Research Article

ROLE OF HALOGEN F---H BONDS IN POTASSIUM TRIFLUOROBORATE SALTS

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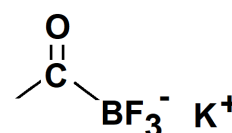| A R T I C L E I N F O	A B S T R A C T
	In this work, the role of halogen F---H bonds in potassium 3-furoyl-trifluoroborate (FTFB), 2-isonicotinoyl-trifluoroborate (ITFB), 5-hydroxypentanoyl-trifluoroborate (HTFB), 5-Br-2-isonicotinoyl-trifluoroborate (Br-ITFB), 6-chloro-2-isonicotinoyl-trifluoroborate (Cl-ITFB), 4-fluorobenzoyl-trifluoroborate (FBTFB) and 2-phenylacetyl-trifluoroborate (PTFB) salts have been studied in gas phase and in aqueous solution by using NBO and AIM calculations with the hybrid B3LYP/6-311++G** method and the SCRF and SM models. In addition, the corrected solvation energy by using ZPVE and non electrostatic terms, volumes and gap values were evaluated as function of molecular weights of salts by using the same level of theory. The AIM calculations show that the IFTB salt present the lower F---H distances in the two media. Evidently, the presence of a pyridine ring linked to C of C=O groups in IFTB favors the formation of halogen interaction, as compared with furyl and phenyl rings. NBO studies show that the higher delocalizations energies of halogen F---H interactions are observed in the Br-ITFB salt in both media together with the ITFB and Cl-ITFB salts. This study evidence clearly that the halogen F---H interaction play a important role in the reactivity and properties of trifluoroborate salts showing that the FTFB salt has lower volume, low corrected solvation energy and is the less reactive while the most reactive Br-ITFB, Cl-ITFB and IFTB salts present high stabilization energies of halogen F---H interactions and high corrected solvation energies. The analyses of the geometrical C-C, C-B, C=O, C-C-B, C-C-O and O-C-B parameters commons at all salts have showed notable influence on the halogen F---H interactions and on the properties of trifluoroborate salts

INTRODUCTION

The trifluoroborate (-BF$_3$) group confers attractive properties to the potassium salts for which the B, K and F atoms present in these species play a very important role in their behaviours in different media because forming 3D arrangement with different coordinations and revealing crystal packing in the solid state of importance in the supramolecular chemistry and in the design of new materials, as reported by different previous studies [1-8]. Hence, these potassium trifluoroborate salts are of great use as reagents in organic synthesis chemistry [9-15]. Thus, the theoretical studies on these salts by using the hybrid B3LYP/6-311++G** level of theory are of great aid to investigate how the different groups linked to trifluoroborate have influence on their reactivities and structural, electronic, topological and vibrational properties [4-8]. In this work, we have particularly investigated the influence of halogen F---H bonds on the properties of seven different potassium trifluoroborate salts which are:

potassium 3-furoyl-trifluoroborate (FTFB), 2-isonicotinoyl-trifluoroborate (ITFB), 5-hydroxypentanoyl-trifluoroborate (HTFB), 5-Br-2-isonicotinoyl-trifluoroborate (Br-ITFB), 6-chloro-2-isonicotinoyl-trifluoroborate (Cl-ITFB), 4-fluorobenzoyl-trifluoroborate (FBTFB) and 2-phenylacetyl-trifluoroborate (PTFB) salts [4-12]. The properties of first four salts were already theoretical and experimentally studied [4-8] while the other three are being investigated from the experimental and theoretical points of view and, for this reasons, their first results are here presented. All those salts present a common group which can be seen in **Scheme 1**. In general, in these salts one of three F atoms located in plane form a halogen F---H bond with a H atom of group linked to C=O group. Thus, the nature and characteristics of these halogen bonds can be theoretically studied by using NBO and AIM calculations with the B3LYP/6-311++G** method [16,17].

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Scheme 1 Common group at all potassium trifluoroborate salts.

Hence, the purposes of this work are: (i) to model and optimize all the structures of those seven salts in gas phase and in aqueous solution [18-20], (ii) to investigate the stabilization energies and their topological properties by using the NBO and AIM2000 programs [21-23], (iii) to compute the gap values by using the frontier orbitals and with these results to predict the behaviours of these salts [24-29], (iv) to predict the corrected solvation energies and, finally, (v) to find correlations and tendencies among the studied properties for the halogen F---H bonds with molecular properties of salts, such as their molecular weights, volumes, F---H distances, solvation energies and reactivities values.

Computational Details

The properties of four potassium 3-furoyl-trifluoroborate (FTFB), 2-isonicotinoyl-trifluoroborate (ITFB), 5-hydroxypentanoyl-trifluoroborate (HTFB), 5-Br-2-isonicotinoyl-trifluoroborate (Br-ITFB) salts were previously published [4-8] and their structures can be seen in Figure 1 while the structures of other three 6-chloro-2-isonicotinoyl-trifluoroborate (Cl-ITFB), 4-fluorobenzoyl-trifluoroborate (FBTFB) and 2-phenylacetyl-trifluoroborate (PTFB) salts were modelled with the *Gauss View* program [30] and later optimized in gas phase and in aqueous solution with the Revision A.02 of Gaussian 09 program, [31] by using the hybrid B3LYP/6-311++G** method [17,18]. Figure 2 shows the structures of Cl-ITFB, FBTFB and PTFB salts. In solution, all the calculations were performed with the integral equation formalism variant polarised continuum method (IEFPCM) and the solvation models [18-20].
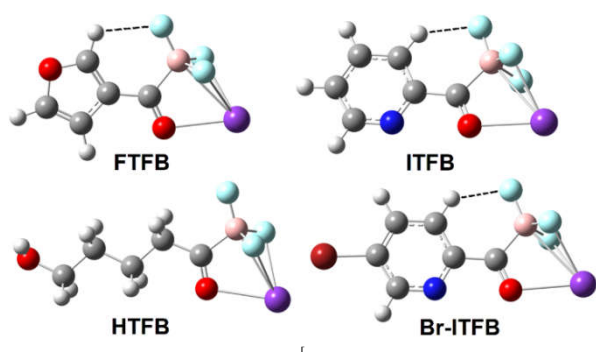

Figure 1 Molecular structures of the potassium 3-furoyl-trifluoroborate (FTFB), 2-isonicotinoyl-trifluoroborate (ITFB), 5-hydroxypentanoyl-trifluoroborate (HTFB) and 5-Br-2-isonicotinoyl-trifluoroborate (Br-ITFB) salts.

The donor-acceptor energy interactions and the topological properties were calculated with NBO and AIM calculations [21-23] at the same level of theory. The reactivities were predicted with the gap values calculated from their frontier orbitals by using the hybrid B3LYP/6-311++G** method [24-29].
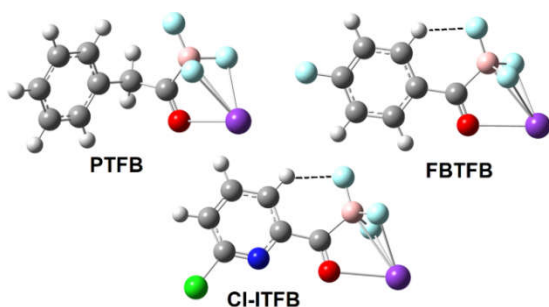

Figure 2 Molecular structure of potassium 6-chloro-2-isonicotinoyl-trifluoroborate (Cl-ITFB), 4-fluorobenzoyl-trifluoroborate (FBTFB) and 2-phenylacetyl-trifluoroborate (PTFB) salts.

RESULTS AND DISCUSSION

NBO and AIM studies of Halogen F---H Bonds in gas and in Aqueous Solution Phases

Different interaction's types are present in all trifluoroborate salts due to the presence of B, K and F atoms and, in particular in this case the halogen F---H interactions were studied and, for these reasons, NBO and AIM calculations were performed for FTFB, ITFB, HTFB, Br-ITFB, Cl-ITFB, FBTFB and PTFB salts in gas and aqueous solution phases by using B3LYP/6-311++G** calculations. [21-23]. First, according to the Bader's theory the topological properties were evaluated in the bond critical points (BCPs) with the AIM2000 program [22,23]. Hence, the calculated electron density, $\rho(r)$ and the Laplacian values, $\nabla^2\rho(r)$ for all salts in both media are presented in **Table 1**. Obviously, the halogen F---H interactions present $\lambda1/\lambda3 < 1$ and $\nabla^2\rho(r) > 0$ and these interactions only were observed for the FTFB, ITFB, Br-ITFB, Cl-ITFB, FBTFB and PTFB salts in both media but for the latter salt that interaction was not observed in aqueous solution. In this work the eigenvalues *(λ1, λ2, λ3)* of the Hessian matrix were not presented because the values can be observed in the previous papers reported [4-8]. Thus, **Table 1** summarize the analyses in the BCPs of $\rho(r)$, $\nabla^2\rho(r)$ and the distances corresponding to the F---H bonds of the FTFB, ITFB, Br-ITFB, Cl-ITFB, FBTFB and PTFB salts in gas and aqueous solution phases by using B3LYP/6-311++G** calculations. Note that HTFB do not present halogen F---H interactions in both media while in PTFB shows interaction in gas phase but not in solution.

Table 1. Analysis of the Bond Critical Points (BCPs) and distances corresponding to the F---H bonds of potassium 3-furoyl-trifluoroborate (FTFB), 2-isonicotinoyl-trifluoroborate (ITFB), 5-hydroxypentanoyl-trifluoroborate (HTFB), 5-Br-2-isonicotinoyl-trifluoroborate (Br-ITFB), 6-chloro-2-isonicotinoyl-trifluoroborate (Cl-ITFB), 4-fluorobenzoyl-trifluoroborate (FBTFB) and 2-phenylacetyl-trifluoroborate (PTFB) salts in gas and aqueous solution phases by using B3LYP/6-311++G** calculations.

Halogen F---H Bonds							
B3LYP/6-311++G** method							
Gas Phase							
Parameter (a.u.)	FTFB[b]	ITFB[c]	Br-ITFB[d]	Cl-ITFB[a]	PTFB[a]	FBTFB[a]	HTFB[e]
$\rho(r)$	0.0117	0.0170	0.0167	0.0169	0.0069	0.0166	0
$\nabla^2\rho(r)$	0.0477	0.0672	0.0670	0.0661	0.0260	0.0649	0
Distances (Å)	2.348	2.125	2.132	2.132	2.578	2.142	2.830
Aqueous Solution							
Parameter (a.u.)	FTFB	ITFB	Br-ITFB	Cl-ITFB	PTFB	FBTFB	HTFB
$\rho(r)$	0.0122	0.0166	0.0153	0.0160	0	0.0161	0
$\nabla^2\rho(r)$	0.0549	0.0640	0.0604	0.0622	0	0.0622	0
Distances (Å)	2.390	2.148	2.202	2.162	3.172	2.160	2.837

[a]This work, [b]From Ref [4], [c]From Ref [5], [d]From Ref [7,8], [e]From Ref [6]

The presence of CH$_2$ groups between the BF$_3$K groups and the H atoms in both salts justify clearly the absence of halogen bonds in the two salts, as shown in Figures 1 and 2. The behaviors of halogen interactions for all salts in both media can be easily seen in Figure 3 together with the distances involved in those halogen bonds. Evaluating first the distances

involved in the halogen bonds, we observed that in HTFB due to the CH$_2$ group the F---H distances in this salt is higher than the other ones, especially in solution due to solvent, justifying strongly the absence of halogen F---H bonds in this salt in both media. However, in PTFB the highest F---H distance of 3.172 Å in solution explain the absence of halogen interaction in this medium. Here, IFTB in both media present the lower distances in the two media. Evidently, the presence of a pyridine ring linked to C of C=O groups in that salt favours the formation of halogen interaction, as compared with furyl and phenyl rings (FTFB, Br-ITFB, Cl-ITFB, FBTFB and PTFB). Comparing the Br-ITFB and Cl-ITFB, it is observed that the Br salt present higher distance than the Cl salt, then, lower density values are expected for the Br salt, as compared with the Cl salt. Here, the higher size of Br atom and the higher electronegativity of Cl atom justify the differences observed between both salts in both media. If now the densities are analyzed from Table 1 and Figure 3 for all salts in both media, obviously, for HTFB in both media and for PTFB in solution are not observed values of densities but the higher densities values for the low F---H distances are expected. Here, due to the reasons explained before, the Cl-ITFB salt present higher densities than the Br salt.
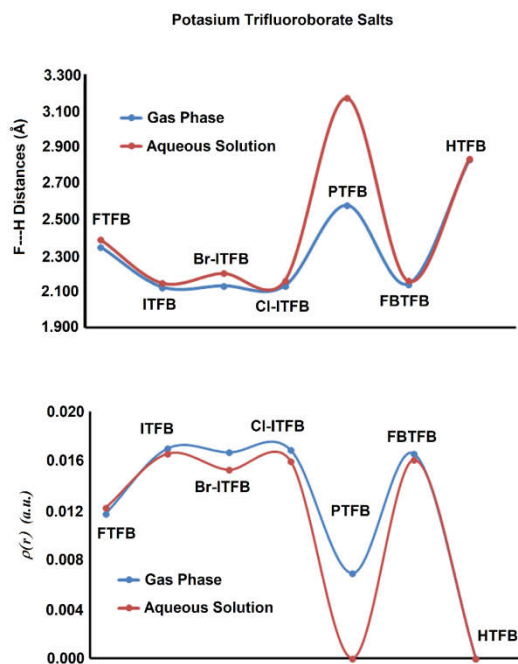
delocalizations of all salts are strongly dependent on the medium because in solution the values decrease, as compared with the values in gas phase.

Table 2 Main delocalization energies (in kJ/mol) for the potassium 3-furoyl-trifluoroborate (FTFB), 2-isonicotinoyl-trifluoroborate (ITFB), 5-hydroxypentanoyl-trifluoroborate (HTFB), 5-Br-2-isonicotinoyl-trifluoroborate (Br-ITFB), 6-chloro-2-isonicotinoyl-trifluoroborate (Cl-ITFB), 4-fluorobenzoyl-trifluoroborate (FBTFB) and 2-phenylacetyl-trifluoroborate (PTFB) salts in gas and aqueous solution phases by using B3LYP/6-311++G** calculations.

B3LYP/6-311++G**							
Delocalization (kJ/mol)	**Gas Phase**						
	FTFB[b]	**ITFB**[c]	**Br-ITFB**[d]	**Cl-ITFB**[a]	**PTFB**[a]	**FBTFB**[a]	**HTFB**[e]
$F \rightarrow \sigma^*C\text{-}H$	0	6.52	10.83	6.35	1.00	5.68	0
	Aqueous solution						
Delocalization (kJ/mol)	**FTFB**[b]	**ITFB**[c]	**Br-ITFB**[d]	**Cl-ITFB**[a]	**PTFB**[a]	**FBTFB**[a]	**HTFB**[e]
$F \rightarrow \sigma^*C\text{-}H$	0	5.73	5.56	5.27	0.71	5.47	0

[a]This work, [b]From Ref [4], [c]From Ref [5], [d]From Ref [7,8], [e]From Ref [6]
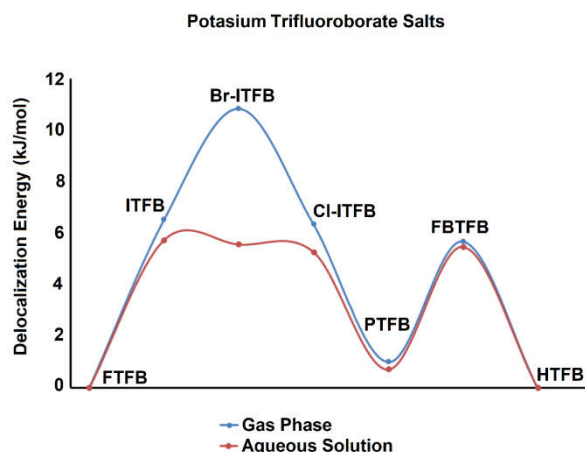

Figure 4 Main delocalization energies corresponding to halogen F---H interactions of the FTFB, ITFB, HTFB, Br-ITFB, Cl-ITFB, FBTFB and PTFB salts at the B3LYP/6-311++G** level of theory.

This study support the higher delocalizations energies for the halogen F---H interactions of those salts where a pyridine ring are linked to the C atoms of C=O groups while, on the contrary, in those salts with furyl and phenyl rings the interactions are null or have low values.

Properties and Reactivities of salts in both Media

The above NBO and AIM studies have evidenced that ITFB salt and their derivatives Br-ITFB and Cl-IFTB present the strongest halogen F---H interactions with higher densities values, lower distances between the related F and H atoms and, higher stabilization energies. Hence, the molecular weights, volumes, corrected solvation energy by using ZPVE and non electrostatic terms and reactivities values of each salt were analyzed in order to find some correlations in their properties that can explain why those ITFB salts show strong halogen F---H interactions. Thus, in Table 3 are summarized the molecular weights, volumes, corrected solvation energies, dipole moments and gap values for the FTFB, ITFB, HTFB, Br-ITFB, Cl-ITFB, FBTFB and PTFB salts by using B3LYP/6-311++G** calculations. Here, the volumes in gas

Figure 3 Behaviours of F---H distances (upper) and densities values (bottom) corresponding to halogen F---H interactions of the FTFB, ITFB, HTFB, Br-ITFB, Cl-ITFB, FBTFB and PTFB salts at the B3LYP/6-311++G** level of theory.

NBO calculations were also performed to study the halogen F---H interactions observed in all salts in both media by using the NBO program [21] with the B3LYP/6-311++G** method. Hence, these results for all salts are presented in Table 2 while in Figure 4 are shown the different behaviours of these interactions in all salts in both media. The Br-ITFB salt present the higher values in gas phase together with the ITFB and Cl-ITFB salts while newly in the HTFB salt and also in the FTFB salt are not observed halogen F---H interactions nor in gas phase neither in aqueous solution, as can be seen in both Table 2 and Figure 4. In solution, the strong interaction observed in Br-ITFB decrease strongly showing higher values ITFB than the other ones. Here, it is easily observed that the main

phase of all salts were calculated with the Moldraw program at the same level of theory [32].

Table 3 Molecular weights, volumes, corrected solvation energies and gap values for the potassium 3-furoyl-trifluoroborate (FTFB), 2-isonicotinoyl-trifluoroborate (ITFB), 5-hydroxypentanoyl-trifluoroborate (HTFB), 5-Br-2-isonicotinoyl-trifluoroborate (Br-ITFB), 6-chloro-2-isonicotinoyl-trifluoroborate (Cl-ITFB), 4-fluorobenzoyl-trifluoroborate (FBTFB) and 2-phenylacetyl-trifluoroborate (PTFB) salts by using B3LYP/6-311++G** calculations.

		Potasium trifluoroborate salts		
Salts	**MW (g/mol)**	**B3LYP/6-311++G** Method**		
		Volumen (Å^3)	**ΔG_c (kJ/mol)**	**Gap (eV)**	**μ (D)**
FTFB[b]	201.8	229.0	-85.65	5.05	7.79
HTFB[e]	207.8	252.9	-108.98	4.99	8.4
ITFB[c]	212.8	220.3	-94.58	4.39	5.56
PTFB[a]	225.8	259.2	-87.35	4.81	7.98
FBTFB[a]	229.8	250.7	-81.54	4.69	8.54
Cl-ITFB[a]	247.3	260.5	-93.03	4.32	5.64
Br-ITFB[d]	291.7	248.0	-88.81	4.30	6.89

[a]This work, [b]From Ref [4], [c]From Ref [5], [d]From Ref [7,8], [e]From Ref [6]

On the other hand, in Figure 5 are graphed the volumes, corrected solvation energies and gap values as functions of their corresponding molecular weights in increasing order. Analyzing first the volumes, it is observed that the ITFB salt presents the lower value than the other ones including than the FTFB salt which presents a furyl ring linked to the C atoms of C=O groups. Hence, the ITFB salt generates a strong halogen interaction with higher density and lower F---H distance. The higher volume values are observed in the Cl-ITFB and PTFB salts. If now the corrected solvation energies are evaluated as function of molecular weights, the higher and most negative value (-108.98 kJ/mol) is observed for the HTFB salt while the lower value for the FBTFB salt (-81.54 kJ/mol). Then, the ITFB salt and their derivatives Br-IFTB and Cl-IFTB also present high corrected solvation energies values and probably, for these reasons, these salts decrease the densities values in aqueous solution, as observed in Figure 3.
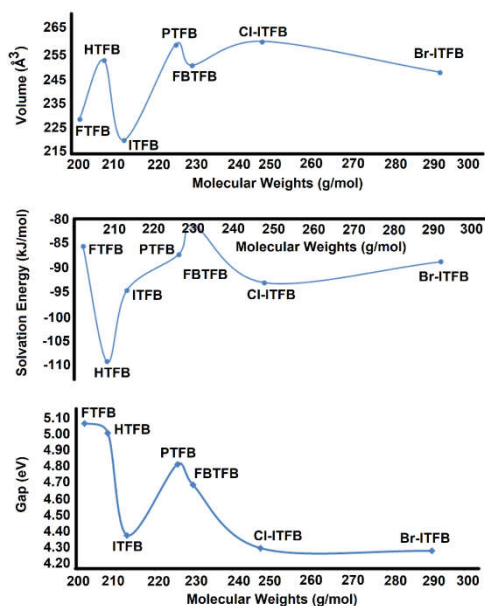

Figure 5 Variations of volumes (upper), corrected solvation energies (medium) and gap values (bottom) calculated at the B3LYP/6-311++G** level of theory as function of molecular weights of the FTFB, ITFB, HTFB, Br-ITFB, Cl-ITFB, FBTFB and PTFB salts.

When the gap values are analyzed the ITFB salt and their derivatives Br-IFTB and Cl-IFTB present the lower values and, hence, these salts are the most reactive than the other ones while the FTFB and HTFB salts are the less reactive. Other property studied for all salts as function of molecular weights in increasing order are the dipole moment values in gas phase which are presented in Table 3. **Figure 6** shows the variations of the dipole moment values against to their corresponding molecular weights. The figure shows clearly that the lower dipole moment values are observed for the ITFB salt and their derivatives Cl-IFTB and Br-IFTB, hence, these salts with low dipole moment values are the most reactive indicating clearly that there are certain dependence of this property with the reactivities of salts.
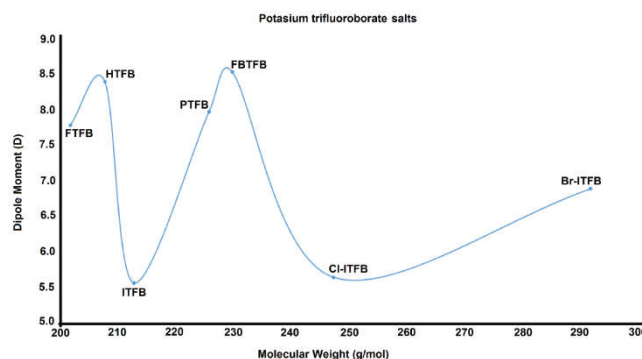

Figure 6 Variations of dipole moment values calculated at the B3LYP/6-311++G** level of theory as function of molecular weights of the FTFB, ITFB, HTFB, Br-ITFB, Cl-ITFB, FBTFB and PTFB salts.

Geometrical Parameters Common at all salts

The studies performed before have evidenced that the most reactive ITFB salt and their derivatives Cl-IFTB and Br-IFTB show low dipole moment values and strong halogen F---H interactions where, in particular, the ITFB salt has the lower volume in gas phase. Hence, in order to investigate what geometrical parameters have higher influence on the properties of seven trifluoroborate salts, the bonds C-C, C-B and C=O lengths and bonds C-C-B, C-C-O and O-C-B angles commons at all salts were analyzed in function of molecular weights. The common parameters are shown in scheme 1. In Table 4 are presented these parameters calculated in gas phase by using the B3LYP/6-311++G** method.

Table 4 Common geometrical parameters corresponding to the potassium 3-furoyl-trifluoroborate (FTFB), 2-isonicotinoyl-trifluoroborate (ITFB), 5-hydroxypentanoyl-trifluoroborate (HTFB), 5-Br-2-isonicotinoyl-trifluoroborate (Br-ITFB), 6-chloro-2-isonicotinoyl-trifluoroborate (Cl-ITFB), 4-fluorobenzoyl-trifluoroborate (FBTFB) and 2-phenylacetyl-trifluoroborate (PTFB) salts in gas phase by using B3LYP/6-311++G** method.

Salts	**MW g/mol**	**B3LYP/6-311++G** Method**					
		Bond lengths (Å)			**Bond angles (º)**		
		C-C	**C=O**	**C-B**	**C-C-B**	**C-C-O**	**O-C-B**
FTFB[b]	201.8	1.463	1.247	1.649	123.7	118.5	117.6
HTFB[e]	207.8	1.510	1.238	1.648	120.8	120.2	118.9
ITFB[c]	212.8	1.509	1.235	1.659	126.2	118.1	115.5
PTFB[a]	225.8	1.525	1.235	1.651	122.1	118.9	118.9
FBTFB[a]	229.8	1.489	1.245	1.657	126.4	118.1	115.3
Cl-ITFB[a]	247.3	1.509	1.233	1.659	126.1	117.9	115.9
Br-ITFB[d]	291.7	1.509	1.235	1.658	126.1	118.1	115.6

[a]This work, [b]From Ref [4], [c]From Ref [5], [d]From Ref [7,8], [e]From Ref [6]

In Figure 7 are graphed the variations of those parameters as a function of molecular weights. First, we analyzed the bond C-C lengths from Fig.7a, the higher values are observed for the HTFB and PTFB salts, as expected because both salts present CH_2 groups and, for these reasons, in both salts are not observed halogen F---H interactions.
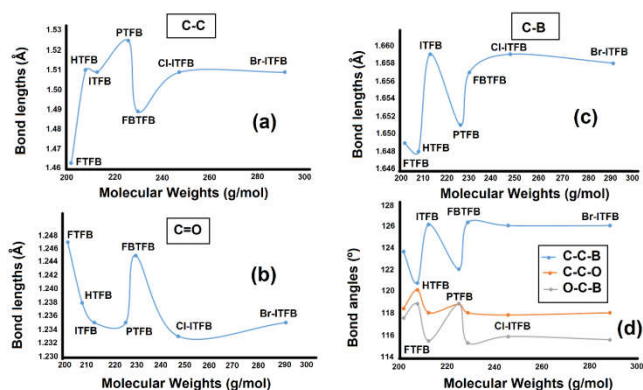

Figure 7 Variations of geometrical parameters calculated at the B3LYP/6-311++G** level of theory as function of molecular weights of the FTFB, ITFB, HTFB, Br-ITFB, Cl-ITFB, FBTFB and PTFB salts.

Then, the ITFB salt together with their derivatives Cl-IFTB and Br-IFTB show practically the same C-C distances revealing that the incorporations of Cl and Br atoms in the pyridine rings linked to C-C bonds practically don't have influence on those distances while the lower value in the FTFB salt could have influence on the low volume, lower solvation energy and higher gap value, lower F---H distance and, as a consequence a low density it is observed in the halogen F---H interaction of this salt. However, the C-C distance value can have influence on the F---H distance of halogen F---H interaction observed in the FBTFB salt, as can be seen from Fig. 1. If now the bonds C=O lengths are analyzed from Fig.1b, we can see that the lower values or the higher double bond character of these bonds are evidenced in the ITFB salt together with their derivatives Cl-IFTB and Br-IFTB and also, in PTFB, while the FTFB and FBTFB salts with higher C=O distances present the low solvation energies and high dipole moment values. When the bonds C-B lengths are analyzed we observed that the ITFB salt together with their derivatives Cl-IFTB and Br-IFTB show the higher values while HTFB, FTFB and PTFB present the lower values. Therefore, when higher is the distance between both C and B atoms lower value it is observed in the F---H distance and, hence, the halogen F---H interactions is strong. Thus, higher electronic density in the bond critical points are observed and higher stabilization energies in the halogen F---H interaction are expected. Evaluating the bond C-C-B, C-C-O and O-C-B angles, the higher C-C-B angles are in agreement with the higher C-B distances observed for the ITFB salt together with their derivatives Cl-IFTB and Br-IFTB while the lower values in the O-C-B angles are strongly related to the lower C=O distances corresponding thus, the lower values to the ITFB salt and their derivatives Cl-IFTB and Br-IFTB. Hence, these studies suggest clearly the dependence of the commons geometrical parameters on the properties of halogen F---H interactions and, hence, on the properties of trifluoroborate salt. Other very important result obtained from this study is that the change of Cl atom by Br in the pyridine ring of the ITFB salt modify notably the molecular weight of salt but few changes in the geometrical C-C, C-B, C=O, C-C-B, C-C-O and O-C-B parameters are observed, as evidenced from Figure 7.

CONCLUSIONS

In the present work, the role of halogen F---H interactions present in the potasium trifluoroborate salts were theoretically evaluated by using NBO and AIM calculations in gas phase and in aqueous solution by using B3LYP/6-311++G** method and the SCRF and SM models. In addition, the corrected solvation energy by using ZPVE and non electrostatic terms, volumes and gap values were evaluated as function of molecular weights of salts by using the same level of theory. The AIM calculations show that the IFTB salt present the lower F---H distances in the two media. Evidently, the presence of a pyridine ring linked to C of C=O groups in IFTB favours the formation of a halogen interaction, as compared with furyl and phenyl rings of other salts. NBO studies show that the higher delocalizations energies of halogen F---H interactions are observed in the Br-ITFB salt in both media together with the ITFB and Cl-ITFB salts. This study evidence clearly that the halogen F---H interaction play a important role in the reactivity and properties of trifluoroborate salts showing that the FTFB salt has lower volume, low corrected solvation energy and is the less reactive while the most reactive Br-ITFB, Cl-ITFB and IFTB salts present high stabilization energies of halogen F---H interactions and high corrected solvation energies. The studies of dipole moments values show that the lower dipole moment values are observed for the ITFB salt and their derivatives Cl-IFTB and Br-IFTB, which are the most reactive salts and with high solvation energy values indicating clearly that there are certain dependence of this property with the reactivities of salts and their solvation energies. Probably, the ITFB salt with strong halogen F---H interaction is the most reactive due to its low dipole moment value and to the presence of pyridine ring that increase the reactivity. On the other hand, the presence of CH_2 groups between the BF_3K groups and the H atoms in the HTFB and PTFB salts justify the absence of halogen F---H interactions in both media. Besides, in both HTFB and PTFB salts are observed high dipole moment values and, for these reasons, both salts show low reactivities together with the FBTFB salt. The analyses of the commons geometrical C-C, C-B, C=O, C-C-B, C-C-O and O-C-B parameters at all salts have showed notable influence on the halogen F---H interactions and on the properties of trifluoroborate salts where the ITFB, Cl-IFTB and Br-IFTB salts show practically the same C-C distances and higher C=O and C-B distances values revealing few changes in the distances when the Cl and Br atoms are incorporated to the pyridine rings. The evaluation of bond C-C-B, C-C-O and O-C-B angles have revealed that the ITFB, Cl-IFTB and Br-IFTB salts present higher C-C-B angles and lower O-C-B angles values suggesting the clear dependence of the commons geometrical parameters on the properties of halogen F---H interactions and, hence, on the properties of trifluoroborate salt. Additionally, the change of Cl atom by Br in the pyridine ring of the ITFB salt modify notably the molecular weight of salt but few changes in the geometrical C-C, C-B, C=O, C-C-B, C-C-O and O-C-B parameters are observed.

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