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The structure and energetics of $[B, C, F, H_3]^+$: quantum chemistry shows multiple minima

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Abstract

There is a marked paucity of reliable energetics data for ions containing boron, carbon, fluorine and hydrogen. Even one of the conceptually most simple ions, $[B, C, F, H_3]^+$, is poorly understood because its sole measurement is part of a 40-year-old electron impact study on CH_3BF_2. Intuition suggests this ion has the structure $[CH_3BF]^+$. What else could it be—it is isoelectronically related to the well-known CH_3CN, $[CH_3CO]^+$ and $[CH_3N_2]^+$? What about $[BH_3CF]^+$, isoelectronic to the well-known BH_3CO and $[BH_3CN]^-$? We use high level quantum chemical calculations in the current study to disclose 10 minima: $[CH_3BF]^+$ is the most stable and $[BH_3CF]^+$ is not even a minimum. Derived quantitative energy differences and qualitative reasoning are used for the understanding of the various isomeric forms of the $[B, C, F, H_3]^+$ ion, and by inference and extension in future studies, other ions containing boron, carbon and fluorine.

Keywords: Organoborane halide; QCISD(T); Hydrogen bonds; Hydrogen bridges; Isomeric structures; Isoelectronic species

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1. Introduction

We start with acknowledging that ions with the composition $[B, C, F, H_3]^+$ are all but unknown and uncharacterized. An appearance energy of 15.05 ± 0.10 eV has been reported [1] for such an ion arising from electron impact on the organoborane halide derivative CH_3BF_2. The general lack of reliability of such measurements as earlier practiced (see, for example, the preliminary text in [2]) and the lack of thermochemical knowledge of organic derivatives of the boron fluorides [3] conspire to give not more than a plausible estimate of the enthalpy of formation of this ion.

We say "this ion" as though it is structurally unique. The most probable structure of the species formed in the above ion formation and fragmentation process is $[CH_3BF]^+$, produced by simple B–F cleavage. As suggested, much as BF is related to CO, N_2 and CN^-, this ion is related to $[CH_3CO]^+$, $[CH_3N_2]^+$ and CH_3CN, archetypal examples of acylating agents, biologically active electrophiles and mutagens/carcinogens, and aprotic dipolar solvents. It is also similar to CH_3BO, which is the major product in a matrix isolation study of the reaction between

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laser-ablated boron atoms and methanol [4]. An isomeric form of $[B, C, F, H_3]^+$ with the B–C bonded connectivity $[BH_3CF]^+$ also appears to be a reasonable species. CF^+ is isoelectronic to CO and CN^- and we recognize this new ion as related to BH_3CO and $[BH_3CN]^-$, particularly well-known stabilized forms of the otherwise unisolable simple borane BH_3.

Such recognition resulted in the quantum chemical comparison [5] of the related derivatives of the likewise unisolable and even simpler BH, $[HBCF]^+$ and its derivatives HBCO and $[HBCN]^-$. Such calculations showed a variety of possible structures, both cyclic and the expected acyclic. This suggested there might be a variety of structures for $[B, C, F, H_3]^+$ other than just the above described $[CH_3BF]^+$ and $[BH_3CF]^+$. This possibility is realized. The current paper is a quantum chemical study of the structure and energetics of these species. Multiple minima are found. Many surprises abound.

2. Computational details

Ab initio molecular orbital calculations were performed with use of the Gaussian 98 suite of programs [6]. The minima on the singlet potential energy surface (PES) of $[B, C, F, H_3]^+$ were mapped out utilizing both Møller–Plesset second-order perturbation MP2 calculations [7,8] and quadratic configuration interaction QCISD calculations [9] together with the aug-cc-pVDZ basis set [10,11]. Based on other studies of the features of PES [12–14] computed energies were then improved by single-point QCISD(T)/aug-cc-pVTZ calculations for both sets of geometries. The quadratic configuration interaction theory QCISD(T) includes all single and double excitations plus perturbative corrections for the triple excitations [9]. The equilibrium structures were characterized by harmonic vibrational frequency calculations at the MP2/aug-cc-pVDZ and QCISD/aug-cc-pVDZ levels. The vibrational frequencies are unscaled.

The aug-cc-pVDZ and aug-cc-pVTZ correlation-consistent basis sets developed by Dunning and co-workers [10,11] have been optimized for best performance with correlated calculations. They are valence double-zeta or triple-zeta basis sets with polarization and diffuse functions on all atoms. Since this family of basis sets was developed in a systematic way, many properties converge asymptotically as the size of the basis set increases.

3. Results and analysis of results

Ten minima have been located on the singlet PES of $[B, C, F, H_3]^+$. The isomers are illustrated in Fig. 1. They have been numbered in order of decreasing stability. The relevant geometrical parameters for the isomers are given in Table 1 for both the MP2/aug-cc-pVDZ and QCISD/aug-cc-pVDZ optimizations. The remaining bond lengths differed by less than 0.007 Å for the two sets of data; the remaining bond angles and dihedral angles differed by less than 1.3°. The point group for isomers **4** and **9** changes from C_1 for the MP2 optimizations to C_s for the QCISD optimizations. This change in symmetry leads to some of the largest deviations in the geometrical parameters obtained with the two procedures.

Only two of the covalently-bound structures, **1** and **2**, have a terminal fluorine atom. Six of the structures have a fluorine bridge, with CFB, CFH and BFH combinations all represented. Two of the structures have unconventional hydrogen bonds, in which the carbon atom is either the electron-donating atom or the proton-donating atom. Isomer **10** has a $C–H\cdots B$ hydrogen bond, whereas isomer **7** has a $B–H\cdots C$ hydrogen bond. We have designated these linkages as three-center/four-electron hydrogen bonds as opposed to three-center/two-electron hydrogen bridges since the $X–H\cdots Y$ angles are linear or nearly so rather than significantly bent. Many other connectivities have been examined for $[B, C, F, H_3]^+$. Surprisingly, no structures containing a tetracoordinate boron atom were observed at minima. The only equilibrium structure that contains a BH_3 moiety is **7**, the hydrogen-bonded ion $[H_2B–H\cdots C–F]^+$. All of our attempts to locate the $[H_3B–C–F]^+$ isomer have proved futile, since it rearranges without

Table 1
Selected geometrical parameters for the [B, C, F, H_3]$^+$ system[a]

Structure	Bond lengths (Å)	Bond angles (°)	Dihedral angles (°)
$[H_3C–BF]^+$, **1** C_{3V}	CB: 1.500 [1.506] BF: 1.251 [1.251]	CBF: 180.0 [180.0]	
$[H_2B–CFH]^+$, **2** C_s	CB: 1.580 [1.588] CF: 1.270 [1.273]	BCF: 120.2 [120.3]	HBCF: ±90.9 [±91.0]
$[H_3C–FB]^+$, **3** C_s	CF: 1.674 [1.682] BF: 1.484 [1.488]	CFB: 136.5 [138.1]	HCFB: ±60.5 [±60.5]
$[H_2C–B–FH]^+$, **4** C_1 [C_s]	CB: 1.378 [1.392] BF: 1.466 [1.476]	CBF: 178.4 [161.3]	HFBC: 2.3 [0.0] HCBF: 88.5 [±97.2] HCBF: −93.1
$[HF–C(H)–BH]^+$, **5** C_1	CB: 1.429 [1.433] CF: 1.585 [1.618]	FCB: 110.1 [108.5] HCB: 143.1 [145.7]	HBCF: −123.5 [−108.4] HBCH: 68.0 [84.8] HFCB: 108.5 [109.0]
$[H_2B–F–CH]^+$, **6** C_s	CF: 1.534 [1.558] BF: 1.562 [1.544]	CFB: 118.6 [119.5] HCF: 118.6 [94.0]	
$[H_2BH\cdots CF]^+$, **7** C_s	CF: 1.226 [1.235] BH: 1.341 [1.352] C···H: 1.440 [1.426]	BHC: 162.0 [162.3] HCF: 104.6 [104.4]	
$[H_2C(B)–FH]^+$, **8** C_s	CB: 1.725 [1.738] CF: 1.672 [1.719]	FCB: 99.7 [99.2]	HFCH: ±58.6 [±58.3]
$[H_2C–F–BH]^+$, **9** C_1 [C_s]	CF: 1.500 [1.485] BF: 1.516 [1.555]	CFB: 166.8 [149.9] HCF: 106.5 [108.8] HCF: 106.8 [108.8]	HBFC: −173.1 [180.0] HCFB: 64.7 [±75.4] HCFB: −79.0
$[HC(F)H\cdots BH]^+$, **10** C_1	CF: 1.256 [1.257] CH: 1.140 [1.135] H···B: 2.153 [2.191]	CHB: 176.1 [176.1] HBH: 180.0 [180.0]	HBHC: 135.0 [161.0] HCHB: 180.0 [180.0] FCHB: 0.1 [−0.2]

[a] MP2/aug-cc-pVDZ and QCISD/aug-cc-pVDZ data (in brackets).

barrier to isomer **2**. We must conclude that $[H_3B–C–F]^+$, which is related to BH_3CO and $[BH_3CN]^-$, does not exist. Likewise, the structures with connectivity $[H_3B–F–C]^+$, $[H_2B(F)–C–H]^+$ and $[H_2B–H\cdots F–C]^+$ converted to **1**, **1** and **7**, respectively. All possible CFB three-membered ring systems were considered but they all rearranged to one of the stable acyclic systems. For example, c-H_2CFBH converted to **1**. Structures with one bridged hydrogen, two bridged hydrogens and an X–H···H–Y moiety were also unstable.

Table 2 gives the energies at 0 K and the enthalpies, entropies, and Gibbs free energies at 298 K for the system [B, C, F, H_3]$^+$. The relative energies, enthalpies, entropies and Gibbs free energies for the 10 stable structures are collected in Table 3. The QCISD(T)/aug-cc-pVTZ//MP2/aug-cc-pVDZ and QCISD(T)/aug-cc-pVTZ//QCISD/aug-cc-pVDZ data are provided in the tables. Any differences in the MP2/aug-cc-pVDZ//MP2/aug-cc-pVDZ and/or QCISD/aug-cc-pVDZ//QCISD/aug-cc-pVDZ results are discussed below.

The QCISD(T)/aug-cc-pVTZ total energies and relative thermochemical values show very little dependence on which set of equilibrium geometries is utilized to compute them. Despite differences in bond lengths of as much as 0.04 Å and differences in bond angles of as much as 25° (Table 1), the QCISD(T)/aug-cc-pVTZ relative energies, enthalpies and free energies generally agree to within 3 kJ/mol. The only structure for which the deviation in the two sets of data is larger (≈10 kJ/mol) is **9**, one of the ions for which the point group changes (Table 1).

The relative energies and enthalpies of the 10 ions are essentially equivalent at all four calculational levels (Table 3). The other isomers gain stability in contrast to **1** when entropy effects are taken into account. However, the enthalpy contributions are so dominant that the entropy contributions do not change the trends in free energy compared to the trends in enthalpy (Table 3).

The most stable ion is $[CH_3BF]^+$, that is the ion analogous to $[CH_3CO]^+$, $[CH_3N_2]^+$ and CH_3CN. Isomer **1** is most stable regardless of which calculational method is used, and it is more stable than the other isomers by at least 330 kJ/mol. The relative stabilities of the six lowest energy structures are identical for all four calculational levels, and the order remains the same whether it is based on energies, enthalpies, or Gibbs free energies (Tables 2 and 3). In contrast, although the four structures with highest energy remain in a separate group, their relative stabilities depend on the level of calculation. Ions **7** and **8** switch places in the stability order since their energies, enthalpies and free energies sometimes deviate by less than 1 kJ/mol. The two lower level calculations place isomer **10** below **9**; however, increasing the size of the basis set and improving the correlation level interchanges their stabilities (Tables 2 and 3). In fact, obtaining QCISD(T)/aug-cc-pVTZ single-point energies reverses the relative energies of these two structures by as much as 80 kJ/mol. This change is observed for both sets of geometries.

For the 10 isomers we have located, only the two most stable isomers, $[CH_3BF]^+$ and $[H_2BCFH]^+$, have just one unsaturated atom (B for **1** and C for **2**). All of the other isomers have two or more unsaturated or over-saturated atoms (Fig. 1). In addition, **1** and **2** are the only two ions without either a non-terminal fluorine atom or hydrogen bonding.

The low stability of **9** was initially surprising to us. Utilizing our best data (Tables 2 and 3), the only structure higher in energy than **9** is the hydrogen-bonded structure **10**. Even isomer **7**, the other hydrogen-bonded isomer, is about 15 kJ/mol more stable than

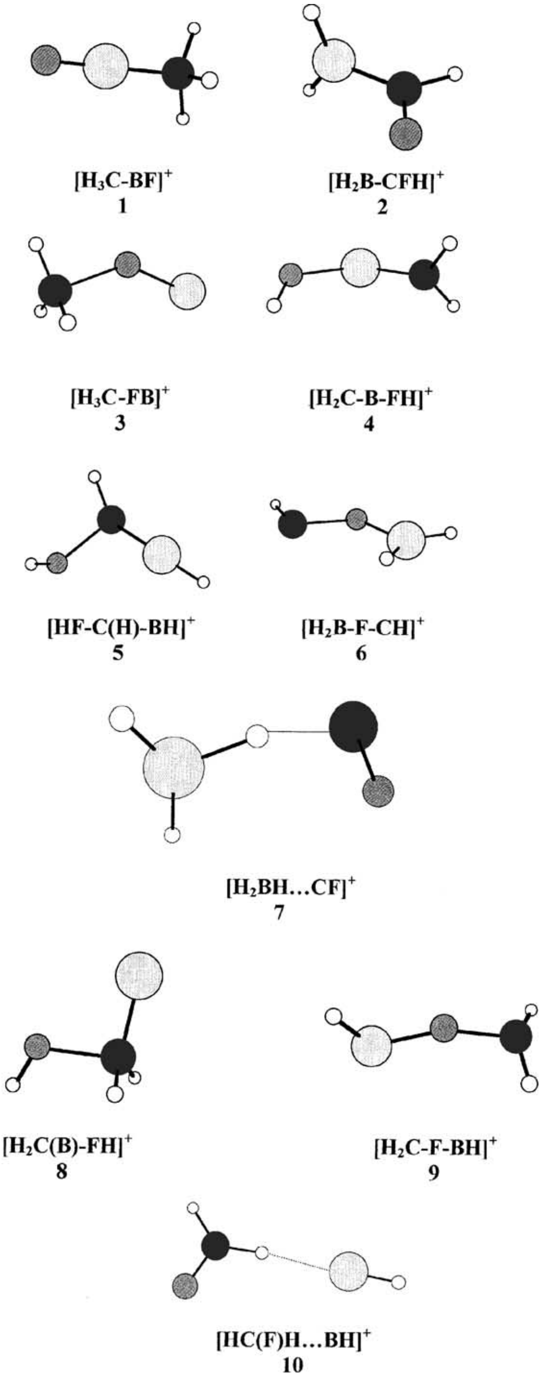


Fig. 1. Ball and stick representations of the 10 $[B, C, F, H_3]^+$ isomers. The degrees of grayness are: C > F > B > H. The sizes of the balls are: B > C > F > H.

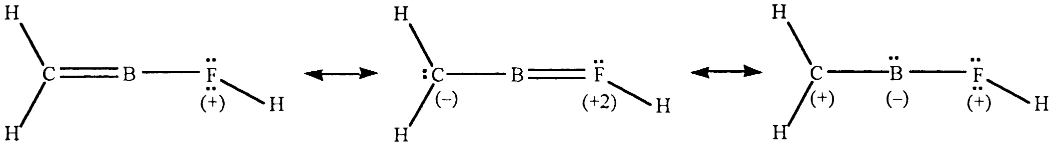
Table 2
Total energies, enthalpies, entropies, and free energies for the [B, C, F, H_3]$^+$ system[a]

Structure	E (0 K)	H (298 K)	G (298 K)	S (298 K)
[H_3C–BF]$^+$	−164.054749	−164.0538049	−164.0820319	59.409
1	[−164.054813]	[−164.0538690]	[−164.0821010]	[59.419]
[H_2B–CFH]$^+$	−163.9145340	−163.9135900	−163.9434340	62.813
2	[−163.9146954]	[−163.9137504]	[−163.9436184]	[62.862]
[H_3C–FB]$^+$	−163.8932817	−163.8923367	−163.9250157	68.779
3	[−163.8933523]	[−163.8924083]	[−163.9264133]	[71.570]
[H_2C–B–FH]$^+$	−163.8897037	−163.8887597	−163.9197317	65.185
4	[−163.8893447]	[−163.8884007]	[−163.9194197]	[65.286]
[HF–C(H)–BH]$^+$	−163.8541165	−163.8531725	−163.8835925	64.024
5	[−163.8540839]	[−163.8531399]	[−163.8837629]	[64.453]
[H_2B–F–CH]$^+$	−163.8179468	−163.8170028	−163.8479448	65.123
6	[−163.8183870]	[−163.8174430]	[−163.8484910]	[65.347]
[H_2BH···CF]$^+$	−163.8106128	−163.8096688	−163.8435748	71.362
7	[−163.8107955]	[−163.8098515]	[−163.8437785]	[71.406]
[H_2C(B)–FH]$^+$	−163.8093952	−163.8084512	−163.8399232	66.238
8	[−163.8092468]	[−163.8083028]	[−163.8399858]	[66.682]
[H_2C–F–BH]$^+$	−163.8032012	−163.8022562	−163.8343272	67.497
9	[−163.8070042]	[−163.8060602]	[−163.8381642]	[67.570]
[HC(F)H···BH]$^+$	−163.7907303	−163.7897863	−163.8231783	70.280
10	[−163.7908605]	[−163.7899165]	[−163.8235825]	[70.857]

[a] QCISD(T)/aug-cc-pVTZ//MP2/aug-cc-pVDZ and QCISD(T)/aug-cc-pVTZ//QCISD/aug-cc-pVDZ data (in brackets). Energies, enthalpies, and free energies in Hartrees; entropies in J/(mol K).

9. A more careful examination of the equilibrium geometries of **9** and **10** shows that these two ions can be considered to consist of the same two groups [H_2CF]$^+$ and BH. These groups are connected to each other with a B–F bond in **9** and a B···H bond in **10**. With regard to ion **9**, BH is known to be a Lewis acid but the [H_2CF]$^+$ fragment is undoubtedly a poor Lewis base. With regard to ion **10**, BH is now the electron donor and the [H_2CF]$^+$ fragment is the proton donor in the weak C–H···B hydrogen bond. An extension of this analysis that may further our understanding of the poor stability of **9** is to compare **9** with **6**. The only difference in the connectivities of these two cations is that a H atom is bonded to C instead of B in **9** (ignore the differences in bond angles and bond lengths). Yet **9** is far less stable than **6**. This difference in stability can be explained by considering **6** as a complex of H_2BF (a better Lewis base than [H_2CF]$^+$) and CH$^+$ (a better Lewis acid than BH).

The optimum bond lengths collected in Table 1 suggest that several of these structures may have some double bond character. Lanzisera and Andrews have found evidence for C=B bonds in their studies of laser-ablated boron reacting with C_2H_6 [15] and CH_3X, X = F, Cl, Br [16]. The products of these reactions were identified by obtaining matrix infrared spectra for several isotopic combinations and density functional frequency calculations. The major product in the first reaction is CH_3BCH_2 [15]; two of the major products in the latter reactions are H_2CBX and HCBX [16]. Although CH_3BF was not detected in the matrix, CH_3BCl and CH_3BBr were both observed [16]. The results indicate that, unlike the CB bonds in CH_3BCl and CH_3BBr, one CB bond in CH_3BCH_2 and the CB bonds in H_2CBX and HCBX are double bonds. Based on the BP86/6-311G(d) data, the C=B double bond is about 0.2 Å shorter than the C–B single bond. If the C–B bond in the analogous ion **1**, [CH_3BF]$^+$, is used as the reference bond for ions containing a bridged boron atom, the reference C–B bond length for our systems is 1.506 Å (QCISD/aug-cc-pVDZ data, Table 1). Although the CB bonds in isomers **4** and **5** are not 0.2 Å shorter than the bond in **1**, these bonds may have some double bond character.



Scheme 1.

In contrast, Lanzisera and Andrews' calculations show that the BF bonds in H_2CBF and HCBF are only 0.03 Å shorter than the corresponding bond in CH_3BF. They interpret these data as indicating that the BF bonds are single bonds, i.e., the F atom does not donate a lone pair of electrons into the empty p-orbital on boron [16]. The results for the $[B, C, F, H_3]^+$ system are quite different. Although there is no good reference structure for the B–F bond in these isomers, we observe a wide range of lengths for that bond (Table 1). In particular, our results suggest that the BF bond in ion **1** may exhibit some dative bonding. We note that Lanzisera and Andrews' data can also be interpreted as indicating that all three molecules have a common B–F bond order greater than one but less than that found in our cationic species with their even more electron-deficient boron.

Table 3
Relative energies, enthalpies, entropies, and free energies for the $[B, C, F, H_3]^+$ system[a]

Structure	ΔE (0 K)	ΔH (298 K)	ΔG (298 K)	ΔS (298 K)
$[H_3C–BF]^+$	0.0	0.0	0.0	0.0
1	[0.0]	[0.0]	[0.0]	[0.0]
$[H_2B–CFH]^+$	367.8	367.8	363.5	3.4
2	[367.5]	[367.5]	[363.2]	[3.4]
$[H_3C–FB]^+$	423.5	423.5	411.8	9.4
3	[423.5]	[423.5]	[408.4]	[12.2]
$[H_2C–B–FH]^+$	432.9	432.9	425.7	5.8
4	[434.0]	[434.0]	[426.7]	[5.9]
$[HF–C(H)–BH]^+$	526.2	526.2	520.5	4.6
5	[526.5]	[526.5]	[520.2]	[5.0]
$[H_2B–F–CH]^+$	621.1	621.1	614.0	5.7
6	[620.1]	[620.1]	[612.7]	[5.9]
$[H_2BH\cdots CF]^+$	640.4	640.4	625.5	12.0
7	[640.0]	[640.0]	[625.1]	[12.0]
$[H_2C(B)–FH]^+$	643.6	643.6	635.0	6.8
8	[644.1]	[644.1]	[635.1]	[7.3]
$[H_2C–F–BH]^+$	659.8	659.8	649.7	8.1
9	[650.0]	[650.0]	[639.8]	[8.2]
$[HC(F)H\cdots BH]^+$	692.5	692.5	679.0	10.9
10	[692.3]	[692.3]	[678.1]	[11.4]

[a] QCISD(T)/aug-cc-pVTZ//MP2/aug-cc-pVDZ and QCISD(T)/aug-cc-pVTZ//QCISD/aug-cc-pVDZ data (in brackets). Energies, enthalpies, and free energies in kJ/mol; entropies in J/(mol K).

Isomers **8** and **3** are used as the reference isomers for the C–F bond, since these bonds involve a tetracoordinate carbon atom and are presumably single bonds. For the QCISD/aug-cc-pVDZ data, the C–F bond length is 1.719 Å in **8** and 1.682 Å in **3**. The C–F bonds in all of the other isomers are considerably shorter, decreasing in length by as much as 0.4 Å, and may have some double bond character.

The possibility of double bond character in these isomers is supported by the existence of reasonable Lewis structures that contain double bonds. The three most reasonable resonance forms for cation **4** are presented in Scheme 1. Resonance structures with a +2 formal charge have been included to accommodate the octet rule and the total ion charge of +1. Similar types of resonance forms can be drawn for each of the remaining cations without hydrogen bonds. Seven of these eight isomers have at least one Lewis structure with a single formal charge of +1. No such Lewis structure can be drawn for **9**, which is another way to rationalize its poor stability. Only the two most stable ions **1** and **2** have a resonance form for which the +1 formal charge is on the more electropositive C or B atom.

4. Summary

In summary, the following points were made:

1. Ten minima have been located on the PES of $[B, C, F, H_3]^+$. Although both cyclic and acyclic

structures were considered, only acyclic structures were identified at minima. Two of the isomers have unconventional hydrogen bonds involving the carbon atom and six have a bridged fluorine atom.

2. With the exception of isomer **9**, the MP2/aug-cc-pVDZ and QCISD/aug-cc-pVDZ potential surfaces are quite flat in the regions near the minima. Although there are differences in the equilibrium structures obtained at the two levels of calculation, especially in the dihedral angles, the QCISD(T)/aug-cc-pVTZ single-point energies based on the two sets of geometries generally agree to <1.5 kJ/mol. The deviation is 10 kJ/mol for isomer **9**, one of the two isomers that belongs to a different point group at the two levels.
3. Improving the correlation level altered the relative stabilities of some of the isomers.
4. The most stable structure **1** is $[CH_3BF]^+$, which is related to $[CH_3CO]^+$, $[CH_3N_2]^+$ and CH_3CN. Efforts to locate $[BH_3CF]^+$, which is related to BH_3CO and $[BH_3CN]^-$, proved futile. The surprising instability of structure **9** $[H_2C–F–BH]^+$ has been rationalized on the basis of the $[H_2CF]^+$ fragment being a poor Lewis base and the BH fragment being a weak Lewis acid.
5. Some of the structures may have some double bond character.

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