)	-0.76	0.90	6.73	7.93	...	...
$\Delta Z$	0.07	0.03	0.05	0.03	$\Delta Z$	0.08
Channel	$\Delta ZPE$	MBPT(2)	MBPT(4)	CCSD	CCSD(T)	
$\text{BF}_4^- \rightarrow \text{BF}_3 + \text{F}^-$	0.08	3.50	3.50	3.59	3.58 <sup>c</sup>	
$\text{AlF}_4^- \rightarrow \text{AlF}_3 + \text{F}^-$	0.06	4.97	4.97	5.07	5.06 <sup>d</sup>	
$\text{AlF}_4 \rightarrow \text{AlF}_3 + \text{F}$	0.025	0.20	0.21	0.22	0.25	
$\text{BF}_4 \rightarrow \text{BF}_3 + \text{F}$	0.014	0.06	0.06	0.05	0.07	

The geometries are optimized at the CCSD(T), MBPT(4) and HFDF(T)BLYP (for  $\text{BF}_3$ ) levels. Dissociation energies are corrected for the corresponding Zs. All values are in eV.

<sup>a</sup>The  $X_\alpha$  vertical detachment energies for  $\text{BF}_4$  and  $\text{AlF}_4$  are the same (6.2 eV) [5].

<sup>b</sup>CCSD + T is a short form of the CCSD + T(CCSD) method [10].

<sup>c</sup>Experimental data are  $3.42 \pm 0.41$ ,  $3.12 \pm 0.22$ ,  $3.99 \pm 0.26$ ; see Ref. [32,33] and [34], respectively.

<sup>d</sup>Experimental value is 5.05 [30].

The experimental dissociation energy of  $\text{AlF}_4^-$  to  $\text{AlF}_3 + \text{F}^-$  (see Ref. [30] and references therein) is rather large and matches our value computed at the CCSD(T) level. Experimental estimates [32–34] of the  $\text{F}^-$  affinity to  $\text{BF}_3$  show a large dispersion, being consistent with our CCSD(T) value within experimental error bars.

The dissociation energy of  $\text{AlF}_4$  equals 5.8 kcal/mol at the CCSD(T)/6-311 + G(2d) level, making an increase in 1.4 kcal/mol with respect to the value computed at the MBPT(4)/6-31 + G(d) level [7]. This increase lends further support for the existence of bound  $\text{AlF}_4$ .  $\text{BF}_4$  is less stable than  $\text{AlF}_4$  by 4.2 kcal/mol and forms a rather weakly bound complex  $\text{BF}_3 * \text{F}$ . The  $\text{BF}_4^-$  anion is less stable than  $\text{AlF}_4^-$  by a quantity which is close to the difference in the  $A_{\text{ad}}$ s of  $\text{AlF}_3$  and  $\text{BF}_3$ .

#### 4. Conclusion

The results of our computations at the CCSD(T)/6-311 + G(2d) level of theory allow several conclusions:

(1)  $\text{BF}_3^-$  is metastable with respect to the decay channel  $\text{BF}_3 + e$ , whereas the  $\text{AlF}_3^-$  is thermodynamically stable and the  $A_{\text{ad}}$  of  $\text{AlF}_3$  equals 0.90 eV.

(2) Both  $\text{BF}_4^-$  and  $\text{AlF}_4^-$  anions are rather stable with respect to the detachment of  $\text{F}^-$  (by 3.58 and 5.06 eV, respectively). The reduced stability of  $\text{BF}_4^-$  could be responsible for higher sensitivities of  $\text{BF}_4^-$ -based salts.

(3) The  $\text{BF}_3 * \text{F}$  (bound by 1.6 kcal/mol) and  $\text{AlF}_3 * \text{F}$  (bound by 5.8 kcal/mol) complexes are superhalogens with the adiabatic electron affinities of 6.75 and 7.93 eV, respectively.

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