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The cooperativity between hydrogen and halogen bond in the XY···HNC···XY (X, Y = F, Cl, Br) complexes

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Abstract The cooperativity between hydrogen and halogen bonds in XY···HNC···XY (X, Y = F, Cl, Br) complexes was studied at the MP2/aug-cc-pVTZ level. Two hydrogen-bonded dimers, five hydrogen-bonded dimers, and ten trimers were obtained. The hydrogen- and halogen-bonded interaction energies in the trimers were larger than those in the dimers, indicating that both the hydrogen bonding interaction and the halogen bonding interaction are enhanced. The binary halogen bonding interaction plays the most important role in the ternary system. The hydrogen donor molecule influences the magnitude of the halogen bonding interaction much more than the hydrogen bonding interaction in the trimers with respect to the dimers. Our calculations are consistent with the conclusion that the stronger noncovalent interaction has a bigger effect on the weaker one. The variation in the vibrational frequency in the HNC molecule was considered. The NH antisymmetry vibration frequency has a blue shift, whereas the symmetry vibration frequency has a red shift. A dipole moment enhancement is observed upon formation of the trimers. The variation in topological properties at bond critical points was obtained using the atoms in molecules method, and was consistent with the results of the interaction energy analysis.

Keywords Hydrogen bond · Halogen bond · Cooperativity · Frequency shift · Dipole enhancement · Bond enhancement

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Introduction

Noncovalent bonding interactions play an important role in crystal packing, molecular recognition, biological processes, and reaction selectivity [1, 2]. Hydrogen bonding is a well-known noncovalent interaction, which has attracted much attention and a significant amount of experimental and theoretical research [3–5]. Another noncovalent interaction, called halogen bonding, has been confirmed to play an essential role in biochemistry and crystal chemistry [6–9]. Recently, the reason why halogen-bonded complexes can be formed was explained by Politzer et al. [10–13], who recognized that halogen bonding involves the interaction of positive σ-holes—positive regions of electrostatic potential along the direction of the covalent bond to the halogen—with negative sites on other molecules.

A great many works have been published that study the cooperative effects in systems where two or more noncovalent interactions coexist [14–20]. Recently, Alkorta et al. [21, 22] defined a new concept, namely synergetic stability, to stress the importance of the interplay between noncovalent interactions in ternary systems. Both hydrogen and halogen bonding are electrostatically driven noncovalent interactions, which suggests that cooperative effects between hydrogen and halogen bonds should be observable. There is plenty of theoretical and experimental evidence showing the simultaneous presence of hydrogen and halogen bonds [23–27]. Lankau et al. [23] studied theoretically the cooperativity between hydrogen and halogen bonds in X···HCN···Y (X: C_2H_2, H_2O, NH_3, HCl, HCN, HF; Y: HF, BrF, Br_2) complexes. Voth and co-workers [26] found that halogen bonds were geometrically perpendicular to, and energetically independent of, hydrogen bonds that share a common carbonyl oxygen acceptor by performing an analysis of crystal structures of biomolecules.

Hydrogen isocyanide (HNC) is a highly reactive specie discovered in 1867. Alkorta et al. [28] carried out theoretical calculations incorporating a Cambridge Structural Database (CSD) search to prove that HNC is a good proton acceptor. Quantum chemical investigations indicate that the ability of the HNC proton donor is stronger than that of its proton acceptor [28]. Li et al. have published several papers [29–31] investigating the cooperativity of noncovalent complexes containing HNC. Their results show significant cooperativity between both types of hydrogen bonds, such as HNC···HNC···HNC, HF···HNC···HNC, H_3C···HNC···HNC, and H_3N···HNC···HNC. Thus, although the cooperative effect of hydrogen bonds in HNC ternary systems has been well studied, the interplay between hydrogen- and halogen-bonded interactions in the trimer of HNC has not been the focus of experimental and theoretical methods.

The present paper reports on a study of the XY···HNC···XY (X, Y = F, Cl, Br) complex with ab initio calculations. In order to gain insight into synergistic effects, XY···HNC (hydrogen bonds) and HNC···XY (halogen bonds) dimers were calculated. Topological properties were studied using the atoms in molecules (AIM) theory [32]. We believe that our theoretical study will enrich the knowledge on cooperativity in multiple noncovalent interactions.

Methods

Full geometry optimizations of the XY···HNC, HNC···XY, and XY···HNC···XY complexes were performed at the MP2/aug-cc-pVTZ level. The corresponding frequency calculations were carried out at the same level to ensure that the structures of the complexes are true minima. No basis set superposition errors (BSSE) were computed since it has been shown that uncorrected MP2/aug-cc-pVTZ energies lie between the corrected and uncorrected MP2/aug-cc-pVQZ energies [33]. The calculations were carried out by the GAUSSIAN 03 program suite [34]. The bonding characteristic of the complexes were analyzed using AIM theory. AIM analysis was performed with the AIMAll software package [35] using the MP2/aug-cc-pVTZ wave functions as input.

For convenience, hydrogen-bonded dimers are denoted by A-B, and halogen-bonded dimers are denoted by B-C; A-B-C represents trimers. Here B is HNC, and A and C are XY (X, Y = F, Cl, Br). The hydrogen bonding and halogen bonding interaction energies in the dimers were calculated using Eqs. 1 and 2, respectively

$$\Delta E_{AB} = E_{AB} - (E_A + E_B) \quad (1)$$

$$\Delta E_{BC} = E_{BC} - (E_B + E_C) \quad (2)$$

The hydrogen bonding and halogen bonding interaction energies in trimers are given in Eqs. 3 and 4, respectively

$$\Delta E_{AB}' = E_{ABC} - (E_A + E_{BC}) \quad (3)$$

$$\Delta E_{BC}' = E_{ABC} - (E_C + E_{AB}) \quad (4)$$

where E_{ABC} is the total energy of the ternary system, and E_A, E_{BC}, E_C, and E_{AB} are the energies of the binary and monomeric systems.

The interaction energy of the ternary system was calculated using Eq. 5

$$\Delta E_{ABC} = E_{ABC} - (E_A + E_B + E_C) \quad (5)$$

Results and discussion

Energies and geometries

Not all the dihalogens could form hydrogen- or halogen-bonded complexes with HNC. Two hydrogen-bonded and five halogen-bonded complexes were obtained in our calculations: ClF···HNC, BrF···HNC, HNC···F_2, HNC···Cl_2, HNC···Br_2, HNC···ClBr, and HNC···BrCl. Because hydrogen and halogen bonding interactions are electrostatically driven, we calculated the molecular electrostatic potential (MEP) of F_2, Cl_2, Br_2, FCl, ClBr, BrF, and BrCl. The corresponding values of MEP maxima and minima are collected in Table 1. A positive "σ-hole" was detected in the F_2, Cl_2, Br_2, and ClBr molecules. The ClBr molecule has two different "σ-holes", and two halogen-bonded complexes were formed between ClBr and HNC. Although the BrF and ClF molecules also have large positive values of MEP on the surfaces of the larger halogen atoms, we did not obtain the conventional F-Cl (Br)···CNH halogen-bonded complexes. Instead, special halogen-shared interactions, F···Cl(Br)···CNH, were found, which have been studied very recently by Del Bene [36]. Because our aim was to investigate the F-Cl(Br)···CNH

Table 1 Maxima and minima of the molecular electrostatic potential (MEP; in kcal mol^{-1}) of F_2, Cl_2, Br_2, BrCl, ClF, and BrF at 0.001 a.u. isosurfaces calculated at the MP2/aug-cc-pVTZ level[a]

MEP	F_2	Cl_2	Br_2	BrCl	ClF	BrF
Maxima	12.6	27.0	29.3	19.5(Cl) 35.8 (Br)	46.0	56.7
Minima	-	-	-	-	−8.2	−13.8

[a] Only values involved in hydrogen and halogen bonding are given

halogen bonding interaction, we considered only hydrogen bonds between FCl(Br) and HNC, not involving halogen bonds. The optimized structures and geometrical parameters of the dimers are shown in Fig. 1. The interaction energy of the hydrogen-bonded complexes was calculated to be −2.246 and −3.243 kcal mol^{-1} for the ClF···HNC and BrF···HNC dimers, respectively. For halogen bonding, the interaction energies were −1.078, −3.159, −5.422, −6.445, and −2.677 kcal mol^{-1} for the HNC···F_2, HNC···Cl_2, HNC···Br_2, HNC···ClBr, and HNC···BrCl dimers, respectively. One can see that the order of interaction energies is consistent with that of the MEP.

From the above results on dimers, ten stabilizing trimers were obtained. The optimized structures and geometrical parameters of the ternary system investigated (ClF···HNC···F_2, ClF···HNC···Cl_2, ClF···HNC···Br_2, ClF···HNC···ClBr, ClF···HNC···BrCl, BrF···HNC···F_2, BrF···HNC···Cl_2, BrF···HNC···Br_2, BrF···HNC···ClBr, and BrF···HNC···BrCl) are shown in Fig. 2. One can see that both the F···H and C···X (X = F, Cl, Br) distances have decreased in the trimers compared to the dimers. The interaction energies and the cooperative energies are given in Table 2. It is obvious that the hydrogen- and halogen-bonded interaction energies in the trimers are larger than those in the dimers, which indicates that both the hydrogen bonding interaction and the halogen bonding interaction are enhanced. The absolute increment and relative increment percentage of the hydrogen- and halogen-bonded interaction energies in the trimers with respect to the dimers are gathered in Table 3.

It is important to note that the absolute increments of the hydrogen bonding interaction and the halogen bonding interaction have identical values [37]. That is to say, $\Delta\Delta E_{AB} = \Delta E_{AB}' - \Delta E_{AB} = \Delta\Delta E_{BC} = \Delta E_{BC}' - \Delta E_{BC} = \Delta\Delta E$. The relative increments of these interactions were defined as $P_{AB}=100\%*\Delta\Delta E/\Delta E_{AB}$, and $P_{BC} = 100\%*\Delta\Delta E/\Delta E_{BC}$. The values of $\Delta\Delta E$ become larger in the order of ClF(BrF)···HNC···F_2< ClF(BrF)···HNC···ClBr< ClF(BrF)···HNC···Cl_2< ClF(BrF)···HNC···Br_2< ClF(BrF)···HNC···BrCl. This is consistent with the order of interaction energy of the halogen-bonded dimers, indicating that binary halogen bonding interaction plays the most important role in the ternary system. The stronger hydrogen bonding interaction makes the halogen bonding interaction in the same trimer more stabilizing. For example, the ClF···HNC complex is less stabilizing than the BrF···HNC complex, and the absolute increment of the halogen bonding interaction is smaller in the ClF···HNC···F_2 (0.086 kcal mol^{-1}) complex than in the BrF···HNC···F_2 (0.123 kcal mol^{-1}) complex. Similar results are obtained in other ternary systems.

It is interesting to investigate how halogen bonding influences the hydrogen-bonded interaction, and how hydrogen bonding affects halogen-bonded interactions. In the ClF···HNC···C trimer, the participation of the C molecule makes the magnitude of hydrogen bonding increases greater than those of halogen bonding except for the ClF···HNC···F_2 (3.8% vs 8.0%) complex. For the BrF···HNC···C ternary system, the relative increment of hydrogen bonding is stronger than that of halogen bonding only in the BrF···HNC···Br_2 (22.9% vs 13.7%) and BrF···HNC···BrCl (27.2% vs 13.7%) complexes. There results can be attributed to the relative magnitude of the interaction energies in the hydrogen- and halogen-bonded

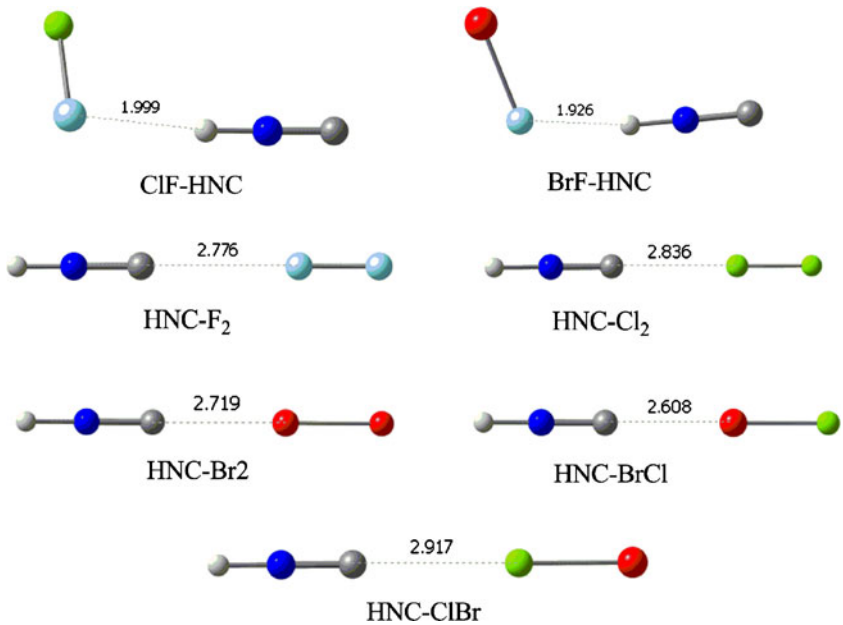

Fig. 1 MP2/aug-cc-pVTZ optimized geometries of the binary system

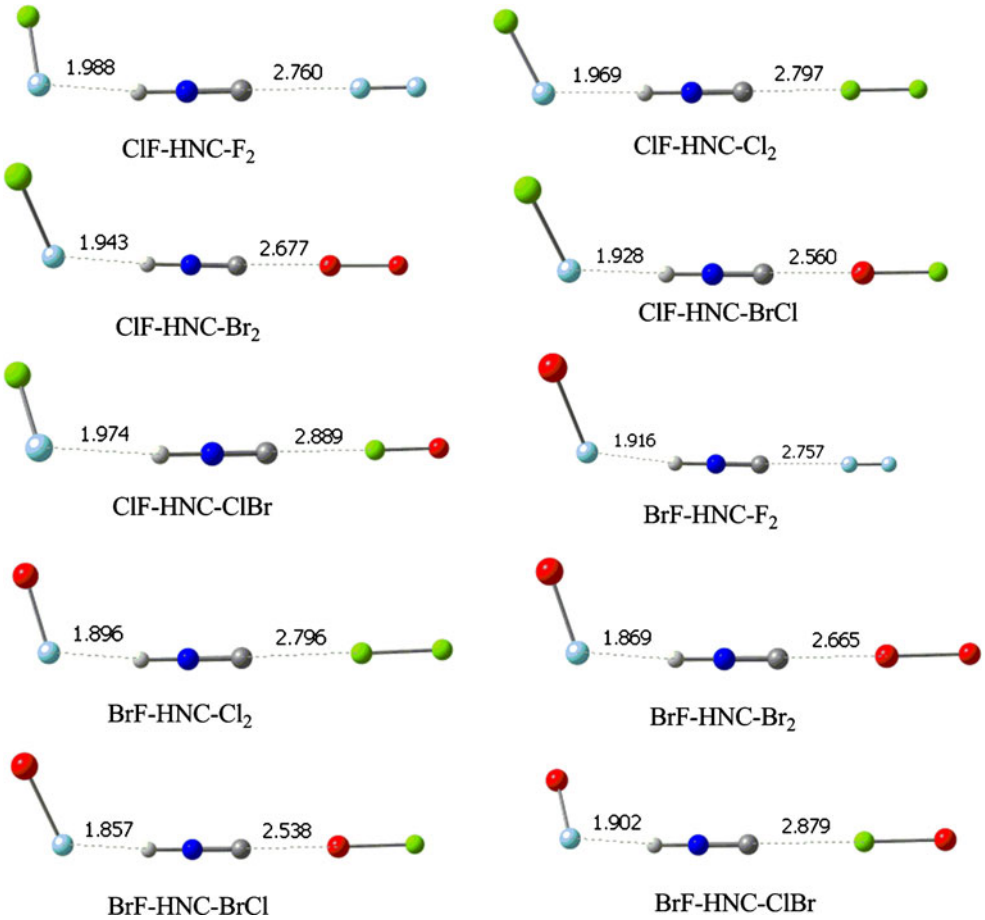

Fig. 2 MP2/aug-cc-pVTZ optimized geometries of the ternary system

dimers. The absolute value of the interaction energy of the HNC···F_2 complex is smaller than that of the ClF···HNC complex, and the HNC···Br_2 and HNC···BrCl complexes are more stabilizing than the BrF···HNC complex. Our calculations are consistent with the conclusion that the stronger noncovalent interaction has a bigger effect on the weaker one [31].

The cooperative energy (E_{coop}) [21, 22] is applied here to evaluate the cooperativity of the hydrogen bonds and halogen bonds in their ternary systems. Cooperative

Table 2 Interaction energies and cooperative energies (in kcal mol^{-1}) in the ternary system[a]

Complex	ΔE_{ABC}	$\Delta E_{AB}'$	$\Delta E_{BC}'$	ΔE_{AC}	E_{coop}
ClF-HNC-F_2	-3.409	-2.332	-1.164	0.042	-0.127
ClF-HNC-Cl_2	-5.691	-2.531	-3.445	0.069	-0.349
ClF-HNC-Br_2	-8.217	-2.796	-5.972	0.195	-0.744
ClF-HNC-BrCl	-9.323	-2.878	-7.077	0.446	-1.078
ClF-HNC-ClBr	-5.170	-2.496	-2.926	0.025	-0.272
BrF-HNC-F_2	-4.444	-3.366	-1.201	0.046	-0.169
BrF-HNC-Cl_2	-6.818	-3.658	-3.575	0.060	-0.476
BrF-HNC-Br_2	-9.409	-3.987	-6.166	0.202	-0.946
BrF-HNC-BrCl	-10.569	-4.125	-7.326	0.502	-1.383
BrF-HNC-ClBr	-6.264	-3.632	-3.021	0.024	-0.368

[a] The various energies have been defined in the text

Table 3 The absolute (in kcal mol^{-1}) increment and relative increment percentage of the hydrogen and halogen bonding in trimers with respect to dimers[a]

Complex	$\Delta\Delta E$	P_{AB}	P_{BC}
ClF-HNC-F_2	-0.086	3.8%	8.0%
ClF-HNC-Cl_2	-0.285	12.7%	9.0%
ClF-HNC-Br_2	-0.550	24.5%	10.1%
ClF-HNC-BrCl	-0.632	28.1%	9.8%
ClF-HNC-ClBr	-0.250	11.1%	9.3%
BrF-HNC-F_2	-0.123	3.8%	11.4%
BrF-HNC-Cl_2	-0.415	12.8%	13.1%
BrF-HNC-Br_2	-0.744	22.9%	13.7%
BrF-HNC-BrCl	-0.882	27.2%	13.7%
BrF-HNC-ClBr	-0.389	12.0%	14.5%

[a] $\Delta\Delta E$, P_{AB}, and P_{BC} are defined in the text

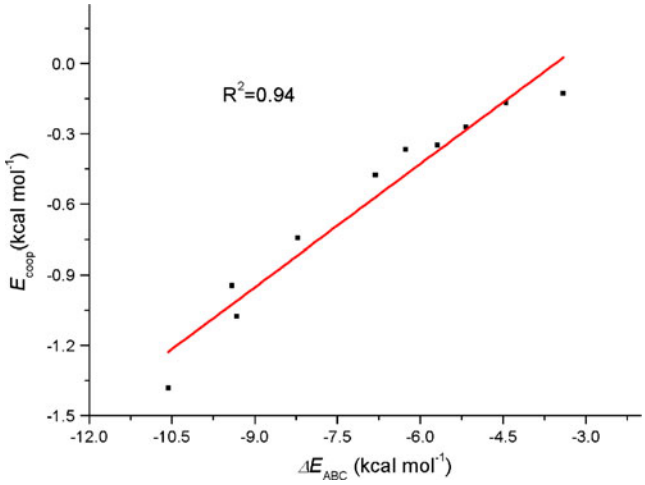

Fig. 3 Correlation between ΔE_{ABC} and E_{coop}

energies were calculated using Eq. 6

$$E_{coop} = \Delta E_{ABC} - \Delta E_{AB} - \Delta E_{BC} - \Delta E_{AC} \quad (6)$$

where ΔE_{AC} is the interaction energy of molecules A and C in the geometry they adopt in the trimer. A negative cooperativity indicates that the two interactions work in concert with each other and enhance each other's strength, while a positive value indicates that the two interactions work anti-cooperatively. From Table 2, it can be seen that all the values of E_{coop} are negative, indicating an overall stabilization of the interactions in ternary complex with respect to the binary complexes, in agreement with the above analysis of the interaction energy. In the ternary systems, the absolute values of E_{coop} increase in the order of ClF(BrF)···HNC···F_2< ClF(BrF)···HNC···ClBr < ClF(BrF)···HNC···Cl_2< ClF(BrF)···HNC···Br_2< ClF(BrF)···HNC···BrCl. For trimers containing the same halogen bond donor, the absolute values of E_{coop} are larger in BrF trimers than in ClF trimers. A good correlation was found between E_{coop} and ΔE_{ABC} (R^2=0.94), as shown in Fig. 3.

Table 4 Frequency of NH antisymmetry vibration and the symmetry vibration (in cm^{-1}) of the HNC molecule in the dimers and trimers

Complex	$\nu_{antisym}$	ν_{sym}
ClF-HNC	2,017.95	3,755.74
BrF-HNC	2,017.56	3,723.06
HNC-F_2	2,021.98	3,815.69
HNC-Cl_2	2,031.77	3,808.09
HNC-Br_2	2,044.32	3,803.08
HNC-BrCl	2,052.89	3,800.70
HNC-ClBr	2,027.05	3,809.29
ClF-HNC-F_2	2,024.52	3,751.42
ClF-HNC-Cl_2	2,035.52	3,743.41
ClF-HNC-Br_2	2,049.39	3,720.53
ClF-HNC-BrCl	2,058.05	3,710.49
ClF-HNC-ClBr	2,031.68	3,740.73
BrF-HNC-F_2	2,023.30	3,716.74
BrF-HNC-Cl_2	2,035.85	3,699.58
BrF-HNC-Br_2	2,048.61	3,678.10
BrF-HNC-BrCl	2,057.97	3,665.30
BrF-HNC-ClBr	2,031.62	3,705.28

Table 5 Dipole moment enhancement (in Debye) upon complex formation, and cooperativity parameter as defined by Eq. 7

Complex	ΔD_{ABC}	ΔD_{AB}	ΔD_{BC}	D_{coop}
ClF-HNC-F_2	0.2645	-0.0763	0.2871	0.0537
ClF-HNC-Cl_2	1.2857	-0.0763	1.0083	0.3537
ClF-HNC-Br_2	2.1902	-0.0763	1.9163	0.3502
ClF-HNC-BrCl	2.6032	-0.0763	2.1967	0.4828
ClF-HNC-ClBr	-0.0045	-0.0763	-0.0897	0.1615
BrF-HNC-F_2	0.2533	-0.1070	0.2871	0.0732
BrF-HNC-Cl_2	1.1302	-0.1070	1.0083	0.2289
BrF-HNC-Br_2	2.2656	-0.1070	1.9163	0.4563
BrF-HNC-BrCl	2.7464	-0.1070	2.1967	0.6567
BrF-HNC-ClBr	0.0416	-0.1070	-0.0897	0.2383

Vibrational analysis and dipole moment enhancement

The frequency shift in infrared spectroscopy is a useful tool for the characterization of hydrogen- and halogen-bonded complexes. Here, we focused on two vibration modes: the NH antisymmetry vibration and the symmetry vibration in the HNC molecule [29]. The corresponding results are summarized in Table 4. The frequency of the NH antisymmetry vibration and the symmetry vibration in the HNC monomer is 2016.95 and 3821.08 cm^{-1}, respectively. It is seen that the NH antisymmetry vibration frequency has

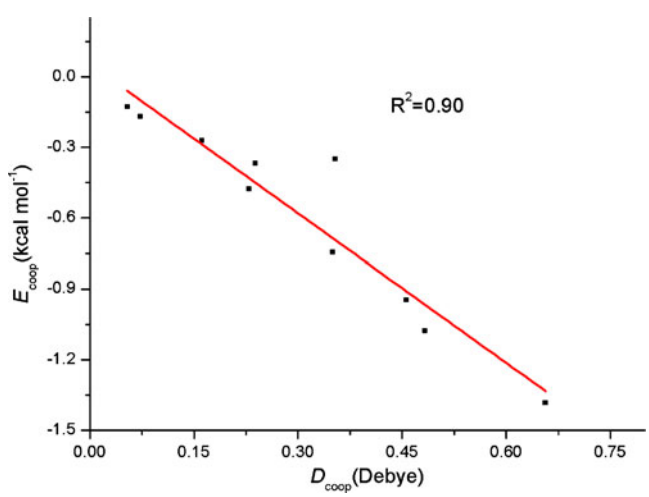

Fig. 4 Correlation between D_{coop} and E_{coop}

a blue shift, whereas the symmetry vibration frequency has a red shift. Compared to the binary system, the NH antisymmetry vibration frequency in the ternary system increases in the following order: ClF(BrF)···HNC···F_2< ClF(BrF)···HNC···ClBr < ClF(BrF)···HNC···Cl_2< ClF(BrF)···HNC···Br_2< ClF(BrF)···HNC···BrCl, and the symmetry vibration frequency decreases in the opposite order. This result is consistent with the above analysis of interaction energy and cooperative energy. Similarly, the halogen bond donor has a stronger influence on the variation in vibration frequency than the hydrogen bond acceptor.

We also studied the effect of complex formation on the dipole moment values of the binary and ternary systems. The results are presented in Table 5. According to Alkorat et al. [22], a cooperative parameter was defined for the dipole moment enhancement due to complex formation in Eq. 7

$$D_{\text{coop}} = \Delta D(\text{ABC}) - \Delta D(\text{AB}) - \Delta D(\text{BC}) \quad (7)$$

where the corresponding ΔD is calculated as the difference between the dipole moment in the cluster and the sum of the isolated monomers in their optimized geometries. One can see from Table 5 that a dipole moment enhancement is observed upon formation of the trimers, with a positive D_{coop}, which indicates that the dipole moment enhancement in the trimers is larger than that observed as the sum of the two dimers. It is noteworthy that not all D_{coop} values are consistent with E_{coop}. For example, E_{coop}(ClF···HNC···Cl_2) is larger than E_{coop}(ClF···HNC···Br_2), but D_{coop}(ClF···HNC···Cl_2) is smaller than D_{coop}(ClF···HNC···Br_2). Despite such exceptions, a good correlation was also obtained between E_{coop} and D_{coop} (R^2=0.90), as shown in Fig. 4.

Table 6 Variation in electron charge density ($\Delta\rho$, a.u.) and Laplacian (ΔL, a.u.) in the trimers A-B-C with respect to the dimers A-B and B-C at the MP2/aug-cc-pVTZ level measured at the bond critical point (BCP)

Complex	$10^2\times\Delta\rho_1$	$10^2\times\Delta\rho_2$	$10^2\times\Delta L_1$	$10^2\times\Delta L_2$
ClF-HNC-F_2	0.0441	0.0463	0.1525	0.2000
ClF-HNC-Cl_2	0.1032	0.1726	0.3913	0.3999
ClF-HNC-Br_2	0.2422	0.2645	0.7927	0.4041
ClF-HNC-BrCl	0.3130	0.3771	1.0075	0.4481
ClF-HNC-ClBr	0.1046	0.1039	0.3542	0.2494
BrF-HNC-F_2	0.0499	0.0547	0.1430	0.2328
BrF-HNC-Cl_2	0.1533	0.1781	0.4398	0.3948
BrF-HNC-Br_2	0.3083	0.3458	0.8376	0.5140
BrF-HNC-BrCl	0.3719	0.5612	1.0033	0.6510
BrF-HNC-ClBr	0.1221	0.1428	0.3511	0.3421

AIM analysis

AIM theory is based on a topological analysis of the electron charge density and its Laplacian, and has been applied successfully to the characterization of hydrogen bonds and halogen bonds of different strengths in a wide variety of molecular complexes [38–40]. With this in mind, we performed a topological analysis to gain more insight into the cooperativity of these ternary systems. Table 6 collects the values of electron density and the Laplacian computed at the bond critical points (BCP) for the ternary systems. In addition, we also give the variation of these values with respect to the values obtained for the binary systems [22]. It can be seen that all the values of $\Delta\rho$ are positive, indicating a reinforcement of the interactions because this implies that the value of ρ is larger in the trimers than in the dimers. Furthermore, the values of ΔLapacian are also positive. All these results are in accordance with former investigations into interactive distance and interaction energy indicating that both the

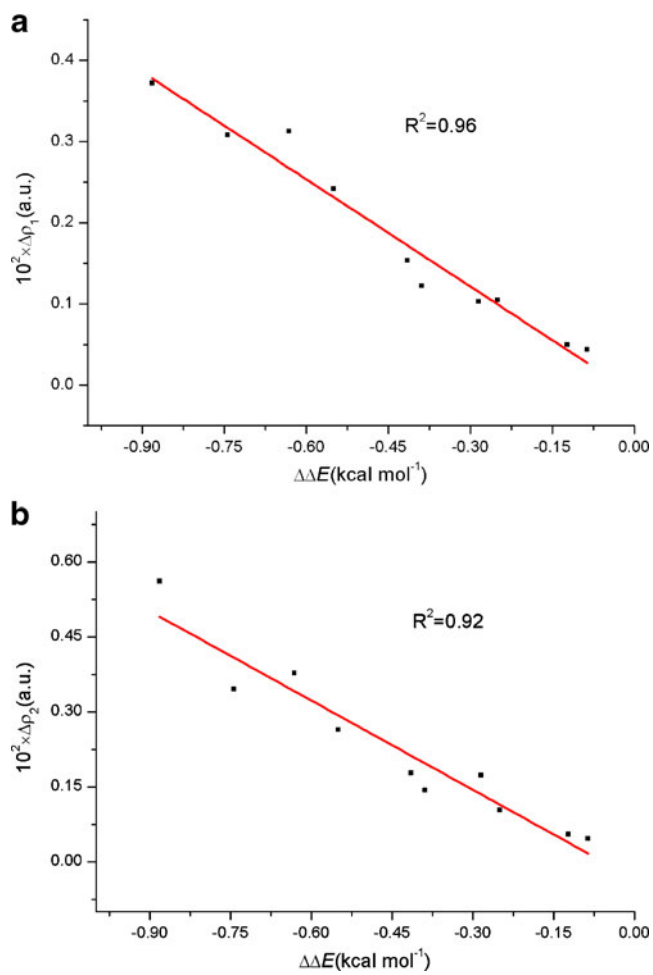

Fig. 5 Correlation between $\Delta\Delta E$ and the variation in electron charge density at the bond critical point (BCP) in trimers with respect to dimers

hydrogen bonding interaction and the halogen bonding interaction are enhanced. It is noteworthy that the variation in $\Delta\rho$ in the ternary system is consistent with the variation in $\Delta\Delta E$, for which a good correlation is presented in Fig. 5.

Conclusions

We investigated cooperativity between hydrogen and halogen bonds in XY···HNC···XY (X, Y = F, Cl, Br) complexes using the MP2/aug-cc-pVTZ method. The interaction energies of the dimers are in accordance with the MEP. Both hydrogen bonding interactions and halogen bonding interactions are enhanced in trimers with respect to dimers. The stronger noncovalent interaction has a bigger effect on the weaker one, as verified by our analysis of the relative increment in the interaction energy. The variation in vibrational frequency in the HNC molecule was considered. The NH antisymmetry vibration frequency has a blue shift, whereas the symmetry vibration frequency has a red shift. A dipole moment enhancement is observed upon formation of trimers, which is consistent with the cooperative energy. Similar results were obtained by performing AIM analysis.

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