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Theoretical Analysis of Solid-Phase F-F, Br-O, and Br-Br Interactions

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In order to learn more about the nature of the FF, BrBr, and BrO interactions in crystalline 1-bromo-2,3,5,6-tetrafluoro-nitrobenzene (BFNB), a quantum chemistry analysis was conducted. This system was chosen because it has properties that are similar to those of halogen bonds in crystals and biological systems. The poor electrophilic activity of fluorine atoms may be due to their modest positive electrostatic potentials (VS,max +1 kcal mol-1). Calculations based on atomic and molecular quantum theory place the electron density at the FF critical spots in the range of 0.004-0.006 au, whereas the values of 2BCP are all positive and fall in the range of 0.023-0.031 au. This suggests that the nature of all FF interactions in crystalline BFNB is weak and primarily electrostatic. Energy decomposition analysis (EDA) is used to investigate the character of intermolecular interactions. Our findings suggest that nuclear magnetic resonance characteristics undergo significant modifications while transitioning from the solitary gas phase molecule model to crystalline BFNB, particularly for those nuclei involved in intermolecular interactions. The strength of these alterations at each nucleus is, of course, proportional to the relative importance of its role in the interactions.

Keywords: Hydrogen bonding, DFT, NMR, QTAIM, and electrostatic potential

INTRODUCTION

Substantial contributions are made by non-covalent interactions in a wide variety of chemical processes [1–5], including supramolecular chemistry, molecular recognition, bioligical structure, and crystal packing of molecules. Hydrogen bonding interactions, which often include two electronegative elements with lone electron pairs on one of them, are by far the most prevalent type of covalent contact. Unconventional hydrogen bonding, on the other hand, includes interactions between electrons in the C-H-Y, X-H-C, and X-H-- configurations [6]. R-XB interaction is a universal description of halogen bonds [7,8], where X is an electrophilic halogen atom (usually chlorine, bromine, or iodine) and B is any negative site such as a Lewis base, the area of an aromatic molecule, or an anion. In most cases, the R-XB angle is very near to 180 degrees, indicating that the halogen bond is a very directed interaction. Despite the fact that halogen bonds and hydrogen bonds share many chemical and physical features [9–13], it was fascinating to see that halogen bonding won out in a competitive identification procedure [14]. The existence of an electropositive crown at the top of the halogen atom pointed toward the electron donor explains the stability of the halogen bond [15], even if the halogen atom X and halogen bond electron donor B engaged in a halogen bond may have a net negative charge. The halogen's polarization along the elongation of the covalent link produces a positive potential, or "-hole" [16]. Extensive experimental studies [17–19] and theoretical calculations [20–26] show that the polarizability and electronegativity of a halogen atom determine the positivity of the -hole and the strength of the halogen bond that is formed between the atoms of the same element.

Multiple research teams have only recently presented evidence for weak closed-shell bonding interactions between halogens using

features of form and power [27-30]. The coordination of halogens to carbon has begun to take on certain patterns. It has been proposed [31] to differentiate between halogen-halogen interactions of types I and II (Scheme 1). Closed-shell bonding interaction between chlorine atoms in neighboring molecules is proposed by Tsirelson et al. [32] as a possible explanation for

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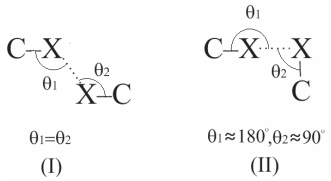
this crystalline form of chlorine. The F atom is often disregarded from XX bonding because of its high electronegativity and low polarizability. F is most likely to function as a halogen bond acceptor because the electron density distribution around it is almost spherical rather than anisotropic. Recent research [33–35] has demonstrated, however, that under certain conditions the fluorine atom is capable of forming non-covalent XX bonds and can also influence recognition and self-assembly processes. In an electron density analysis of crystalline pentafluorobenzoic acid at 110 K employing multipolar refinement, Bach and coworkers [36] have revealed weak intermolecular FF interactions. The FF bonding is revealed to exhibit all the features of a closed-shell weak interaction, according to the analysis of bond route connecting to saturated fluorine atoms performed by Matta et al. [37]. Calculated electron densities at the FF bond critical point were found to correlate with the through-space fluorine-fluorine spin-spin coupling constant, JFF, in six fluorinated organic compounds by Alkorta and Elguero [38].

The purpose of this research is to use QCA and QTAIM [39] to investigate the nature of the FF, BrBr, and BrO interactions in solid 1-bromo-2,3,5,6- tetrafluoro-4-nitrobenzene (BFNB), as shown in Fig. 1. Furthermore, the influence of these intermolecular interactions on the calculated BFNB 19F and 79Br NMR parameters is investigated. The halogen-halogen and halogen-bond interactions observed in crystal structures and biological molecules inspired the choice of this system. Theoretical research into the nature and strength of halogen-halogen and halogen bond interactions will greatly benefit the development of novel materials and potent pharmaceuticals incorporating halogenated compounds.



Scheme 1. Classification of halogen-halogen bonds

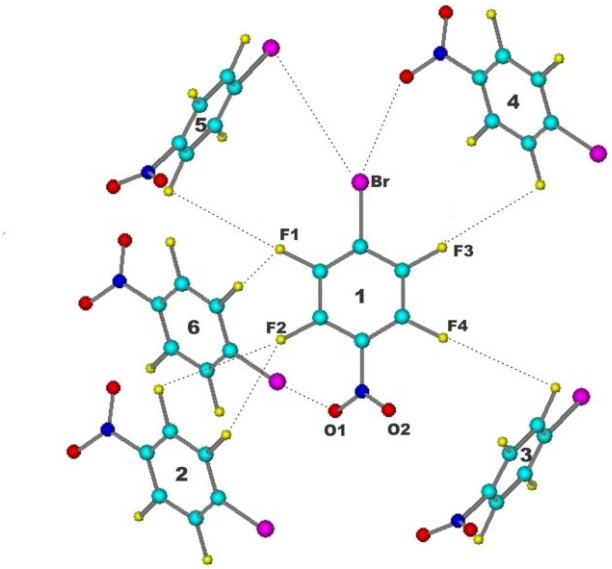


Fig. 1. Crystalline structure of BFNB. The dashed linesindicate intermolecular halogen bonds.

compounds.

Computational Details

The GAMESS software package [40] was used for all the computations. The standard basis set of 6-311++G** was used for the density functional theory (DFT) computations, together with the density functionals B3LYP [41] and M06-2X [42]. Since B3LYP is the most popular option, it was chosen, and M06-2X was included since it performs very well for halogen bonding interactions [43]. At the same theoretical level, the electrostatic potential of the BFNB molecule was calculated with M06-2X/6-311++G** optimized geometry. An experimental X-ray crystal structure for BFNB [44] was utilized to build the model cluster for this investigation. Both the M062X and MP2/6- 311++G** levels of theory were used to calculate the interaction energies between BFNB monomers. Interaction energies were adjusted using the basis set superposition error (BSSE) obtained using the counterpoise approach [45]. Interaction energies were deconstructed using [46] to learn more about the

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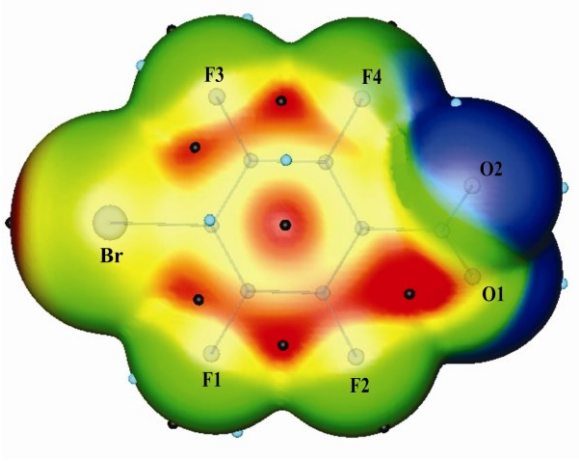
properties of intermolecular interactions.

$$E_{\text{int}} = E_{elst} + E_{exch-rep} + E_{pol} + E_{disp}$$



describes the repulsive exchange-repulsion component deriving from the Pauli exclusion principle, and Eexchrep is the electrostatic term representing the classical Coulumb interaction of the occupied orbitals of one monomer with those of another monomer.

represent polarization and dispersion terms in a mathematical expression.
At the B3LYP and M06-2X/6-311++G** theory levels, the gauge- included atomic orbital (GIAO) technique has been used to derive the absolute chemical shielding tensors at the locations of 19F and 79Br nuclei [47]. Bond critical points (BCPs) were located and characterized using the QTAIM [39] in terms of electron density, BCP, its Laplacian, 2BCP, and energy density. The AIM2000 software program [48] was used for all electron density investigations.

RESULTS AND DISCUSSION

Geometries

The electrostatic VS(r) map for the surface of the isolated BFNB molecule, as shown in Figure 2, has been assessed. The WFA code [49] locates the maximum (VS,max) and minimum (VS,min) potentials, which are depicted in the image. The oxygen atoms have the lowest electrostatic potential on the BFNB surface (VS,min = -28.5 (O1) and -27.0 (O2) kcal mol-1), respectively). These occur on the NO2 plane and can be explained by the fact that the electrical densities of the unshared electron pairs in oxygen superimpose on one another. Towards the end of the Br atom along the C-Br bond vector, there is a cap of positive electrostatic potential (VS,max = +43.1 kcal mol-1), which is surrounded by an electroneutral zone and then a huge domain of electronegative potential. This is the most noticeable characteristic of Fig. 2. Since these halogen-positive regions are symmetrical along the C-X axis and surrounded by regions with a negative electrostatic potential, we call them "-holes." When this positive area comes into contact with an electronegative atom or group, a Fig. 2 can form. The electron density of BFNB molecules was mapped electrostatically (0.001 e au-3) on the surface. The energy levels (kcal mol-1) for each color are as follows: red > 26.1, yellow 7.9-26.1, green -10.0-7.9, and blue -10.0. The highest and lowest points on the surface are shown by the black and blue circles, respectively.

strongly directed communication. The weak electrophilic behavior of fluorines is further explained by the fact that they have weak positive -holes (VS,max +1 kcal mol-1). Formation of additional fluorine-centered halogen-bonded compounds has also been attributed to this mechanism [50].
Positive -holes in halogens are confined to the halogen-covalent bond extensions, as was previously illustrated. This clarifies the bonding directionality that is characteristic of halogens. Fig. 1 shows a schematic representation of the crystalline BFNB under study. FF interactions, like BrO and BrBr interactions, can be categorized as either type I or type II. Intermolecular

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distances between FF pairs are 2.86 to 3.01 angstroms. Most of them are less than or close to the total of the vdW radii of the constituent atoms (2.94) [51], which is consistent with these interactions being weak noncovalent forces. To further illustrate this notion, consider the BrBr contact, which occurs between the positive -hole of one bromine and the negative lateral side of another. Examination of the data indicates that the BrBr interactions do not significantly contribute to the stability of the crystal packing since the internuclear distances are somewhat larger than the vdW radius sum of the two bromine atoms (3.70) [51]. As can be seen in Fig. 1, the three-dimensional molecular network of BFNB is formed due to the existence of short BrO connections in the crystal structure of BFNB. When compared to the total of the van der Waals radii (3.37), the distance between BrO (3.15) is much less.

It has been questioned whether or not the fluorine short connections found in solid BFNB are the product of FF contacts or some other noncovalent interaction. Politzer and coworkers [52] have examined the characteristics of fluorine-centered halogen bonding in both the gaseous and crystalline states. The authors used statistical analyses of data from the Cambridge Structural Database (CSD) to show that the ability of fluorine to act as a halogen bond donor in solids is most likely to manifest itself when no stronger competing interactions determine the crystal packing. However, systems in which fluorine is located near highly electron withdrawing groups may benefit from a positive -hole and the consequent halogen bond. Only 34 (2.05%) of the compounds found in a recent search on the CSD by Barceló-Oliver et al. [33] demonstrate FF connections of type II, despite the fact that 1658 compounds are found with FF distances up to 3.0. Thus, type I interactions may be used to describe the vast majority of FF interactions in the crystalline phase. This finding runs counter to the idea [35] that only type II connections are stabilizing and that type I contacts are created only by tight packing.

QTAIM Analysis

Non-covalent interactions of varying intensities have been effectively characterized in a wide range of molecular systems using the QTAIM [53–57]. BCP characteristics are used by QTAIM to classify the kind of contact between two atoms as either covalent (or "open-shell") or closed-shell (such as ionic, van der Waals, or HBs). BCP, the value of at a BCP, provides a rough estimate of binding strength [39]. While the closed-shell and covalent types of bonds are easily distinguished,

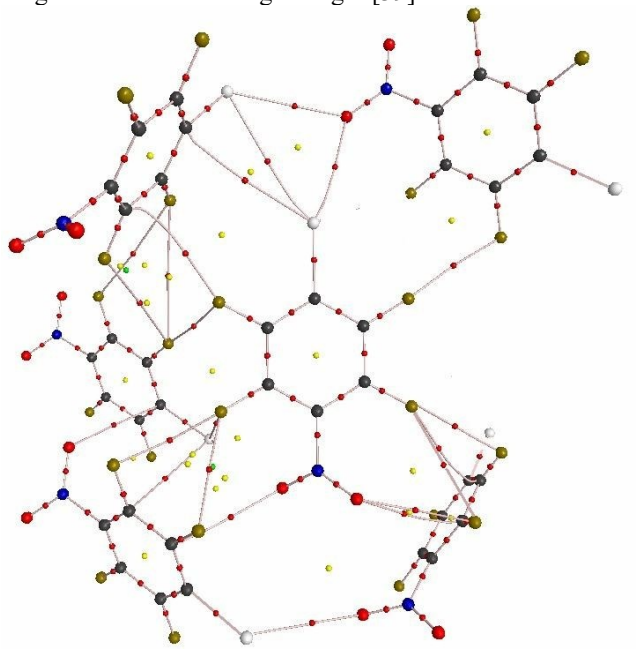

Fig. 3. Molecular graph of crystalline BFNB, *solid lines* indicate bond paths and *large circles* correspond to attractors, *small red* ones to BCPs.

There can be no contact until the local electronic energy density, HBCP, is established. In their study, Rozas et al. [58] found that the Laplacian of the electron density at the BCP (2BCP) may be used to categorize the nature of the interaction. This indicates that the covalent character is established for contacts of high strength (2BCP 0 and HBCP 0), partly covalent character is defined for interactions of medium strength (2BCP > 0 and HBCP 0), and weak interactions (2BCP > 0 and HBCP > 0) are mostly electrostatic. Therefore, the "degree of covalency" existing in an encounter may be inferred from the size of HBCP.

In Figure 3, we can see that there is a BCP and a bond route between every pair of atoms involved in an FF, BrBr, or BrO contact. All of the estimated values for 2BCP are positive, ranging from 0.023 to 0.034 au, whereas the values for BCP are

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in the 0.004 to 0.009 au range. This suggests that the two atomic basins are not particularly similar and that there will be only a little amount of delocalization between the basins of the two corresponding atoms. It was discovered, however, that the BCP value is

BrO's bond strength is somewhat greater than that of BrBr and FF. This lends credence to the theory that the anisotropy of the electron charge distribution of the X atom (in its role as a Lewis acid) and the magnitudes of the VS,min of B (in its role as a Lewis base) are linked to the strength of the halogen bond. Similar electron densities have been observed for other critical sites, such as H-F-F-F [59], C-F-C-C in difluorinated aromatics [37], and H3C-H-F-CH3 [60]. At the FF critical point, the electron density appears to be proportional to the distance between molecules (Fig. 4a). Our computational investigation of solid BFNB concludes that the connections present may be described as weak yet stabilizing interactions.

Somewhat covalent interactions have been linked to positive values for 2BCP and negative values for HBCP, as demonstrated by previous research [58]. Absolute ratio of kinetic energy density to potential energy density, -GBCP/VBCP, is another method for determining the character of contact. If the ratio of -GBCP to VBCP is more than 1, then the interaction is noncovalent. However, if the ratio of GBCP to VBCP is less than 1, then the connection is only partially covalent. Table 1 shows that all FF, BrBr, and BrO interactions are weak and primarily electrostatic in nature due to the tiny values of BCP, the positive values of the 2BCP, - GBCP/VBCP > 1, and the virtually negative values of HBCP. Particularly, it can be shown that the HBCP values obtained for the FF interactions are around 0.010 au, which is somewhat less than that for the BrO BCP. This demonstrates that the FF bond is mostly electrostatic, providing more evidence for the importance of this sort of interaction in halogen bonds. Table 1 further shows that the kinetic energy is larger than the potential energy density at the BCP, as indicated by the computed -GBCP/VBCP values, for all the FF, BrBr, and BrO interactions investigated here. The relationships between the F-F distance and the HBCP, VBCP, and GBCP energetic topological parameters are shown in Figure 4b. It is clear that the changes in these parameters are monotonic; as the FF distance reduces, the GBCP rises, the VBCP falls, and the HBCP hardly shifts at all. In addition, our numbers accord well with those found in the literature for weak FF interactions [37].

Interaction Energies and Energy DecompositionAnalysis (EDA)

The solid-phase stabilizing energy between BFNB monomer dimeric fragments is investigated here. The five BFNB dimers' interaction energies computed with the all-electron MP2 and M06- 2X techniques in the 6-311++G(d,p) basis set are listed in Table 2 below. Examining the interaction energies reveals some intriguing details. No.1No.4 is the most stable BFNB dimer because it contains one C-BrO contact of length 3.15 and one FF interaction of length 3.01. At the MP2/6-311++G(d,p) level, the interaction energy for this dimer is measured to be -5.85 kcal mol-1. The M06-2X produces results that are quite close to those of the M06, while the interaction energy is a little higher. The stabilization energies calculated using MP2 for additi onal BrO interactions are consistent with these findings [8]. In dimer No. 1No. 2, the stabilization energy acquired for each FF contact is around -1.8 kcal mol-1. As with earlier theoretical investigations in the literature [33,35], the contribution of each FF contact to the overall interaction energy of the other dimers is notable. For the dimer 13, where just one FF contact is established, the calculated interaction energies are -1.07 kcal mol-1 at the MP2 level and -2.24 kcal mol-1 at the M06-2X/6-311++G** level of theory. However, as compared to the stability caused by BrO and FF bonds, that generated by BrBr creation is essentially negligible. This is because the total of the vdW radii is somewhat smaller than the long BrBr distanc es. The average interaction energy for BrBr is -2.49 kcal mol-1 [61], according to a study of solid 2,6-dibromo-4-nitroaniline.

We next ran EDA calculations to break down the interaction energies into relevant physical components including electrostatic, polarization, dispersion, and exchange-repulsion energies [40] to learn more about the nature of the interactions. Decomposing the interaction energy was done using Eq.

In-depth computational (1) explanation. Table 2 displays the outcomes of our investigation on dimers. The electrostatic, polarization, and dispersion factors all contribute to stability, as shown in the table. The exchange-repulsion energy surpasses the electrostatic energy in absolute value for all investigated dimers.

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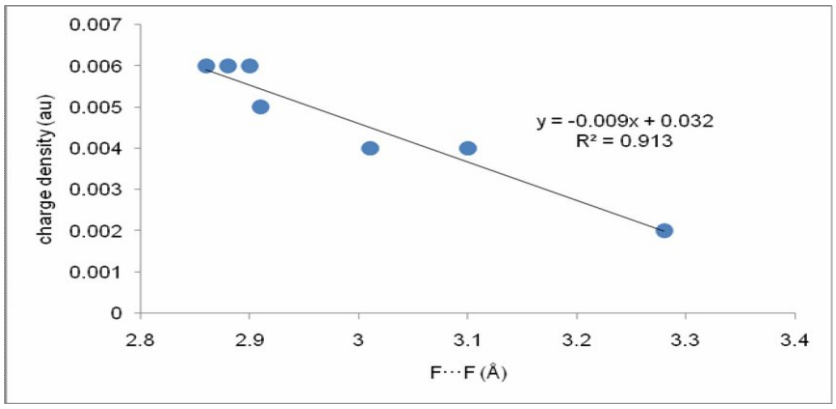
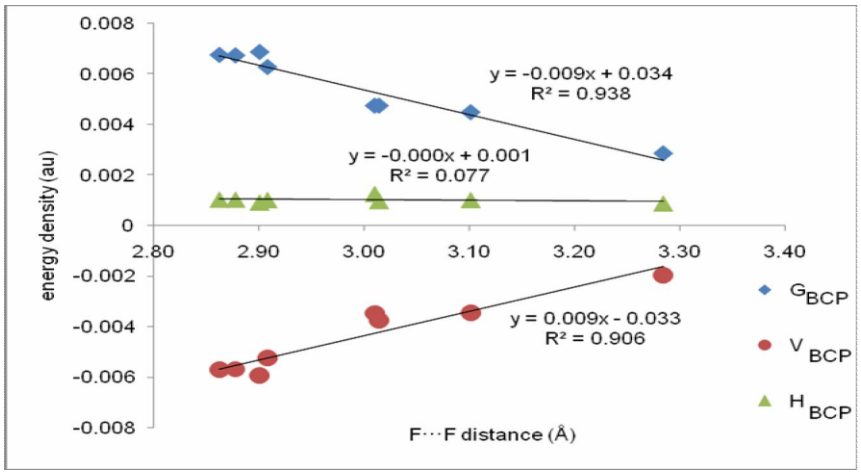


(a)



(b)

Fig. 4. Correlation between F···F distances and (a) electron density, (b) different energy density terms at the corresponding BCPs.

Table 1. Intermolecular Distances r, Angles θ, and Calculated (M06-2X/6-311++G**) Electron Density ρ_{BCP}, its Laplacian $\nabla^2\rho_{BCP}$, Total Electronic Density H_{BCP} and the Absolute Ratio of G_{BCP} and V_{BCP} for Crystalline BFNB

Interaction	r(Å)	θ(°)	ρ_{BCP} (au)	$\nabla^2\rho_{BCP}$ (au)	H_{BCP} (au)	$-G_{BCP}/V_{BCP}$
CF1(1)···F2(5)	2.91	169.50	0.005	0.029	0.0010	1.19
CF1(1)···F2(6)	3.01	174.02	0.004	0.024	0.0010	1.25
CF2(1)···F3(2)	2.90	127.88	0.006	0.031	0.0009	1.15
CF2(1)···F4(2)	2.86	176.05	0.006	0.031	0.0010	1.18
CF3(1)···F3(4)	3.01	174.04	0.004	0.023	0.0010	1.26
CF4(1)···F3(3)	2.88	168.68	0.006	0.031	0.0010	1.18
CBr(1)···Br(4)	3.88	147.61	0.005	0.016	0.0009	1.42
CBr(1)···O2(5)	3.15	155.89	0.009	0.033	0.0012	1.20
O2(1)···Br(6)C	3.15	155.89	0.009	0.034	0.0012	1.20

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Table 2. Calculated Interaction Energies and EDA Results for Different BFNB Dimers[a]

dimer	$E_{int}^{M\ 06-2X}$	E_{int}^{MP2}	E_{elst}	$E_{exch-rep}$	E_{pol}	E_{disp}
No. 1-No.2	-4.22	-3.60	-2.71	2.94	-1.95	-1.88
No. 1-No.3	-2.24	-1.97	-1.78	2.24	-1.28	-1.15
No. 1-No.4	-6.55	-5.85	-2.13	3.16	-2.61	-4.27
No. 1-No.5	-4.81	-4.31	-1.90	2.63	-1.93	-3.11
No. 1-No.6	-6.69	-5.58	-2.04	3.05	-2.48	-4.11

[a]All energies and energy terms in kcal mol^{-1}.

Table 3. Calculated NMR Parameters for ^{19}F and ^{79}Br Nuclei of Crystalline BFNB[a,b]

Nuclei	M062X		B3LYP	
	σ_{iso}	$\Delta\sigma$	σ_{iso}	$\Delta\sigma$
F1	298 (306)	131 (159)	298 (301)	125 (143)
F2	310 (324)	185 (194)	310 (318)	181 (165)
F3	303 (306)	138 (159)	302 (301)	132 (143)
F4	318 (324)	179 (194)	317 (318)	171 (165)
Br	2016 (2118)	866 (881)	2032 (2052)	859 (985)

[a]The numbers within the parenthesis are referred to the isolated gas phase monomer. [b]The values out of parenthesis are referred to the crystalline phase.

Stabilizing interactions are produced by high levels of attractive polarization and dispersion energy. It is observed that the electrostatic and polarization components of the interaction energy are the most stabilizing for the vast majority of the FF. The dispersion energy accounts for 47% of the total stabilization energy in the No.1-No.4 dimer. The electrostatic attraction between FF bound dimers accounts for around 42% of the total attraction, as shown by EDA. The polarization aspect of this interaction, on the other hand,

BFNB possesses 19F and 79Br nuclei in its gaseous and crystalline states, respectively. Some intriguing tendencies may be easily derived from the estimated data. NMR parameters show significant changes when moving from the model of an isolated molecule to that of a target molecule in a cluster, for those nuclei that engaged in the intermolecular interactions. The strength of these alterations at each nucleus is, of course, proportional to the relative importance of its role in the interactions. However, when comparing and contrasting

while dispersion provides 30% to the stability of these and for various nuclei of the BFNB in gas-phase, comprises 28% of the total attractive forces

structures. In conclusion, electrostatic forces play a crucial role in FF interactions. Dispersion and polarization effects, rather than electrostatic forces, are thought to be primarily responsible for the expected stabilities of the BrBr and BrO halogen bonds.

NMR Parameters

Parameters for the degree of shielding (iso) and anisotropy () at the sites of

intermolecular actions, which are mostly deshielding, are credited with the crystalline lattice [62]. When comparing the iso and values derived for crystalline BFNB using the 6-311++G** basis set using the M06-2X and B3LYP techniques, it is clear that they are quite close to one other.

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Four separate fluorine sites may be seen in the crystal structure of BFNB [44] as shown in Figure 1. All of the iso(19F) values for the monomer BFNB are between 306 and 324 ppm (using the M06-2X technique), as shown in Table 3, while the values for the dimer BFNB are between 325 and 332 ppm.

The F2 and F4 atoms are more protected than the others. Fluorine sites in the monomer BFNB have been shown to have distinct iso and values, suggesting that these discrepancies must result from environmental factors. The results show that the predicted NMR parameters at the fluorine sites are affected by intermolecular FF interactions, but that this effect is not uniform across the four F nuclei. Table 3 shows that the iso(19F) of F2 varies by 14 ppm depending on whether the BFNB molecule is in the gas phase or the crystal lattice, as determined using M06-2X/6-311++G** calculations. However, when moving from a single monomer to the target molecule in a cluster, the relevant value reduces by around 9 ppm. These dramatic shifts highlight the role of the FF contacts in bolstering the crystalline BFNB's weak intermolecular connections. It has been determined that the iso parameter for the F2 atom in crystalline BFNB is 310 ppm. When the whole cluster is considered, a value is obtained that is thought to be similar to that of fluorinated benzene derivatives [63]. In contrast, the intermolecular interactions are reflected less strongly in the 19F NMR parameters for the remaining F atoms. The two distinct FF interactions in crystalline BFNB are shown to be influenced by F1 in Figure 1. Weak FF interactions cause an 8 ppm drop in iso(F1) when going from a monomer to a cluster target molecule. From the monomer to the cluster, the value similarly lowers by 28 ppm. This is because the solid-phase intermolecular interactions of BFNB engage this nucleus only to a minor extent.

As mentioned above, the CBr(1) also contains the target molecule's Br atom.crystalline BFNB has Br(4) and CBr(1)O2(5) intermolecular halogen bonding interactions. When comparing the isolated model to the hexamer cluster, there are inconsistencies in the NMR characteristics at this position, more so than what is seen for 19F nuclei. From the monomer to the clustered target molecule, iso at the Br atom's location decreases by 98 ppm, as calculated by the M06-2X/6-311++G** method. Additionally, the value of at this location is reduced from 881 ppm (in monomer) to 866 ppm (in cluster).

CONCLUDING REMARKS

Here, we detail the results of a comprehensive computational investigation of the intermolecular interactions in crystalline BFNB, conducted with the use of quantum chemical simulations. Crystalline BFNB has FF distances in the range of 2.86 to 3.01. Consistent with their having weak interactions, the majority of them are smaller than or close to sums of the vdW radii of the various atoms. The computed values of BCP fall between 0.004 and.009 au, while the values of 2BCP are all positive and lie between 0.023 and 0.034 au. This suggests that the two atomic basins are not particularly similar and that there will be only a little amount of delocalization between the basins of the two corresponding atoms. The electron density and kinetic energy density at the associated BCPs show a reasonable connection with the FF distances. The EDA findings highlight the extraordinary reliance of the FF interactions on electrostatic forces. Dispersion and polarization effects, rather than electrostatic forces, are thought to be primarily responsible for the expected stabilities of the BrBr and BrO halogen bonds. Calculations using nuclear magnetic resonance (NMR) data show that the chemical shielding parameters at the 19F and 79Br sites are affected by the FF, BrBr, and BrO intermolecular interactions. This proves that the 19F and 79Br NMR parameters are good parameters to use when describing the nature of these interactions in crystalline BFNB.

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