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Selected boron, aluminum, and gallium trihalide and trihydride anions

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ABSTRACT

Ab initio methods with flexible orbital basis sets are used to examine the electron binding strengths of trifluorides, tri-chlorides, and tri-hydrides of B, Al, and Ga. The adiabatic electron affinities are found to increase with increasing atomic number of the central atom. For any given central atom M (M = B, Al, Ga), the adiabatic and vertical electronic stability for MCl_3 is larger than that of the corresponding MF_3. The tri-hydrides have quite different electron binding strengths than the corresponding tri-halides. BH_3 has a very small EA (ca. 0.02 eV) and its anion is planar whereas the tri-halide anions and AlH_3^- and GaH_3^- are non-planar. AlH_3 and GaH_3 have considerably smaller EAs (ca. 0.3 eV) than the Al and Ga tri-halides (0.9–1.8 eV). In all, these anions provide species whose electron binding strengths span a considerable range (0.3–1.8 eV).

1. Introduction

Molecular anions exhibit a wide range of electronic stabilities, depending on the strength of the potential responsible for the excess electron's binding [1–4]. Apart from metastable anions whose electronic energies lie above those of their corresponding neutral parents, the vertical electron detachment energies (VDEs) of negatively charged molecular ions described in the literature thus far span the range of 0.001–13.87 eV [1,3,5]. One class of weakly bound anions (i.e., those with VDEs in the range of a few to a few hundred cm^{-1}) is dipole-bound species in which the extra electron is attracted to the dipole field of its neutral parent but whose binding energy often is enhanced by dispersion stabilization [6,7]. In contrast, strongly bound anions [8] have electron binding energies exceeding the electron affinity of the chlorine atom (3.62 eV) [9] and may approach 14 eV in certain cases (e.g., $Sb_3F_{16}^-$, $H_{12}F_{13}^-$) [5,10].

Although many commonly recognized molecules have already been investigated with respect to their ability to form stable anions (see Ref. [3] in which a huge body of the experimental and theoretical data as of 2002 are collected), many systems remain either unstudied or controversial. Borane (trihydridoboron, BH_3) and alane (aluminum hydride, AlH_3) are two examples that could be of interest because the former is believed to be a reaction intermediate in the pyrolysis of diborane (leading to higher boranes) [11] while the latter plays a reducing agent role in organic synthesis [12]. Moreover, various boron and aluminum containing molecules (mainly hydride and halide salts) are used as components in classical and secondary batteries and novel rechargeable storage systems [13–19]. However, literature reports describing the possibility of an excess electron binding by fluorinated and chlorinated borane and alane and the gallium analogs (i.e., BF_3, BCl_3, AlF_3, $AlCl_3$, GaF_3, and $GaCl_3$) are either scarce or lacking. Schwartz and Allen predicted positive eigenvalues for the lowest unoccupied molecular orbitals (LUMO) of both BH_3 and BF_3, which suggested the instability of their corresponding anions [20]. A similar conclusion about the electron affinity of BH_3 was reached by Carmichael in 1987 on the basis of *ab initio* calculations [21], whereas contradictory results were presented by Wickham-Jones et al. who measured the photoelectron spectrum of the BH_3^- anion and estimated the adiabatic electron affinity (EA) of borane to be slightly positive (0.038 ± 0.015 eV) [22]. The electronic stability of BH_3^- was supported theoretically by Gutsev and Bartlett (who stressed the importance of including zero-point energy corrections) [23], by Christe and co-workers [24] who found the anion to be stable by 0.03 eV, and more recently by the Jena group [25] who found the anion to be stable by ca. 0.04 eV. As far as the electronic stabilities of BF_3^- and BCl_3^- are concerned, the coupled-cluster calculations reported in Ref. [24] led to a positive EA (0.49 eV) for BCl_3 and negative (−0.56 eV) EA for BF_3, with the latter result meaning the BF_3^- anion is not electronically stable. The available data regarding the AlH_3^-, AlF_3^-, and $AlCl_3^-$ anions are even more scarce and include the report of alane radical anions in solution and rather outdated (and thus perhaps less reliable) theoretical predictions of the structure and energetics of the AlH_3^- [26,27]. For GaH_3^-, GaF_3^-, and $GaCl_3^-$, we are unaware of any recent studies of their possible stability.

Hence, in this contribution we provide results of detailed considerations regarding the stability of the BH_3^-, BF_3^-, BCl_3^-, AlH_3^-, AlF_3^-,

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AlCl$_3^-$ GaH$_3^-$, GaF$_3^-$, and GaCl$_3^-$ anions established on the basis of correlated *ab initio* calculations using flexible atomic orbital basis sets.

2. Methods

The equilibrium structures and corresponding harmonic vibrational frequencies of closed-shell neutral BH$_3$, BF$_3$, BCl$_3$, AlH$_3$, AlF$_3$, AlCl$_3$, GaH$_3$, GaF$_3$, and GaCl$_3$ and their daughter doublet anions were determined by applying the quadratic configuration interaction method with single and double substitutions (QCISD) [28–30] using the 6-311++G(3df,2pd) [31,32] basis sets. The vertical electron detachment energies (VDEs) and the adiabatic electron affinities (EAs) were calculated by employing the supermolecular approach (i.e., by subtracting the energy of the anion from that of the neutral).

The reliability of the QCISD/6-311++G(3df,2pd) approach was verified by comparing the resulting VDEs and EAs to the corresponding VDEs and EAs calculated by using the coupled-cluster method with single, double, and non-iterative triple excitations (CCSD(T)) [33–36] and the same 6-311++G(3df,2pd) basis set (with all orbitals included while computing the correlation energies). Since the VDEs and EAs obtained using the QCISD method differ from those calculated with the CCSD(T) technique usually by 0.01–0.04 eV (larger differences of 0.06–0.07 eV were noted only for the EA of GaF$_3$ and the VDE of GaCl$_3^-$), we are quite confident that our excess electron binding energies predicted by applying the QCISD approach remain reliable. Since the CCSD(T) analytic gradients and force constants are not implemented in the computational package we have available, we decided to carry out the calculations (geometry optimizations, harmonic frequencies, etc.) using the QCISD method instead.

The (very small) adiabatic electron affinity of BH$_3$ could not be properly described at the QCISD/6-311++G(3df,2pd) level used to treat the other systems; such a treatment led to a negative EA which we knew to be incorrect. Thus, in this particular case, we used the CCSD(T) method [33–36] together with a much larger quintuple-zeta aug-cc-pV5Z basis set [37–41] to evaluate the electronic energies of both neutral BH$_3$ and its daughter BH$_3^-$ anion at equilibrium geometries taken from the QCISD/6-311++G(3df,2pd) calculations (the zero-point energy corrections were also estimated by applying the QCISD/6-311++G(3df,2pd) approach).

The potential energy profiles of the neutral and anionic species as functions of an angle θ (see Fig. 1) describing the deformation of the MX$_3$ units away from planarity were calculated at the QCISD/6-311++G(3df,2pd) level by relaxing the bond lengths (assuming C$_{3v}$ symmetry constraints) for each value of θ.

Since we used methods based on an unrestricted Hartree–Fock (UHF) starting point, it was important to make sure that little (if any) artificial spin contamination enters into the final wave functions. We computed the expectation value $\langle S^2 \rangle$ for the states studied in this work and found values not exceeding 0.7561 for doublet anionic species (at the UHF level). Hence, we are confident that spin contamination is not large enough to significantly affect our findings.

All calculations were performed with the GAUSSIAN09 (Rev. A.02) package [42].

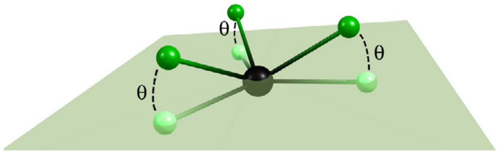

Fig. 1. The definition of the θ angle which indicates the distortion of the C$_{3v}$-symmetry (pyramidal) structure from planarity.

3. Results

In Figs. 2–5 we display the energies of the neutral MX$_3$ and anionic MX$_3^-$ species as functions of sin (θ), where θ is the deformation angle defined in Fig. 1. For each species, the electronic energy of the anion at its optimized geometry defines the zero (reference point) of energy. Notice that all energy profiles appear to depend quadratically on sin (θ) at least for values of sin (θ) near the minima of the neutrals and anions.

For each energy profile, the total zero-point energy (i.e., including the zero-point energy for all vibrational modes) is shown by the upper horizontal line, and the zero-point energy associated with the puckering degree of freedom is shown by the lower

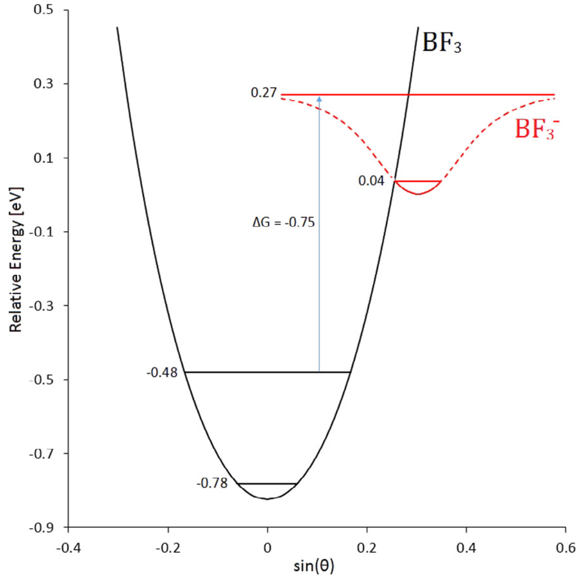

Fig. 2a. Energies of BF$_3$ and BF$_3^-$ as functions of sin (θ). Lower horizontal lines represent zero-point energy along the puckering mode; higher horizontal lines show total zero-point energies.

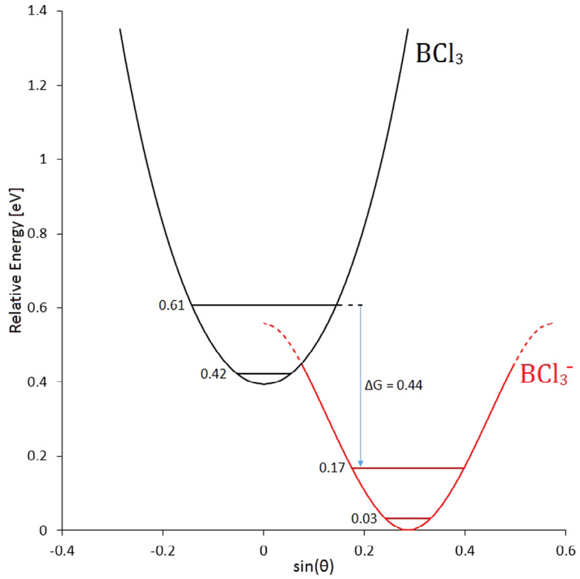

Fig. 2b. Energies of BCl$_3$ and BCl$_3^-$ as functions of sin (θ). Lower horizontal lines represent zero-point energy along the puckering mode; higher horizontal lines show total zero-point energies.

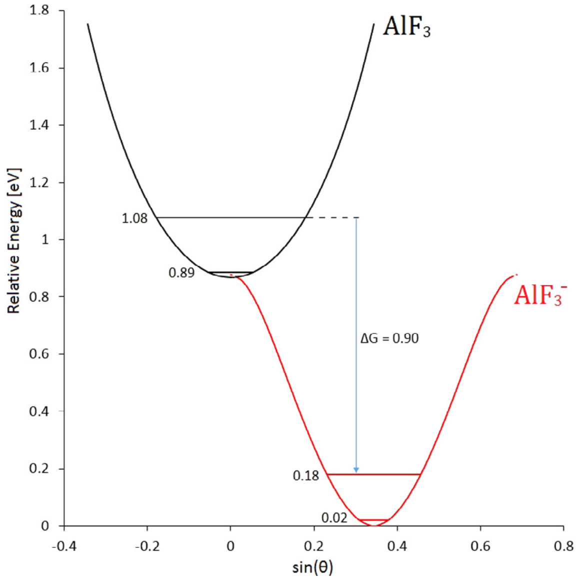

Fig. 3a. Energies of AlF_3 and AlF_3^- as functions of $\sin(\theta)$. Lower horizontal lines represent zero-point energy along the puckering mode; higher horizontal lines show total zero-point energies.

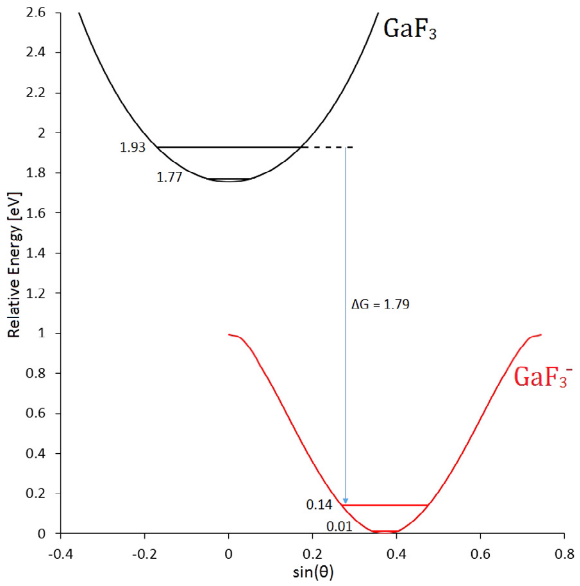

Fig. 4a. Energies of GaF_3 and GaF_3^- as functions of $\sin(\theta)$. Lower horizontal lines represent zero-point energy along the puckering mode; higher horizontal lines show total zero-point energies.

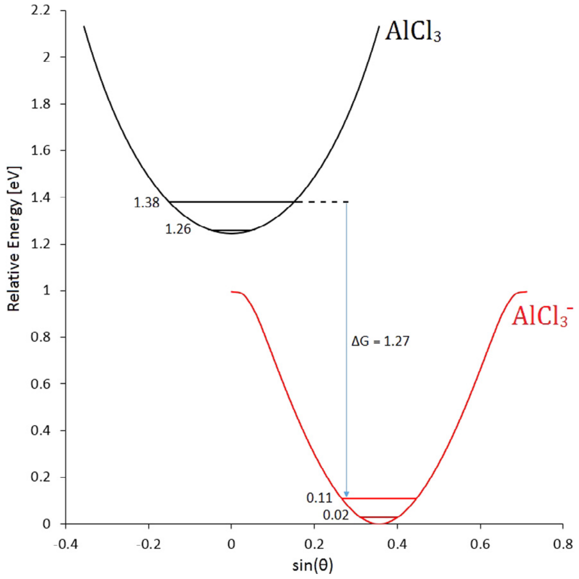

Fig. 3b. Energies of $AlCl_3$ and $AlCl_3^-$ as functions of $\sin(\theta)$. Lower horizontal lines represent zero-point energy along the puckering mode; higher horizontal lines show total zero-point energies.

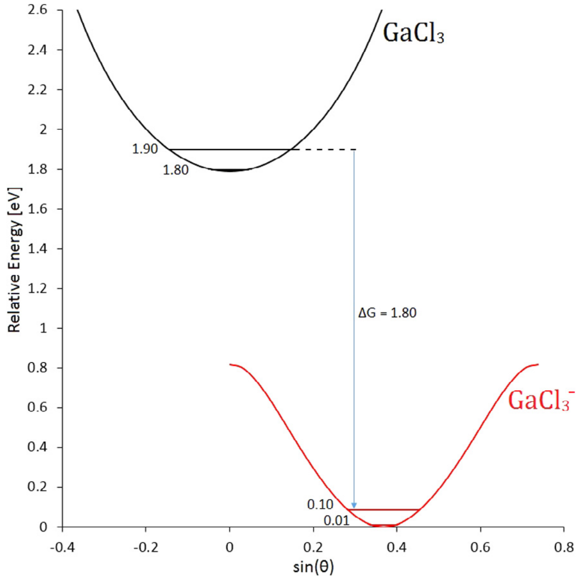

Fig. 4b. Energies of $GaCl_3$ and $GaCl_3^-$ as functions of $\sin(\theta)$. Lower horizontal lines represent zero-point energy along the puckering mode; higher horizontal lines show total zero-point energies.

horizontal line. The values of ΔG were calculated from the (total) zero-point energy of the anion to the (total) zero-point energy of the corresponding neutral. Showing the zero-point energy of the puckering degree of freedom allows us to estimate to what degree this vibrational mode would have to become excited to render the anion electronically unstable, in which case electron detachment should occur.

At geometries where the energy of the anion lies above that of the neutral, the energy profile of the anion is represented by extending the anion's $\sin^2\theta$ profile resulting from our *ab initio* calculations at values of $\sin(\theta)$ for which the anion is stable into the region where the anion is unstable. Of course, these extrapolated energies do not provide accurate representations of the electronic energies of the metastable anions, and they offer no information about the widths (i.e., the inverse of the lifetimes) of these states. However, the energy at which the anion's profile crosses that of the neutral does contain information about to what degree the anion would have to be vibrationally excited along the puckering mode to render the anion unstable to electron detachment.

Before discussing our findings further, it is useful to say a bit about whether the anions treated here are expected to retain the planar D_{3h} geometries that the corresponding neutral parents possess. At the planar geometry of a neutral MX_3 (with M = B, Al, or Ga and X = H, F, or Cl), the lowest unoccupied molecular orbital (LUMO) is expected to be dominated by the 2p, 3p, or 4p orbital component on the central atom. As such, the LUMO has a_2'' symmetry in the D_{3h} point group and is odd under reflection through the plane of the molecule. The Born–Oppenheimer energy of the anion

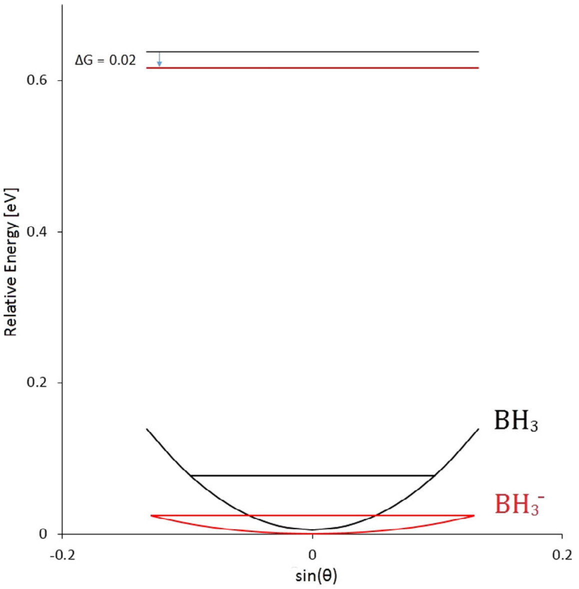

Fig. 5a. Energies of BH_3 and BH_3^- as functions of sin (θ). For BH_3 the profile was constructed from energies computed at the QCISD/6-311++G(3df,2pd) level as with all the other species treated here. For the BH_3^- anion, an energy profile was computed at the QCISD/6-311++G(3df,2pd) level, but then shifted to lower energy to reproduce the CCSD(T)/aug-cc-pV5Z computed adiabatic EA of 0.02 eV.

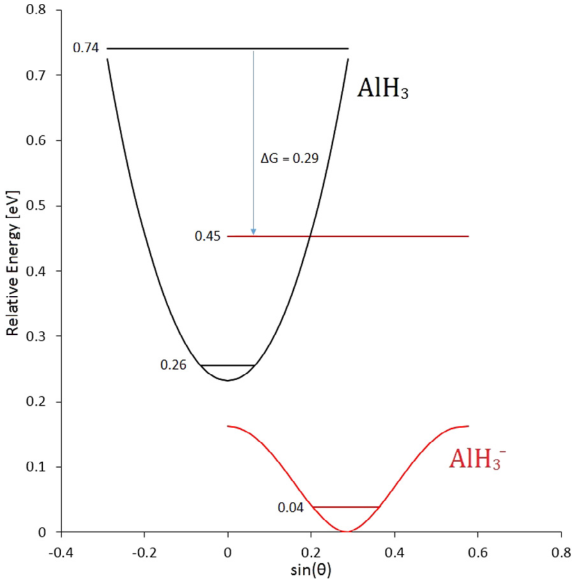

Fig. 5b. Energies of AlH_3 and AlH_3^- as functions of sin (θ). Lower horizontal lines represent zero-point energy along the puckering mode; higher horizontal lines show total zero-point energies.

formed by singly occupying such a LUMO can be expressed as a function of deformation along the puckering mode as follows:

$$E(q) = E(0) + <\psi_{a_2''}\left|\frac{\partial H}{\partial q}\right|\psi_{a_2''}> \delta q$$
$$+\frac{1}{2}\left[<\psi_{a_2''}\left|\frac{\partial^2 H}{\partial q^2}\right|\psi_{a_2''}> + \sum_n \frac{|<\psi_{a_2''}|\frac{\partial H}{\partial q}|\psi_n>|^2}{E(0)-E_n}\right]\delta q^2 + \ldots \quad (1)$$

The gradient $\left\langle\psi_{a_2''}\left|\frac{\partial H}{\partial q}\right|\psi_{a_2''}\right\rangle$ along the puckering mode (q) vanishes because $\frac{\partial H}{\partial q}$ is of odd symmetry under the plane of the molecule whereas the product $\langle\psi_{a_2''}||\psi_{a_2''}\rangle$ is of even symmetry. This means that the anion's energy profile has either a minimum or a maximum along q at the planar geometry, depending on the sign of the quadratic terms in Eq. (1).

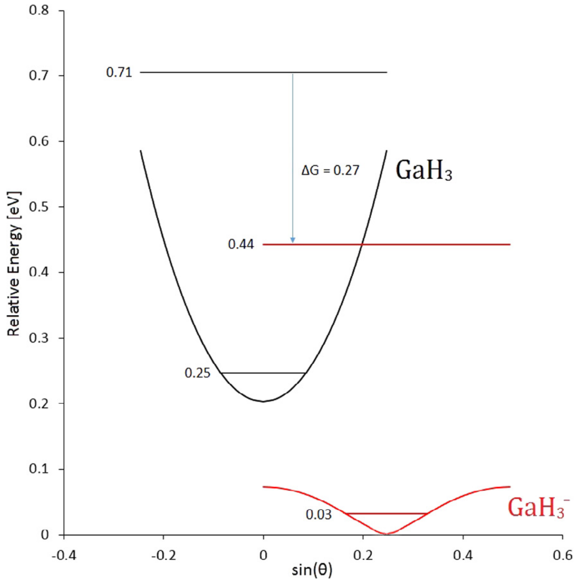

Fig. 5c. Energies of GaH_3 and GaH_3^- as functions of sin (θ). Lower horizontal lines represent zero-point energy along the puckering mode; higher horizontal lines show total zero-point energies.

A likely source of negative curvature along q would be the existence of an excited state ψ_n whose coupling $\left\langle\psi_{a_2''}\left|\frac{\partial H}{\partial q}\right|\psi_n\right\rangle$ to the a_2'' ground state is strong and whose energy E_n is close to that of the ground state $E(0)$. Because $\frac{\partial H}{\partial q}$ is odd under reflection as is $\psi_{a_2''}$, the excited state ψ_n must be of even symmetry. So, to anticipate which anions will remain planar and which will distort, one needs to consider which neutrals are likely to have low-lying orbitals of even symmetry (potentially leading to non-planarity) and which are not (thus retaining planarity). With these considerations in mind, we now present and discuss our findings on the nine neutral MX_3 and anionic MX_3^- species beginning with the halides.

3.1. MX_3 halides and their anions

Clearly, the BF_3^- anion is not expected to exist as a stable species even in its lowest vibrational energy level. The small intrinsic electron affinity of the boron atom combined with the close proximity of the three fluorine ligands likely is the origin of this instability. The instability of the BF_3^- has been also suggested by Grant et al. who predicted a negative electron affinity (−0.56 eV) for its parent neutral molecule at the CCSD(T)/CBS theory level [24]. Moreover, measurements of the adiabatic EA of BF_3 undertaken by Rothe et al. also led to a negative value [43].

In contrast, BCl_3^- is predicted to be a stable anion in its lowest vibrational state and would require substantial vibrational excitation of the puckering mode to reach an internal energy at which electron detachment would be expected. This conclusion agrees with both (i) an experimental evaluation of the adiabatic electron affinity of BCl_3 (0.33 ± 0.20 eV) extracted from the threshold kinetic energy for the $Cs + BCl_3 \rightarrow Cs^+ + BCl_3^-$ reaction (using a crossed molecular beam technique) [43] and (ii) earlier theoretical calculations of the EA performed at the CCSD(T)/CBS level (0.49 eV) [24].

Unlike BF_3^-, AlF_3^- is predicted to be a stable anion and to become electronically unstable only when vibrational motion along the puckering mode brings it into planarity. We believe the possible existence of the AlF_3^- anion has not been raised in the literature thus far, so we have no other data with which to compare.

$AlCl_3^-$ is also predicted to be a stable anion and to remain so even when vibrational motion along the puckering mode brings it into planarity. As with AlF_3, to the best of our knowledge the existence of the $AlCl_3^-$ anion has not been considered in the literature so we have no other data with which to compare.

Notice that for both AlF_3^- and $AlCl_3^-$, the energy profile has zero slope and negative curvature at the planar geometry. As discussed earlier, this suggests that there likely are low-lying vacant orbitals of the corresponding neutral that are even under reflection through the plane of the neutral molecule. Because of the large difference in electronegativity between Al and either F or Cl, a likely candidate for such a low-lying orbital would be the anti-bonding Al-X σ orbital of a'_1 symmetry. The corresponding bonding σ orbital would be strongly polarized toward the halogen nucleus, so its anti-bonding partner would have a large component of Al sp^2 character thus allowing it to couple strongly with the Al 3p (a''_2) orbital to generate the negative curvature.

Both GaF_3^- and $GaCl_3^-$ are predicted to be stable anions and to remain so even when vibrational motion along the puckering mode reaches planarity. To the best of our knowledge the existence of either GaF_3^- or $GaCl_3^-$ has not been considered in the literature so we have no other data with which to compare. As with AlF_3^- and $AlCl_3^-$, these anions' energy profiles have zero slope and negative curvature at the planar geometry probably for the reasons discussed above.

3.2. MX_3 hydrides and their anions

As mentioned in Section 1, we included BH_3^-, AlH_3^-, and GaH_3^- in this study to contrast these anions' behavior to the halogen-containing species and because salts containing anions related to these hydrides have received considerable attention in battery technology and because neutral BH_3 and AlH_3 are important agents in organic synthesis.

One significant difference that could be expected results from the substantial electronegativity differences between H and F or Cl. In particular, B and H have very similar electronegativities, whereas Al and Ga are less electronegative than H.

It is likely that the very similar electronegativities of B and H are why the BH_3^- anion remains planar whereas all the other anions studied here adopt non-planar geometries.

We note that not only are BH_3 and BH_3^- planar but so are [44] CH_3^+ and CH_3 as well as NH_3^+, probably for the reasons explained above.

Based on the CCSD(T)/aug-cc-pV5Z electronic energies obtained for the QCISD/6-311++G(3df,2pd) equilibrium structures of both BH_3 and BH_3^- (corrected by the inclusion of the zero-point vibrational energies), the adiabatic electron affinity of BH_3 of 0.02 eV agrees well with the experimental result of 0.038 ± 0.015 eV (see Ref. [22]) and the earlier theoretical evaluations (0.03 eV) attained by applying either the CCSD(T)/WMR [23] or CCSD(T)/CBS approach [24] (where WMR stands for atomic natural orbital basis of Widmark–Malmqvist–Roos (boron: [14s9p4d3f/7s7p4d3f]; hydrogen: [8s4p3d/6s4p3d]) [45] whereas CBS indicates the complete basis set limit based on the series of calculations employing the aug-cc-pVnZ basis sets, n = D, T, Q) [37–41]). It is worth noting that a B3LYP/6-311+G(d) estimate [25] gives a surprisingly accurate EA value for BH_3 (0.04 eV). However, because we found that high-level *ab initio* calculations with a large basis set were required to properly come close to the experimental EA, this DFT result was probably fortuitous.

These results suggest that AlH_3^- and GaH_3^- should be electronically stable both vertically and adiabatically.

Table 1
Vertical electron detachment energies and adiabatic electron affinities (including zero-point energy corrections) for the nine species studied here evaluated at the level of theory indicated as detailed in Section 2.

Species	QCISD/6-311++G(3df,2pd)	CCSD(T,full)/6-311++G(3df,2pd)
Vertical electron detachment energy (VDE) [eV]		
BH_3^-	<0	0.04[a]
BF_3^-	0.59	0.60
BCl_3^-	1.54	1.52
AlH_3^-	0.38	0.41
AlF_3^-	1.88	1.92
$AlCl_3^-$	2.42	2.43
GaH_3^-	0.29	0.37
GaF_3^-	3.01	2.98
$GaCl_3^-$	3.03	3.10
Adiabatic electron affinity (EA) [eV]		
BH_3	<0	0.02[a]
BF_3	−0.75[b]	−0.74
BCl_3	0.43	0.42
AlH_3	0.29	0.31
AlF_3	0.90	0.94
$AlCl_3$	1.28	1.28
GaH_3	0.27	0.26
GaF_3	1.79	1.72
$GaCl_3$	1.81	1.76

[a] The results obtained using the CCSD(T,full)/aug-cc-pV5Z electronic energies.
[b] As noted in the text, BF_3^- is predicted to be unstable with respect to electron autodetachment.

4. Summary

We have used *ab initio* electronic structure methods with flexible atomic orbital basis sets to examine the extent to which tri-fluorides, tri-chlorides, and tri-hydrides of B, Al, and Ga can bind an excess electron to form an anion. The adiabatic and vertical electronic stabilities of the BX_3^-, AlX_3^-, and GaX_3^- anions (X = F, Cl) manifested in their EA and VDE values, respectively, follow certain trends. Namely, the EAs of BF_3, AlF_3, and GaF_3 increase with increasing atomic number of the central atom – from a negative value characterizing boron tri-fluoride, through a positive EA of 0.90 eV for aluminum tri-fluoride, up to 1.79 eV predicted for GaF_3. An analogous trend is observed for the corresponding tri-chlorides whose EAs grow from 0.43 eV (BCl_3) through 1.28 eV ($AlCl_3$) to 1.81 eV ($GaCl_3$) as we summarize in Table 1. Not surprisingly, the VDE values characterizing the tri-halide anions follow the same trend as the EAs of the corresponding neutral molecules. Hence, the smallest VDEs are predicted for the anions containing boron whereas the VDE values for gallium tri-fluoride and gallium tri-chloride are the largest and slightly exceed 3 eV. In addition, for any given central atom M (M = B, Al, Ga) the adiabatic and vertical electronic stabilities for the MCl_3 tri-chloride system are always larger than those evaluated for the corresponding tri-fluoride compound (MF_3).

The B, Al, and Ga tri-hydrides have quite different electron binding strengths than the corresponding tri-halides. BH_3 has, as was known earlier, a very small EA (ca. 0.02 eV) and its anion retains the planar geometry of its parent neutral unlike the tri-halide anions and AlH_3^- and GaH_3^-, which adopt non-planar geometries. AlH_3 and GaH_3 have considerably smaller EAs (ca. 0.3 eV) than the Al and Ga tri-halides (0.9–1.8 eV) and, as just noted, the AlH_3^- and GaH_3^- anions are non-planar.

Acknowledgement

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