Effects of the Electronegativity of Second Row Elements on Their Bonding to Boron

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ABSTRACT

The effects of electronegativity on the bonding between boron and second row elements are studied in this paper. Calculations using Density Functional Theory (DFT), Moller-Plesset Theory (MP2) and Natural Bonding Orbital (NBO) analysis were performed on BF_3, $B(OH)_3$ and $B(NH_2)_3$ and the localized bonding properties of these molecules were elucidated. All of these molecules showed the absence of pi-bonding and did not obey the octet rule. With decreasing electronegativity of the terminal atoms, F, O and N in BF_3, $B(OH)_3$, $B(NH_2)_3$ there is increasing the propensity of electron donation from these terminal atoms to the empty p-orbital of the central boron. Within the $BH_2{-}F$, $BH_2{-}OH$ and $BH_2{-}NH_2$ series, the amino-borane showed the largest change in relative bond length and angle across this set. Furthermore, the borate anion, $^{-}O{-}B(OH)_2$ was subjected to identical analysis and pi-bond formation was observed. Our results show that a good match orbital energies between the donor and acceptor orbitals are important for pi-bond formation.

KEYWORDS

Electronegativity; Boron Trifluoride; Boric Acid; Triaminoborane; Borate Anion; Octet Rule; Density Functional Theory; Natural Bonding Orbital; Pi-Bond; Double Bond

INTRODUCTION

Chemical bonding is one of the central ideas in chemistry and the octet rule has been used successfully to describe the bonding and reactions in a wide range of substances and this applies to much of organic chemistry and other molecular compounds of the second row elements.[1] This rule state that elements react to form compounds by sharing their valence electrons and stability is achieved when each element has a total of eight valence electrons. (Hydrogen and lithium are exceptions and only requires two). Despite these successes, a number of covalent compounds do not obey this rule. Examples of this violation given in undergraduate-level texts frequently list compounds of beryllium, boron, and elements of the third row.[2,3] To our end, BF_3 was the model example and is the catalyst for our study in this paper. The Lewis structure of this molecule and the associated resonance forms are presented as four structures in **Figure 1** with the non-octet left most structure followed by three resonance structures that obey the octet rule.[1]

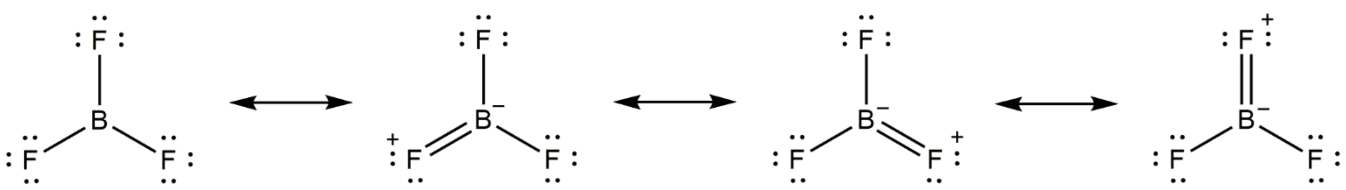

Figure 1. Lewis structure of $BF_3$and associated resonance forms.

A possible reason for the absence of octet in boron of BF_3 may be that the electronegativity (EN) of the terminal fluorine atoms affects their pi-donor strength, i.e. their willingness to donate an electron pair to form a pi-bond to boron.[4] In general, if electron pair donation (pi-bond formation) were to happen between an atom of higher EN to one of lower EN, for example from fluorine to boron, this electron pair would reside mainly around the atom with the higher electronegative[5] fluorine and thus, in essence, may result in the absence of a pi-bond. Indeed, the effects of EN was extensively studied in the boron halides, BF_3 and BCl_3 in relation to their behavior as Lewis acids.[5] These studies though were conducted with terminal atoms of elements down the same group; these atoms have substantial differences in their atomic size and may give rise to other effects.[6] It is hoped that this study would add to the extensive studies on boron compounds. [7,8,9]

In this paper the above hypothesis was tested by replacing the terminal atom with elements across a period, i.e. in order to test the effect of EN of terminal atoms on their ability to form pi-bond to the central B atom, fluorine (F) was replaced with the less EN atoms oxygen (O) and nitrogen (N) and these molecules are shown in **Figure 2.** This approach of using elements across the periodic table has the advantage of bypassing any potential atom size effect as the latter changes slowly across a row. Theoretical calculations, DFT with NBO analysis, were performed to determine the bonding nature between O and N respectively to B in these molecules. With the decreasing EN of O and N, it is anticipated that there will be an increasing tendency of electron donation and potential pi-bond formation to boron. Furthermore, since B, N, O and F are in the same period and thus of similar size, it is anticipated that there will be better overlap and more efficient electron donation potentially leading to better bonding.[10] Although the lack of double bond formation in BF_3 can be rationalized in terms of formal charge, EN was chosen as our starting hypothesis because EN has physical origins in the atomic property of nuclear screen and thus effective nuclear charge,[11] a concept that is more amenable to theoretical studies.

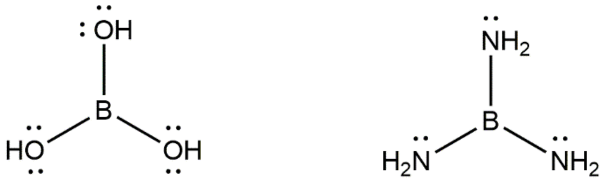

Figure 2. Lewis structures of H_3BO_3 and $B(NH_2)_3$.

METHOD AND PROCEDURES

Geometry optimization – Theoretical calculations were performed using Gaussian 09W.[12] Density functional theory (DFT) with the B3LYP functional using the 6-31+G and 6-311+G (d, p) basis sets as well as Moller Plesset Theory (MP2) using 6-311+G (d, p) basis set were used to optimize the molecular geometry.

Bonding analysis – Natural bonding orbital (NBO) calculations, version 3.1 of this program, were then performed (DFT-B3LYP using the 6-31+G and 6-311+G (d, p) basis sets) on these optimized structures to obtain localized bonding data, i.e. their corresponding Lewis structure. Two different basis-sets were used in all of these calculations and their results were compared to ascertain if there were any basis-set dependent effects which may lead to erroneous results. Both basis-sets contain diffused functions which are essential for molecules with lone electron pairs and vital for anions. The 6-311+G (d, p) basis-set contain polarization functions which allow more flexibility in the atomic orbital in cases where polarization or electron cloud distortions are anticipated.

Interactions between filled NBOs (orbitals with 2 electrons localized on an atom or in a bond between atoms) and empty non-Lewis NBOs (empty orbitals) were also extracted from the NBO calculations. In essence, the extent of pi-bond formation via donation of a lone electron pair of the terminal atoms, F, O, N to B on each of the respective molecules of BF_3, $B(OH)_3$ and $B(NH_2)_3$ was also determined from this interaction data. Delocalization was determined by the partial filling of non-Lewis orbitals and also provided a measure of the degree of departure from the ideal Lewis structure of localized bonds.[13]

Population Analysis – Hirschfeld population analysis for the 3 highest occupied and 3 lowest virtual orbitals were also performed on these molecules using Moller-Plesset (MP2) theory with the 6-311+G (d, p) basis set to obtain the atomic charges on the atoms. Natural Population Analysis (NPA) was also calculated using the same level of theory and basis set for reference purposes.

RESULTS AND DISCUSSION

Molecule→	BF_3		$B(OH)_3$		$B(NH_2)_3$	
Method↓	**B−F (Å)**	**F−B−F ∠ (◦)**	**B−O (Å)**	**O−B−O ∠ (◦)**	**B−N (Å)**	**N−B−N ∠ (◦)**
DFT-B3LYP 6-31+G	1.35158	120	1.38279	120	1.43838	120
DFT-B3LYP 6-311+G(d, p)	1.31766	120	1.36958	120	1.43227	120
MP2 6-311+G(d, p)	1.3825	120	1.37252	120	1.43879	120

Table 1a. Optimized geometry parameters, using DFT and MP2 with the listed basis-set for BF_3, $B(OH)_3$ and $B(NH_2)_3$.

Molecule→	$_2$HB-F		$_2$HB-OH		$_2$HB-NH$_2$	
Method↓	**B−F (Å)**	**H−B−H ∠ (◦)**	**B−O (Å)**	**H−B−H ∠ (◦)**	**B−N (Å)**	**H−B−H ∠ (◦)**
DFT-B3LYP 6-311+G(d, p)	1.32862	120	1.36238	120	1.39124	114

Table 1b. Optimized geometry parameters, using DFT with the listed basis-set for BH_2-F, BH_2-OH and BH_2-NH_2.

Geometry

Geometry optimized bond lengths and angles are presented in **Table 1a** and **1b**. For the series BF_3, $B(OH)_3$, $B(NH_2)_3$ there is little deviation from the trigonal planar structure with 120° bond angles. On the other hand, for the BH_2−F, BH_2−OH and BH_2−NH_2 series, there is a noticeable deviation from the ideal trigonal planar structure for the amino-borane BH_2−NH_2 molecule.

BF_3

Three identical single B−F bonds are obtained from the NBO calculations of this study for BF_3 and this observation and the corresponding bond length are consistent with literature values.[14, 15] The electron occupancy of the three occupied p-orbital localized on each of the F atoms that are parallel, **Figure 3** for the spatial orientation, to the empty p-orbital on B are also listed in this table; depletion of electron population in these p-orbitals is observed when compared to the ideal occupancy value of two electrons. Properties of the empty p-orbital on B are also listed in **Table 2**; delocalization of electron density into this orbital is supported by its' non-zero electron population. The source of this electron density is ascertained from the data in **Table 3**. For BF_3, the major delocalized interactions are between the donor filled p-orbitals on the terminal F atoms and the empty p-orbital on B, listed in **Table 2**. The degree of a donation from each of the terminal F atoms is determined from the occupancy, column 2, of **Table 2** which indicates equal donation from each of the terminal F atoms into B. From this data it is concluded that each F donates roughly 1/10th of an electron to B. The work of See, who proposed a formal trivalent structure for BF_3[14] is well supported by this study and the very limited electron delocalization across the molecular framework giving rise to a very minuscule fractional pi-bond across the p-orbitals are also consistent with the ideas of Straub.[15] The commonly accepted chemical notion that BF_3 does not obey the octet rule is strongly supported by our results.

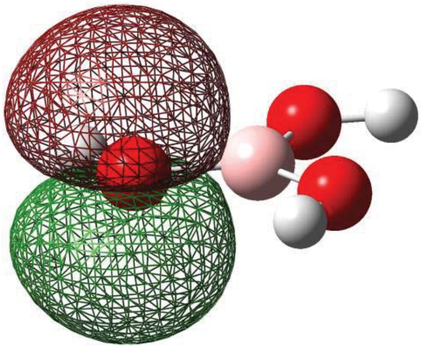

Figure 3. Representative example of the p-orbital on the terminal atom that is parallel to the empty orbital on B. Those described in **Table 1 and 2**.

BF$_3$	Occupancy	Nature of orbital	Atoms involved & % atomic orbital contribution to bond	Hybridization of F
	1.99825 **1.99942**	BD	17.23% Boron and 82.77% Fluorine **18.31% Boron and 81.69% Fluorine**	sp^2 **sp^2**
	1.99825 **1.99942**	BD	17.23% Boron and 82.77% Fluorine **18.31% Boron and 81.69% Fluorine**	sp^2 **sp^2**
	1.99825 **1.99942**	BD	17.23% Boron and 82.77% Fluorine **18.31% Boron and 81.69% Fluorine**	sp^2 **sp^2**
	1.88380 **1.88576**	LP	Fluorine	p
	1.88380 **1.88576**	LP	Fluorine	p
	1.88380 **1.88576**	LP	Fluorine	p
	0.34823 **0.33569**	LP*	Boron	p

B(OH)$_3$	Occupancy	Nature of orbital	Atoms involved & % atomic orbital contribution to bond	Hybridization of O
	1.99583 **1.99627**	BD	20.25% Boron and 79.75% Oxygen **21.44% Boron and 78.56% Oxygen**	sp^2 **sp$^{1.4}$**
	1.99583 **1.99627**	BD	20.25% Boron and 79.75% Oxygen **21.44% Boron and 78.56% Oxygen**	sp^2 **sp$^{1.4}$**
	1.99583 **1.99627**	BD	20.25% Boron and 79.75% Oxygen **21.44% Boron and 78.56% Oxygen**	sp^2 **sp$^{1.4}$**
	1.85823 **1.86137**	LP	Oxygen	p
	1.85823 **1.86138**	LP	Oxygen	p
	1.85823 **1.86137**	LP	Oxygen	p
	0.42410 **0.40383**	LP*	Boron	p

B(NH$_2$)$_3$	Occupancy	Nature of orbital	Atoms involved & % atomic orbital contribution to bond	Hybridization of N
	1.98888 **1.98937**	BD	25.22% Boron and 74.78% Nitrogen **25.93% Boron and 74.07% Nitrogen**	sp^2 **sp$^{1.2}$**
	1.98888 **1.98938**	BD	25.22% Boron and 74.78% Nitrogen **25.93% Boron and 74.07% Nitrogen**	sp^2 **sp$^{1.2}$**
	1.98888 **1.98943**	BD	25.22% Boron and 74.78% Nitrogen **25.93% Boron and 74.07% Nitrogen**	sp^2 **sp$^{1.2}$**
	1.84209 **1.84381**	LP	Nitrogen	p
	1.84209 **1.84384**	LP	Nitrogen	p
	1.84209 **1.84349**	LP	Nitrogen	p
	0.46756 **0.45605**	LP*	Boron	p

Table 2. Localized bonds found in the Lewis structures of BF$_3$, B(OH)$_3$ and B(NH$_2$)$_3$.
Column 1 provides the name of the molecule.
Column 2 gives the occupancy of the orbital.
Column 3 describes the nature of the orbital – BD is bonding, LP is a lone pair, LP* is an empty orbital, *e.g.* a p-orbital.
Column 4 gives the percentage contribution of each atom's atomic orbitals to the bonding orbital (NBO).
Column 5 provides information on the hybridization of the respective atoms involved in the bond. Occupancy of any LP* orbitals reflect a deviation from the ideal Lewis formalism and indicates resonance is present in the molecule.
Entries in **bold** are results using the DFT-B3LYP and 6-311+G (d, p) basis-set while entries in standard font are results from 6-31+G.

Molecule	Donor	Acceptor	S. E	E.N.
BF_3	LP on Fluorine p-orbital	Boron p-orbital	46.88 **44.08**	4.0 (F)
$B(OH)_3$	LP on Oxygen p-orbital	Boron p-orbital	50.34 **50.08**	3.5 (O)
$B(NH_2)_3$	LP on Nitrogen p-orbital	Boron p-orbital	55.13 **52.02**	3.0 (N)

Table 3. Interactions between Lewis orbitals (filled) and non-Lewis (empty) of the respective molecules listed in column 1. It shows the extent of a donation from filled orbitals into empty orbitals and is a measure of the delocalization of electron density. All of the p-orbitals in the table are parallel to the empty p-orbital on B. Note the increasing degree of interaction as one goes from F, O and N.
Column 1 lists the names of the molecules.
Column 2 is the atom containing the filled donor orbital.
Column 3 is the atom containing the empty acceptor orbital.
Column 4 is the Stabilization Energy (S.E) from the donor-acceptor interactions in units of kcal/mol.
Column 5 is the respective electronegativity of each donor.
Entries in **bold** are results using the 6-311+G (d, p) basis-set and entries in standard font are results from 6-31+G.

Molecule	Atomic charge for central Boron atom (Hirschfeld)	Atomic charge for central Boron atom (NPA)
BF_3	0.527606	1.57931
$B(OH)_3$	0.395884	1.37144
$B(NH_2)_3$	0.265733	1.12118

Table 4. Atomic charges were obtained from MP2 calculations with the 6-311+G (d, p) basis set using bot the Hirschfeld and NPA methods.

$B(OH)_3$

Similar to BF_3, formally three single B−O bonds from B to the terminal OH groups are present in $B(OH)_3$. The calculated B−O bond length is comparable top literature value;[11] although the hybridization of O in −OH is expected to be sp^3, there is re-hybridization of these orbitals to generate a p-orbital for overlap with the empty p-orbital on B, column 5 of **Table 2**. These three occupied donor p-orbitals on the O of the terminal −OH groups, parallel to the p-orbital on B, are also listed in **Table 2**. The electron occupancy of these p-orbitals is *more diminished* with a more noticeable increase in the electron occupancy of B for this molecule when compared to BF_3. Even though this electron delocalization has increased, it nonetheless amounts to no more than just 1/7th of an electron donation by each O in $B(OH)_3$ when compared to 1/10th in BF_3; thus, delocalization may have increased with a decrease in EN but is not sufficient to change the established idea that $B(OH)_3$ doesn't obey the octet rule.

$B(NH_2)_3$

Analogous to the above two molecules, formally three single B-N bonds are found in this molecule. The B−N bond length is consistent with literature value.[16] Most notable observation is the *even further diminished* electron occupancy of the p-orbitals on the N of the respective terminal $-NH_2$ groups and the greatest electron occupancy of the empty p-orbital of B in this group of molecules. Once again, the hybridization on the N of $-NH_2$ is expected to be sp^3 but it is seen that there is also substantial re-hybridization to produce a p-orbital for overlap with that on B. These occupied p-orbitals of N are also listed in **Table 1.** This increased delocalization though amounts to no more than roughly just 1/6th of an electron donation from each N's occupied p-orbital into the empty p-orbital of B. Although there is a trend of increasing electron donation from p-orbitals of F, O, and N respectively as a function of decreasing EN, these contributions are insufficient to create a pi-bond in these boron compounds. Thus the octet rule does not apply to the bonding in this molecule.

The trend of increasing electron delocalization as a function of decreasing EN of the terminal atoms is also evident in the trend of atomic charges on B across this series of molecules, see **Table 4.** In order to independently verify the results of the NBO analysis above, atomic charges calculated using Hirschfeld population analysis on the three highest energy filled molecular orbitals and three higher energy virtual orbitals were performed. A trend of decreasing positive atomic charge on B is observed when the terminal atom changes from F to O to N. This observation is consistent with the NBO results of increasing electron density on B for this set of molecules. This trend is also seen in the NPA results which are also included in **Table 4** for reference purposes. Note that in general, different population analysis schemes give different numerical values of atomic charges and cautions should be exercised when comparing absolute values.

An alternative to NBO and Population Analysis in ascertaining the degree of electron donation from the terminal F, O and N to B and thus potential pi-bonding is to study the corresponding relative bond lengths of the BH_2-F, BH_2-OH and BH_2-NH_2 series. The relative bond lengths is defined as the ratio of the length of B−X bond in BX_3 to the length of B−X bond in BH_2X, i.e. (B−X bond in BX_3)/(B−X bond in BH_2X). From the data in **Table 1a and b,** it is observed that there are only small changes in these relative bond lengths across the series except for BH_2-NH_2. Since B and N are neighbors in the periodic table it is expected that they would have better orbital overlap and this observation is consistent with literature results.[9] The calculate BH_2-NH_2 from this study is very close to that of a double bond and warrants further study. A full NBO and Population Analysis on the BH_2-F, BH_2-OH and BH_2-NH_2 series is underway.

Our initial hypothesis that changes in EN may lead to pi-bond formation is incorrect as a change in EN from 4 for F to 3 for O resulted in minuscule change in electron delocalization from the filled p-electrons of the terminal atoms onto the empty p-orbital of B. Undoubtedly there is increased stabilization when the terminal atom changes from F, O and N as seen in the data in **Table 3** but this is not sufficient to create a pi-bond.

$^{-}O-B(OH)_2$

Some insight was gained through this study even though our initial hypothesis proved to be incorrect. The systematic increase in electron delocalization as EN decreased, coupled with the idea that EN is inherently related to the energy of an atom's orbital energy suggested that more efficient electron delocalization may be achieved if the two interacting orbitals have better energy match.[17] Upon inspection of the relative energy levels of the p-orbital on B to those on F, O and N respectively (i.e. orbital energy as a function of nuclear charge), **Figure 4**, a progressively better energy match of F, O and N respectively to that of B[18] is observed.

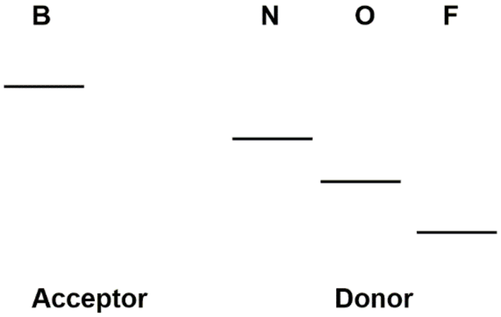

Figure 4. Relative energies of the p-orbitals from B, N, O and F.

Thus, stronger electron delocalization may in principle occur for a chemical species that contained a terminal atom with a donor orbital that is better matched in energy to the acceptor orbital of the central atom.
In order to test this new hypothesis, calculations were performed on the borate ion, $^{-}O-B(OH)_2$, i.e. the anion of $B(OH)_3$. The anion is expected to have a pair of higher energy electrons (i.e. the negative charge residing on the oxygen) compared to the lone pair on a neutral −OH or $-NH_2$ terminal group, and this higher energy pair may thus interact more efficiently with the empty p-orbital of B. Optimized geometric parameters of this anion is given in **Figure 5.** Results from the NBO calculations on the borate ion are given in **Table 5**.

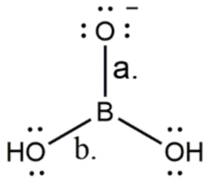

Figure 5. Optimized geometry of the borate ion using DFT-B3LYP 6-311+G (d, p). a = 1.27797 Á and b = 1.46486 Á. The HO−B−O¯ bond angle is 124° and the HO−B−OH bond angle is 112°. At the MP2 6-311+G (d, p) level, the values are: a = 1.28370 Á and b = 1.47068 Á. The HO−B−O¯ bond angle is 125° and the HO−B−OH bond angle is 110°.

$^{-}O-B(OH)_2$	Occupancy	Nature of orbital	Atoms involved & % atomic orbital contribution to bond	Hybridization of Oxygen
	1.91772 1**.92325**	BD	14.45% Boron and 85.55% Oxygen **15.51% Boron and 84.49% Oxygen**	sp **$sp^{1.8}$**
	1.91772 **1.92325**	BD	14.45%Boron and 85.55%Oxygen **15.51% Boron and 84.49% Oxygen**	sp **$sp^{1.8}$**
	1.99283 **1.99385**	BD	22.32% Boron and 77.68% Oxygen **23.41% Boron and 76.59% Oxygen**	sp
	1.99884 **1.99882**	BD	17.83% Boron and 82.17% Oxygen **16.84%Boron and 83.16% Oxygen**	p*

Table 5. Localized bonds found in the Lewis structure of the $^{-}$O-B(OH)$_2$ anion.
*a p-orbital is used on B to form the BD orbital for this entry.
The description of each column is identical to that in **Table 2**.

In this case, four bonds are clearly shown in the NBO analysis. The first two entries in **Table 5** are the single bonds from B to the OH groups while the third and fourth entries are for the sigma single bond between B and O followed by the pi-bond (p-p interaction) between the same two atoms. **Figure 6** provides a visualization of this pi-bond between the terminal O and the central B. Further support for the presence of the pi-bond is seen in the unequal B−O¯ and B−OH bond lengths with the shorter one for the double bond. Previously reported values by Straub are consistent with our results. The magnitude and unequal nature of the HO−B−O¯ and the HO−B−OH bond angles are also consistent and very similar to carbonic acid HO−CO−OH[19] which has is identical structurally to the borate ion.

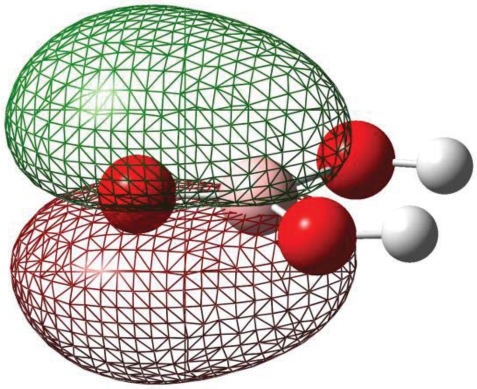

Figure 6. Visualization of the localized pi-bond orbital in the $^{-}$O-B(OH)$_2$ borate anion.

CONCLUSION

This study sought to understand the effects of EN of the terminal atoms on the formation of delocalized pi-bonding to the central B atom in the series BF_3, $B(OH)_3$ and $B(NH_2)_3$. The starting hypothesis that EN played a central role in this delocalization and potential pi-bond formation was shown to be false. Even with fairly large changes in EN, the degree of electron donation from the terminal atoms although increasing was minimal. Despite this, some insight into another factor that influenced pi-bonding in boron compounds was obtained and this insight revealed that improved energy match between the filled donor orbitals of the terminal atoms and the empty p-orbital of boron do lead to pi-bond formation.

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PRESS SUMMARY

Understanding the bonding in the element boron (B) has proven to be a challenge. This paper investigates the effects of electronegativity (EN) on the bonding in B. Different atoms, namely fluorine (F), oxygen (O) and nitrogen (N) respectively are bonded to boron and the nature of the B-F, B-O and B-N bonds are studied theoretical. Since the EN of F, O and N are different, this study may shed light on the effects of changing electronegativity on the bond between B and these other elements.