Inorg. Chem. **1999,** *38,* 4659−4662

Ligand Close-Packing and the Lewis Acidity of BF_3 and BCl_3

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Received June 17, 1999

The unexpected greater Lewis acidity of BCl_3 than BF_3 with respect to strong bases such as NH_3 has been the subject of much discussion. A number of explanations have been proposed, among which the most popular and most widely quoted is that stronger back-donation from fluorine than from chlorine decreases the availability of the otherwise empty 2p orbital on boron from accepting an electron pair from a base. In contrast, toward weak bases such as CO, BF_3 is a stronger Lewis acid than BCl_3. We have reinvestigated the relative acid strengths of BF_3 and BCl_3 toward Lewis bases by calculating geometries and atomic charges for the following adducts: $BF_3{\cdot}NH_3$, $BF_3{\cdot}N(CH_3)_3$, $BF_3{\cdot}OH_2$, $BF_3{\cdot}O(CH_3)_2$, $BCl_3{\cdot}NH_3$, $BCl_3{\cdot}N(CH_3)_3$, $BCl_3{\cdot}OH_2$, and $BCl_3{\cdot}O(CH_3)_2$. Our results show that the halogen ligands remain close-packed throughout the formation of an adduct and that the bond lengths increase accordingly. It takes more energy to lengthen the short strong BF bonds than the longer weaker BCl bonds and it is for this reason that BCl_3 is a stronger Lewis acid than BF_3 toward a strong base such as NH_3. In contrast, in the formation of a complex with a weak base such as CO, the BX_3 is barely distorted from planarity and so the acidity of BF_3 is greater than that of BCl_3 because the charge on boron is greater in BF_3 than BCl_3.

Introduction

It has been well-established by several different experimental methods that the Lewis acidities of the boron halides toward a number of nitrogen and oxygen bases such as $N(CH_3)_3$ and $O(CH_2CH_3)_2$ is $BF_3 < BCl_3 < BBr_3$.[1] Moreover, ab initio calculations have shown that the BN bond in gas-phase $BCl_3{\cdot}NH_3$ is stronger than in $BF_3{\cdot}NH_3$ by 7.7 kcal mol^{-1}.[2] This order is unexpected in view of the decrease in electronegativity from fluorine to chlorine to bromine which would predict a decreasing positive charge on boron in the order $BF_3 > BCl_3 > BBr_3$. This variation in the charge on boron has been confirmed by ab initio calculations for BF_3 and BCl_3 for which NBO charges are $+1.49$ and $+0.29$, respectively,[3] and the AIM charges are $+2.43$[4] and $+1.93$,[5] respectively. The generally accepted explanation for this apparently anomalous order of Lewis acidity is that there is back-donation of charge from one of the 2p orbitals of fluorine to the vacant $2p_z$ orbital of boron, leading to some double bond character for the BF bond in BF_3. In BCl_3, this back-donation is considered to be less important because of a poorer overlap between a chlorine 3p orbital and the boron $2p_z$ orbital. This back-donation makes the $2p_z$ orbital of boron in BF_3 less available for complex formation than that of BCl_3 and hence BF_3 is a weaker acid than BCl_3. However, in a recent paper Brinck[3] showed that the overlap integral of Slater-type boron 2p and fluorine 2p orbitals at the experimental bond length is actually smaller than the corresponding integral for boron 2p and a chlorine 3p orbital. They also showed that the highest-occupied Hartree−Fock π molecular orbital for BCl_3 contains a larger contribution from the boron 2p orbital than the corresponding highest-occupied π molecular orbital in BF_3. These authors therefore proposed an alternative explanation in terms of a concept called charge capacity originally due to Huheey[6] which was formulated as a measure of the ability of a molecule or a group of atoms within a molecule to accept charge. The charge capacities of the boron halides, which were calculated using the experimentally determined electron affinities and ionization potentials, were found to increase in the order $BF_3 < BCl_3 < BBr_3$. From the calculated NBO atomic charges they found that there is a larger charge transfer in the formation of $BCl_3{\cdot}NH_3$ than for the formation of $BF_3{\cdot}NH_3$ and proposed that the increasing charge capacity from BBr_3 to BF_3 is the reason that the acidity of the boron halides increases in this order.[3]

In contrast to the relative Lewis acid strengths toward strong bases, the reverse order, namely that expected on the basis of the charge on the boron atom, has been observed for the weak bases CO, HCN, CH_3CN,[2] and CH_3F.[7]

An extensive theoretical study of the Lewis acid−base conplexes of BH_3, BF_3, BCl_3, $AlCl_3$, and SO_2 has been carried out recently by Frenking et al.[2] Their calculated dissociation energies for eighteen complexes were in good agreement with experimental gas-phase values where these are available. Their calculations confirmed and extended experimental observations that show that the BF and BCl bond lengths in BF_3 and BCl_3 complexes increase with increasing strength of the complex, an important observation that we shall return to.

The purpose of the present paper is to present a simple explanation of the Lewis acid strengths of the boron halides in terms of the recently proposed ligand close-packing (LCP) model.[5,8]

Computational Methods

Standard ab initio and density functional (B3LYP)[9] calculations have been performed on the molecules $BF_3{\cdot}NH_3$, $BF_3{\cdot}N(CH_3)_3$, $BCl_3{\cdot}NH_3$, $BCl_3{\cdot}N(CH_3)_3$, $BF_3{\cdot}OH_2$, $BF_3{\cdot}O(CH_3)_2$, $BCl_3{\cdot}OH_2$, and $BCl_3{\cdot}O(CH_3)_2$.

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10.1021/ic990713m CCC: $18.00

Table 1. Structural Parameters and Nonbonded Interatomic Distances (Å) for $BF_3\cdot NH_3$

	X-ray[a]	microwave[b]	MP2(FC)/TZ2P[c]	this work
B−N	1.60	1.59	1.678	1.685
B−F	1.38		1.367	1.372
N−H			1.012	1.020
∠BNH			110.3	110.2
∠NBF	107		103.9	104.1
∠FBF	111			114.3
∠HNH				108.7
F---F	2.27		2.298	2.305
N---F	2.40		2.406	2.418

[a] Reference 14. [b] Reference 15. [c] Reference 2.

Table 2. Structural Parameters and Nonbonded Interatomic Distances (Å) for $BF_3\cdot N(CH_3)_3$

	X-ray[a]	ED[b]	MP2(FC)/TZ2P[c]	this work
B−N	1.585	1.664	1.661	1.686
B−F	1.39	1.354	1.374	1.377
N−C	1.50	1.468	1.478	1.512
∠BNC	105	110.5	109.4	107.2
∠NBF	112	105.5	105.2	105.5
∠FBF	107	113.1	113.4	113.2
∠CNC	112	108.5	109.5	111.6
F---F	2.24	2.259	2.297	2.299
N---F	2.52	2.410	2.417	2.445

[a] Reference 14. [b] Reference 16. [c] Reference 2.

All geometries have been optimized at the B3LYP level, as implemented in the Gaussian 94 program,[10] using the 6-311+G(2d,p) basis set of Pople,[11] a method which is widely used for calculating charges and densities. Electron densities calculated at B3LYP/6-311+G(2d,p) have been analyzed using the theory of Atoms In Molecules.[12] In this theory, each atom is defined by a region of space bounded by an interatomic surface, and the charge on the atom is calculated by integrating the electron density throughout that region. AIM charges are, in general, larger than those calculated using NBO,[13] the most rigorous of the orbital-based methods for calculating charges. Results of our geometry optimizations are presented in Tables 1−5, with all inernuclear distances in Å and all angles in degrees. Calculated atomic charges are presented in Tables 6 and 7, and the energies of distortion of BF_3 and BCl_3 to pyramidal structures is presented in Table 8.

Table 3. Structural Parameters and Nonbonded Interatomic Distances (Å) for $BCl_3\cdot NH_3$ and $BCl_3\cdot N(CH_3)_3$

	$BCl_3\cdot NH_3$			$BCl_3\cdot N(CH_3)_3$		
	MP2(FC)/ TZ2P[a]	this work	X-ray[b]	ED[c]	MP2(FC)/ TZ2P[a]	this work
B−N	1.606	1.621	1.610	1.652	1.634	1.663
B−Cl	1.833	1.845		1.836	1.841	1.855
N−C				1.497	1.489	1.526
∠BNC					111.0	108.7
∠NBCl	105.0	105.2			107.6	107.7
∠ClBCl	113.5	113.4		110.9	111.3	111.2
∠CNC				108.1	107.9	
Cl---Cl	3.066	3.084		3.025	3.039	3.061
N---Cl	2.732	2.757		2.833	2.806	2.843

[a] Reference 2. [b] Reference 22. [c] Reference 17.

Table 4. Structural Parameters and Nonbonded Interatomic Distances (Å) for $BF_3\cdot OH_2$ and $BF_3\cdot O(CH_3)_2$

	$BF_3\cdot OH_2$		$BF_3\cdot O(CH_3)_2$	
	X-ray[a]	this work	ED[b]	this work
B−O	1.532	1.902	1.75	1.712
B−F	1.388	1.345 × 2, 1.333	1.325	1.355 × 2, 1.363
O−C			1.439	1.446
∠BOC				114.7
∠OBF	106.8	98.3 × 2, 100.8	99.9	102.1 × 2, 103.3
∠FBF	111.5	117.6 × 2, 117.3	117.1	115.1 × 2, 116.1
∠COC			110	113.0
F---F	2.295	2.291 × 2, 2.297	2.26	2.293
O---F	2.347	2.483 × 2, 2.519	2.36	2.396 × 2, 2.421

[a] Reference 18. [b] Reference 19.

Table 5. Calculated Structural Parameters and Nonbonded Interatomic Distances (Å) for $BCl_3\cdot OH_2$ and $BCl_3\cdot O(CH_3)_2$

	$BCl_3\cdot OH_2$	$BCl_3\cdot O(CH_3)_2$
B−O	1.680	1.633
B−Cl	1.814 × 2, 1.836	1.831 × 2, 1.844
O−C		1.462
∠BOC		116.9
∠OBCl	102.6 × 2, 104.0	105.8 × 2, 105.7
∠ClBCl	114.3 × 2, 116.5	113.3 × 2, 112.1
∠COC		110.9
Cl---Cl	306.6 × 2, 308.5	307.0 × 2, 303.7
O---Cl	272.6 × 2, 276.9	276.6 × 2, 277.4

Table 6. Calculated Atomic Charges in Adducts with NH_3 and $N(CH_3)_3$

	$BF_3\cdot NH_3$	$BF_3\cdot N(CH_3)_3$	$BCl_3\cdot NH_3$	$BCl_3\cdot N(CH_3)_3$
q(B)	+2.40	+2.37	+1.92	+1.90
q(N)	−1.07	−1.07	−1.14	−1.01
q(F)	−0.84	−0.84		
q(Cl)			−0.67	−0.67
q(H)	+0.40		+0.41	
$q(CH_3)$		+0.41		+0.37
$q(BX_3)$	−0.12	−0.15	−0.09	−0.11
$q(NR_3)$	+0.12	+0.15	+0.09	+0.11

Results and Discussion

Calculated geometries for $BF_3\cdot NH_3$ and $BF_3\cdot N(CH_3)_3$ are presented in Tables 1 and 2, along with previous experimental[14,15,16] and theoretical[2] results. Our predicted geometries compare favorably with MP2(FC)/TZ2P calculations by Frenking and also with the gas-phase electron diffraction geometry for $BF_3\cdot N(CH_3)_3$, with the exception of the N−C bond length, which is slightly longer than the previous estimates. Our calculated geometries for $BCl_3\cdot NH_3$ and $BCl_3\cdot N(CH_3)_3$ molecules in Table 3 are also in agreement with Frenking's calculations, and for $BCl_3\cdot N(CH_3)_3$ similar agreement is found with the previous electron diffraction data.[17] The N−C bond is again slightly longer at the density functional level than at MP2 and compared to the experimental value. There is little

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Table 7. Calculated Atomic Charges in Adducts with OH_2 and $O(CH_3)_2$

	$BF_3 \cdot OH_2$	$BF_3 \cdot O(CH_3)_3$	$BCl_3 \cdot OH_2$	$BCl_3 \cdot O(CH_3)_2$
q(B)	+2.41	+2.39	+1.92	+1.90
q(O)	−1.10	−1.07	−1.16	−1.06
q(F)	−0.84 × 2, −0.83	−0.85		
q(Cl)			−0.67	−0.67
q(H)	+0.60		+0.62	
q(CH_3)		+0.62		+0.59
q(BX_3)	−0.10	−0.16	−0.09	−0.11
q(OR_2)	+0.10	+0.16	+0.09	+0.11

Table 8. Calculated Differences in Energy (in kJ mol^{-1}) between Planar and Pyramidal Geometries of BF_3 and BCl_3. The Pyramidal Geometries Are Defined by an Assumed XBA Angle Formed with a Lewis Base (A). All Values Are Calculated at B3LYP/6-311+G(2d,p) unless Noted

XBA angle (°)	BF_3	BCl_3
95.0	10.1	8.4
100.0	40.7	34.1
105.0	93.2	78.4
	106.3[a]	90.3[a]
	100.7[b]	82.3[b]
110.0	170.0	143.7

[a] HF/6-31+G(d,p) calculated value from ref 3. [b] MP2/6-31+G(d,p) calculated value from ref 3.

experimental background for the complexes of H_2O and $O(CH_3)_2$ with BF_3 and BCl_3. A crystal structure for $BF_3 \cdot OH_2$[18] and an electron diffraction study of $BF_3 \cdot O(CH_3)_2$[19] are compared with our calculations in Table 4. As has been observed,[20] the bond distances in the solid state are typically much shorter than the gas phase, and the comparison with experiment for $BF_3 \cdot OH_2$ is not a fair one. The calculated C_s geometry of $BF_3 \cdot O(CH_3)_2$ is in good agreement the electron diffraction data. In the calculated geometry of both of these molecules there are two sets of B−F bond distances and angles due to the differing environments of the fluorine lying in the plane of symmetry, and the two fluorines that lie off the symmetry plane. There has been no experimental observation of the chloride analogues of these molecules, $BCl_3 \cdot OH_2$ and $BCl_3 \cdot O(CH_3)_2$; we have calculated their geometries and presented them in Table 5.

Our calculated geometries confirm the accepted order of Lewis acidity for BF_3 and BCl_3. The B−N and B−O bond distances are shorter for the molecules of BCl_3 than they are for the corresponding BF_3 adducts, indicative of a stronger bond between the boron and the nitrogen or oxygen. The distance from boron to fluorine (which is 1.314 Å in BF_3) increases to 1.372 Å on interaction with NH_3, 1.377 Å with $N(CH_3)_3$, 1.349 Å (average) with OH_2, and 1.359 Å (average) with $O(CH_3)_2$. The distance from boron to chlorine (which is 1.750 Å in BCl_3) increases upon interaction with the Lewis bases to 1.845 Å (NH_3), 1.855 Å ($N(CH_3)_3$), 1.825 Å (OH_2, average), 1.837 Å ($O(CH_3)_2$, average), an average increase of 0.05 Å in BF_3 compared with 0.09 Å in BCl_3. The XBX angles similarly are smaller in the adducts than the 120° of planar BF_3 and BCl_3, the average angle in the BF_3 adducts being 115° compared with 113° for BCl_3 adducts.

In our previous studies of ligand close-packing we have published a series of nonbonded radii for atoms coordinated to central cations.[5] The values in coordination to boron are 1.13 Å for F, 1.51 Å for Cl, 1.24 Å for N, and 1.19 Å for O. Thus, if the adducts follow the guidelines for ligand close packing, we would expect interatomic distances of 2.26 Å for F---F, 3.02 Å for Cl---Cl, 2.37 Å for N---F, and 2.32 Å for O---F. All the calculated F---F distances are very close to 2.26 Å, indicating that the fluorine atoms remain close-packed about the boron nucleus. The Cl---Cl distances in all four adducts are also very close to that predicted on the basis of ligand close packing. In keeping with the accepted order of base strengths, the methylated molecules are calculated to form adducts with shorter adduct bond lengths, and greater distortion of the BX_3 group than NH_3 and OH_2. It appears that NH_3 distorts the BX_3 group to a greater extent than OH_2.

Atomic charges for all the atoms have been calculated using the theory of atoms in molecules (AIM). The charges on fluorine and chlorine remain fairly constant across all of the molecules studied. The charge on fluorine is intermediate between the charge on fluorine in BF_3, which is −0.81 and in BF_4^-, which is −0.86. Similarly the charge on chlorine is calculated to be between the values for BCl_3 and BCl_4^- (−0.65 and −0.70, respectively).[5] The charge on boron decreases slightly upon methylation of the adduct. The argument has been put forward that the lower Lewis acidity of BF_3 is due to its poor charge capacity when compared with BCl_3.[3] We can calculate the charges on each molecule in the adduct and hence calculate the charge transfer by summing the charges on the individual atoms. We can see that contrary to this argument, the charge transfer is greater for the fluorides than the chlorides, and BF_3 is actually accepting more electron density from the Lewis bases than BCl_3.

When a boron trihalide acts as a Lewis acid, as the bond forms between the boron and the donor atom the halogen atoms are repelled to the opposite side of the boron atom. They remain in contact with each other, as evidenced by the near-constant halogen−halogen distances which are in accord with the nonbonded distances predicted by the ligand close packing model. As the bond angle decreases the bond lengths increase accordingly. The high strength of the B−F bond, which is due to the large charges on B and F, and the smaller size of the F atom, allowing it to come close enough to boron to form a strong polar bond, mean that more energy is required to distort the BF_3 moiety from planarity. In the case of BCl_3, the bond is not so strong, the chlorine atoms are not as close to the boron nucleus, and the ability of the molecule to distort is much greater, hence the shorter adduct bonds and the greater Lewis acid strength of BCl_3. The "pyramidalization" energy, defined as the difference in energy between planar BX_3 and a geometry where the three XBX angles have been set at 103.5° and the B−X bond distance has been optimized, has been reported by Brinck at the HF and MP2 level.[3] We have calculated the pyramidalisation energies for several degrees of distortion of BF_3 and BCl_3 and presented these energies in Table 8. In accord with the previously calculated values, at the B3LYP level of theory, both small and large distortions of BF_3 require greater energy than distortions of BCl_3. In the case of very weak interactions such as those with CH_3F or CH_3CN the parent molecules are barely distorted, and the interaction is purely electrostatic in nature. This is the reason for the weak interactions having the opposite trends in acid strength to the stronger interactions with amines and ethers.

A strong Lewis base needs to get close to the boron atom to form a bond, and thus repels the fluorides or chlorides. It is questionable whether in the gas phase this approach is close enough to consider the entire molecule to be close-packed, and the oxygen or nitrogen atom of the donating molecule to be in

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contact with the halogen atoms on the boron. The nonbonded interatomic distances are all slightly longer than those predicted by the ligand close packing model, however in the solid state the energy required to repel the halogen atoms to the point where a strong bond can be formed is obtained from the interaction with the condensed medium environment.[20] The increase in molecular dipole moment caused by the shortening of the B−N bond has been observed in polarizable continuum calculations.[21] In the solid state the geometry is close-packed, and the interligand distances are in agreement with those predicted by the ligand close packing model.

Conclusions

We have shown that the difference in Lewis acidity between BF_3 and BCl_3 with strong donor molecules, can be explained on the basis of ligand close packing. As the donor molecule is attracted toward the boron atom by its large positive charge it repels the chlorine or fluorine ligands thus decreasing the XBX angle and increasing the BX bond length while the X---X distances remain constant in accordance with the LCP model. The ease with which this distortion occurs depends on the strength of the BX bonds. BF bonds are stronger and more difficult to stretch than BCl bonds. Hence with strong Lewis bases, such as NH_3, BF_3 is a weaker Lewis acid than BCl_3. Although the F and Cl ligands remain close packed through the formation of the acid−base complex in general the B−N or B−O distances are not short enough that the O or N atoms are also close packed with the halogen ligands. However in the solid-state structures of $BF_3{\cdot}NH_3$ and $BF_3.OH_2$ the medium provides sufficient energy to allow the BF_3 molecule to be distorted to a very nearly tetrahedral geometry and in these cases the F---N and F---O distances show that all four ligands are close packed around the boron. This explanation of the relative acid strengths of BF_3 and BCl_3 is simpler and more quantitative than the back-bonding explanation for which there is little, if any, compelling evidence.

With very weak bases such as CO the Lewis acid BX_3 is barely distorted from its planar geometry so no pyramidalization energy is required and the strength of the acid−base interaction depends only on the charge of the boron atom which is larger in BF_3 than in BCl_3. So for these complexes BF_3 is a stronger acid than BCl_3.

IC990713M

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