



## Theoretical study of molecular interactions of phosphorus ylide with hypohalous acids HOF, HOCl and HOBr

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### ABSTRACT

The molecular interactions of phosphorous ylide (PY) and hypohalous acids HOX (X = F, Cl and Br) were investigated using the MP2 method at 6-311++G(2d,2p) basis set. The patterns including non-classical hydrogen bond H...C, halogen bond X...C, classical hydrogen bonds H...X and H...O, and F...P interactions were found for complex formation between PY and HOX molecules. From the predicted models, stabilities of the X...C and H...C types complexes are greater than other types. Quantum theories of atoms in molecules (AIM) and natural bond orbitals (NBO) methods have been applied to analyze the intermolecular interactions. Good correlations have been found between the interaction energies (SE), the second-order perturbation energies  $E^{(2)}$  and the charge transfer qCT in the studied systems.

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### 1. Introduction

Noncovalent interactions have attracted much attention due to their extensive applications in fields of chemistry, biology, and physics [1]. Hydrogen bond certainly holds the most important position among the intermolecular interactions. It has been demonstrated that the electrostatic interaction, together with induction and dispersion interactions, contributes jointly to the formation of hydrogen bond [2]. A large number of theoretical studies on the structure, stability and vibrational spectra employing *ab initio* and DFT calculations have been undertaken in recent years for the hydrogen-bonded complexes [3–7].

The presence of the partially negative charge on carbon and positive charge on phosphorus atoms in phosphorus ylides make these molecules suitable for acting as both hydrogen bond acceptor (HBA) and hydrogen bond donor (HBD) species. Ylides as HBA have been the subject of a number of studies [8–13]. The HB complexes of these acceptors can show low-barrier hydrogen bond interactions which are particularly short and strong interactions [14].

On the other hand, hypohalous acids are important from an atmospheric chemistry point of view. Since, HOCl and HOBr have been involved in catalytic cycles in the seasonal depletion of the ozone layer in the stratosphere. The hypohalous acids are strong oxidants with potent antibacterial properties [15]. Both HOCl and HOBr react readily with biological molecules including amino

acids, proteins, antioxidants (including thiols), carbohydrates, lipids, and DNA [16,17].

Because of chemical instability of the hypohalous acids that renders the accurate experimental determination of their properties rather difficult, theoretical studies on the properties of these molecules can thus play a very important role and will be in order [18–20]. Therefore, the main focus of the present study is to analyze the key structural for interactions of phosphorus ylide with HOX molecule (X = F, Cl and Br). In the best of our knowledge such studies have not been presented previously. Results of this study also show that intermolecular interactions might affect the ylide structure.

In this work, the 1:1 molecular complexes of PY with HOX molecules have been investigated. The second-order Moller–Plesset perturbation (MP2) with the large basis set 6-311++G(2d,2p) has been employed to determine the equilibrium structure and vibrational frequencies of the interacting complexes.

### 2. Computational methods

Calculations were performed using the Gaussian 03 package of codes [21]. The geometries of the isolated ylide, HOX and their complexes were fully optimized at the MP2/6-311++G(2d,2p) computational level. Harmonic vibrational frequency calculations at MP2/6-311++G(2d,2p) level confirmed the structures as minima and enabled the evaluation of zero-point vibrational energies (ZPVE). The counterpoise procedure [22] was used to correct the interaction energy for basis set superposition error (BSSE). The AIM2000 package [23] was used to obtain bond properties; and

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to plot molecular graphs. The natural bond orbitals (NBO) method [24] implemented within the Gaussian 03 set of codes was applied to perform NBO analysis.

### 3. Results and discussion

Results of geometry optimizations for the PY and its complexes with HOX molecules are given in Tables 1–3 and Fig. 1. Three atoms of HOX could interact with the ylide. The proposed patterns which considered for interaction of HOX molecules with PY are including H...C, X...C, H...X, H...O, and X...P interactions, Scheme 1.

In the first type (I) we have H...C and X...C interactions in which HOX through both its H and X atoms act as Lewis acid or electron acceptor and PY act as Lewis base or electron donor. In the H...C the HOX as a HBD interact with the C atom of the ylide in a HB interaction, while in the X...C type the X atom of HOX acts as electron acceptor where as the C atom of the ylide acts as electron donor in a halogen bond interaction.

The second type (II) the H...X and H...O interactions were found between ylide and HOX. This type is including usual HB interactions in which an H atom of PH<sub>3</sub> role as HBD toward X or O atoms of HOX as HBA.

Eventually, the third model (III) denoted as X...P interaction which was specified to the interaction of P atom of ylide as electron acceptor with F function of HOF as electron donor. Results of calculations show that X...C interactions are stronger than X...P, O...H, and X...H interactions (Table 1).

Results indicate that three hydrogens of PH<sub>3</sub> in the free ylide are not equivalent. They could be classified as P–H<sub>a</sub>, which it is gauche to the CH<sub>2</sub>, P–H<sub>b</sub> and P–H<sub>c</sub> which are anti with respect to the CH<sub>2</sub> (Scheme 2). The P–H<sub>a</sub> (1.426 Å) is longer than P–H<sub>b</sub> and P–H<sub>c</sub> bonds (1.394 Å). The reason of this difference would be interpretable in term of lp(C) → σ\*(P–H) charge transfer, in which electron density from a lone pair electron that located on the C atom goes to the σ\* of (P–H) orbitals. According to natural bond orbital analysis (NBO) the occupancy for σ\*(P–H<sub>a</sub>) is 0.1857e but for σ\*(P–H<sub>b</sub> and P–H<sub>c</sub>) is 0.0526e, Tables 4 and S1. Since lp(C) → σ\* charge transfer for P–H<sub>a</sub> is stronger than P–H<sub>b</sub> and P–H<sub>c</sub>, then P–H<sub>a</sub> is longer and weaker than P–H<sub>b</sub> and P–H<sub>c</sub>.

The S1–S10 complexes have been predicted as results of H...C, X...C, X...P and X...H interactions between H<sub>2</sub>C=PH<sub>3</sub> with hypohalous acids HOF, HOCl and HOBr molecules. However the S1–S5 complexes might be considered as the relevant minima for these interactions but our studies also detects the S6–S10 as weak intermolecular complexes which might be formed between ylide and HOX molecules. Stabilization energies calculated for these complexes show that type I interactions are stronger than two other types (Table 1).

**Table 1**  
BSSE, stabilization energy corrected with ZPE, uncorrected stabilization energy, at MP2/6-311++G(2d,2p).

Complex	BSSE (kcal mol <sup>-1</sup> )	SE (corr.) (kcal mol <sup>-1</sup> )	SE (uncorr.) (kcal mol <sup>-1</sup> )
S1	2.77	-16.89	-18.62
S2	3.05	-12.92	-14.61
S3	2.01	-12.91	-14.72
S4	1.97	-12.51	-14.32
S5	1.89	-12.39	-14.30
S6	0.89	-2.42	-3.08
S7	0.89	-2.23	-2.83
S8	0.68	-1.62	-2.14
S9	0.83	-1.87	-2.29
S10	0.70	-1.59	-2.13

**Table 2**  
Bond lengths (Å) of PY and [PY...HOX] complexes at MP2/6-311++G(2d,2p) level.

Complex	C=P	P–H <sub>a</sub>	P–H <sub>b</sub>	PY...HOX	H–OX	O–X
CH <sub>2</sub> =PH <sub>3</sub>	1.677	1.426	1.394	–	–	–
S1	1.719	1.407	1.388	2.359	0.966	2.013
S2	1.719	1.407	1.388	2.227	0.967	1.938
S3	1.702	1.414	1.389	1.800	1.013	1.708
S4	1.701	1.415	1.390	1.810	1.010	1.834
S5	1.702	1.414	1.389	1.836	1.010	1.443
S6	1.679	1.425	1.392	2.789	0.966	1.850
S7	1.678	1.425	1.392	2.814	0.966	1.720
S8	1.678	1.425	1.392	2.890	0.967	1.436
S9	1.672	1.443	1.393	2.421	0.966	1.860
S10	1.678	1.425	1.392	3.320	0.967	1.437
Free H-O-X	H-O-F (0.966,1.436),	H-O-Cl (0.965,1.718),	HOBr (0.966,1.848)			

#### 3.1. The HOX...C interactions

In the HOX...C type complexes, HOX as Lewis acid interacts with C atom of PY as Lewis base and leads to X...C (S1, S2) and H...C (S3–S5) type complexes (Fig. 1). The results indicated that the halogen bond is stronger than the hydrogen bond (Table 1). This can be understood with the strength of X...C interaction.

The HOX...C interaction decreases the lp(C) → σ\*(P–H) charge transfer and consequently leads to contraction of P–H bonds. P–H bonds show blue shift with complex formation and amount of this blue shift in the HOX...C type complexes (S1–S5) are greater than other type of adducts (Tables 2 and 3). In the free ylide the lone pair on C atom is partly shared with P atom and leads to a bond order greater than 1 for P–C. But in S1–S5 complexes due to halogen and hydrogen bond interaction this lone pair mainly located on the C atom and less shared with the P atom, thus as a result the P–C bond in S1–S5 complexes are longer than free PY. This also has been confirmed by increasing the occupancy of nonbonding orbital on the C atom (0.1643–0.0144e) in S1–S5 complexes relative to the free H<sub>2</sub>C=PH<sub>3</sub>, Tables 5 and S1.

##### 3.1.1. The X...C interactions

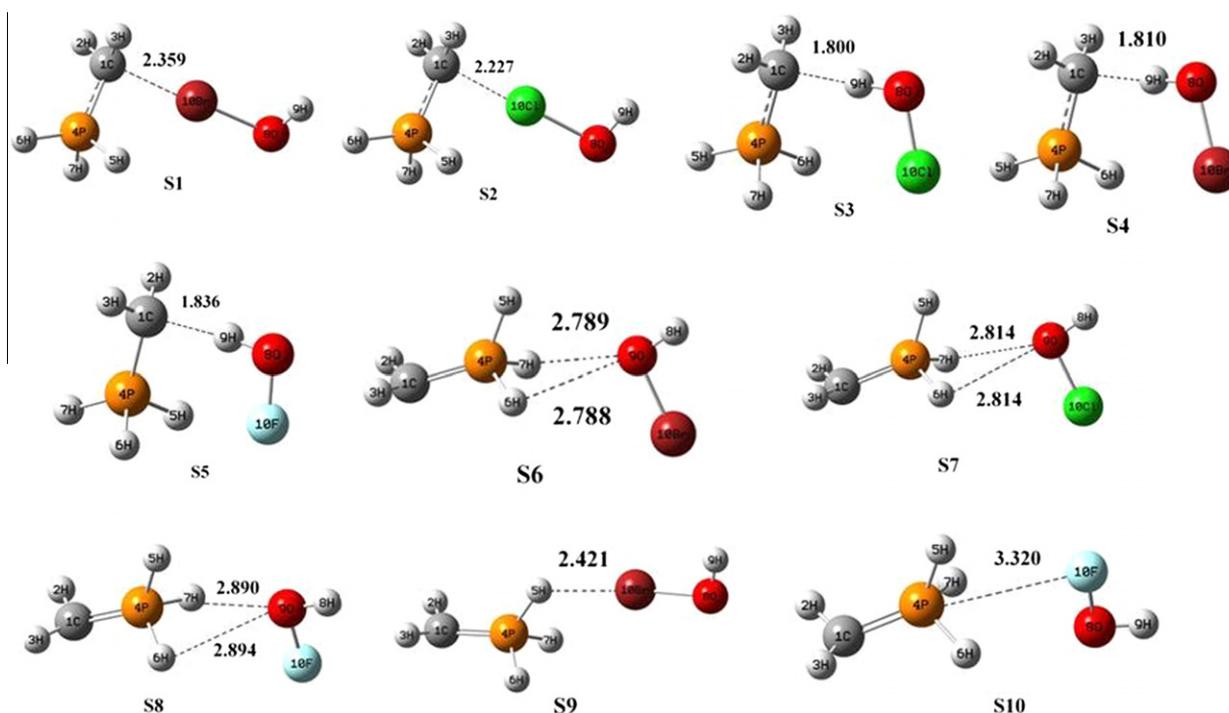
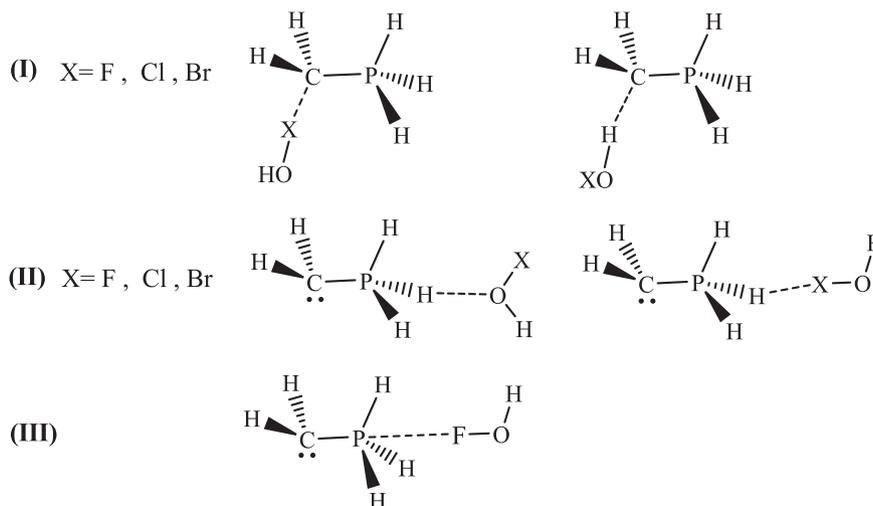
In these interactions, two complexes S1 and S2 have been obtained. The NBO analysis shows that Natural Population Analysis (NPA) charges of the Cl and Br atoms in monomers are positive (NPA charge: 0.216 and 0.305 respectively), see Table S1. On the other hand, C atom of ylide has negative charge, NPA charge -1.215, thus both molecules can interact through halogen bonding and the S1 complex is more stable than S2 (Table 1). The acceptor capacity of σ\* increases for halogens going down the periodic table, F < Cl < Br < I. This effect is attributed to the lower energy of the σ\* orbitals with the heavier elements.

The X...C bond lengths of S1 and S2 complexes are 2.359 and 2.227, respectively (Table 2). In halogen bonded complexes S1 and S2, the NBO analysis shows charge transfer from lp(C) to σ\*(O–X), which leads to elongation of the O–Br and O–Cl bonds (0.165 and 0.22, respectively). Also their stretching frequencies show red shift (200 and 308 cm<sup>-1</sup>) upon complex formation (Table 3). The X...C interaction is along with shortening of P–H bonds, so that these bonds in S1 and S2 complexes are shorter than corresponding bond in the free ylide molecule, in agreement with bond length contractions, P–H bonds show blue shift upon X...C interaction. The blue shift of P–H<sub>a</sub> (160–165 cm<sup>-1</sup>) is more significant than P–H<sub>b,c</sub> (49–54 cm<sup>-1</sup>) (Table 3). Also, data given in Table 2 shows that shortening of P–H<sub>a</sub> (0.019 Å) is more considerable than P–H<sub>b,c</sub> (0.006 Å).

According to previous studies direct contribution in HB is not necessary for blue shift of C–H bonds [25]. Since PH bonds did not participate directly in an H-bond in S1 and S2, thus their blue shifts and contractions are frequently the result of an electronic

**Table 3**Unscaled vibrational frequencies ( $\text{cm}^{-1}$ ) with corresponding intensities (values given in parenthesis,  $\text{km mol}^{-1}$ ) of  $[\text{PY} \cdots \text{HOX}]$  complexes at MP2/6-311++G(2d,2p) level.

Compound	$\nu_{\text{C}=\text{P}}$	$\nu_{\text{PHb}}$	$\nu_{\text{P}-\text{Ha}}$	$\nu_{\text{PY} \cdots \text{HX}}$	$\nu_{\text{H}-\text{OX}}$	$\nu_{\text{O}-\text{X}}$
$\text{CH}_2=\text{PH}_3$	962(48)	2521(44), 2539(26)	2260(318)	–	–	–
S1	896(31)	2570(7), 2590(1)	2420(184)	295(250)	3798(76)	427(175)
S2	898(31)	2572(9), 2593(1)	2425(169)	330(208)	3784(72)	423(335)
S3	920(37)	2556(14), 2574(7)	2363(249)	268(29)	2877(2003)	743(10)
S4	920(36)	2555(13), 2573(7)	2358(254)	259(28)	2916(1964)	648(13)
S5	921(39)	2558(14), 2575(8)	2367(224)	277(35)	2948(1702)	961(5)
S6	960(66)	2531(46), 2551(20)	2264(302)	–	3795(94)	626(15)
S7	961(63)	2531(44), 2551(20)	2263(309)	–	3797(89)	727(11)
S8	961(59)	2532(39), 2551(20)	2261(319)	–	3789(59)	952(1)
S9	971(45)	2528(25), 2549(13)	2113(1404)	–	3795(130)	592(123)
S10	960(58)	2532(39), 2552(21)	2265(300)	–	3789(61)	953(1)
Free H–O–X	H–O–F 3798(48), 954(1), H–O–Cl 3805(83), 731(11), H–O–Br 3799(92), 627(14)					

**Fig. 1.** Schematic representation of  $\text{PY} \cdots \text{HOX}$  complexes optimized at MP2/6-311++G(2d,2p).**Scheme 1.** The possible models for interaction of  $\text{CH}_2=\text{PH}_3$  with  $\text{HOX}$  molecules.



**Table 6**  
Topological parameters for [PY...HOX] complexes at MP2/6-311++G(2d,2p).

	bcp	$\rho$	$\nabla^2$	-Gc	Vc	-Gc/Vc	Hc
S1	C...Br	0.0638	0.0841	0.0352	0.0494	0.7130	0.0142
S2	C...Cl	0.0749	0.0913	0.0427	0.0625	0.6824	0.0199
S3	C...H	0.0494	0.0472	0.0249	0.0379	0.6556	0.0131
S4	C...H	0.0480	0.0490	0.0244	0.0366	0.6674	0.0122
S5	C...H	0.0465	0.0504	0.0238	0.0349	0.6802	0.0112
S6	O...H	0.0051	0.0305	0.0065	0.0054	1.2031	-0.0011
	O...H	0.0075	0.0305	0.0065	0.0054	1.2032	-0.0011
S7	O...H	0.0069	0.0288	0.0061	0.0050	1.2211	-0.0011
	O...H	0.0069	0.0289	0.0061	0.0050	1.2217	-0.0011
S8	O...H	0.0055	0.0249	0.0051	0.0039	1.2822	-0.0011
	O...H	0.0055	0.0253	0.0052	0.0040	1.2868	-0.0011
S9	Br...H	0.0196	0.0522	0.0129	0.0129	1.0039	-0.0002
S10	F...P	0.0049	0.0252	0.0051	0.0038	1.3266	-0.0013

P—H<sub>a</sub>. It was found that the O atom to be a better electron donor than the X atom in HOX.

### 3.2.1. The O...H type complexes

The O...H type complexes return to the  $lp(O) \rightarrow \sigma^*(P-H)$  charge transfer. Interaction of O atom of HOX with P—H<sub>b,c</sub> leads to bifurcated hydrogen bond complexes. The H...O bond distances of S6–S8 complexes are 2.789, 2.814 and 2.890 Å, respectively. Data given in Table 1 shows that stability of these complexes are in the order S6 > S7 > S8. The P—H<sub>a,b,c</sub> bonds in S6–S8 complexes are shorter than corresponding bonds in the free ylide molecule (0.001–0.002), while the P—C bond shows a small lengthening (0.001–0.002). The O—X bond in S8 remained constant but in S6 and S7 indicates a small lengthening (0.002) by H...X interaction (Table 2).

The stretching frequency of O—X and the C—P bonds shows 1–4 cm<sup>-1</sup> red shift. In contrast P—H<sub>b,c</sub> shows blue shift (10–12) in S8

and S9 that is greater than predicted blue shift for P—H<sub>a</sub> (1–4 cm<sup>-1</sup>) in S6–S8 complexes. The red shifts of H—X in S6–S8 complexes are 4, 8 and 9 cm<sup>-1</sup> which are small comparing to P—H<sub>b,c</sub>.

### 3.2.2. The X...H type complexes

The S9 complex was produced from interaction of  $lp(Br) \rightarrow \sigma^*(P-H_a)$ . This interaction causes to elongation of the P—H<sub>a</sub> bond (0.017) and red shift (147 cm<sup>-1</sup>) of its stretching frequency. Also the O—X bond show about 0.012 elongations and its stretching shifted about 35 cm<sup>-1</sup> to lower energies. In contrast, the C—P and P—H<sub>b</sub> bonds have about 9 and 10 cm<sup>-1</sup> blue shift with complex formation (Tables 2 and 3).

### 3.3. The X...P interaction

In the base of NBO analysis in free HOF the F atom bear negative charge (-0.192e) and the P atom of ylide positive charge (1.077e). Presence of these situations in free molecules makes conditions favorable for appearing the novel F...P weak interaction. Therefore, in the P...F type complex, the F atom of HOF as electron donor interacts with P atom of PY as electron acceptor and leads to S10 complex.

The P...F bond distances of S10 complex is 3.320 Å. This P...F interactions didn't have a considerable effect on previous H—C, C—P and P—H bonds in the PY molecule. Also the H—O and O—X bonds length remained unchanged after complex formation. The red shifts of H—O and O—X in S10 complex with respect to the free H—O—X molecule is negligible.

## 4. AIM analysis

The atom in molecules (AIM) theory [23] is applied here to analyze the characteristics of the intermolecular critical points (BCP)

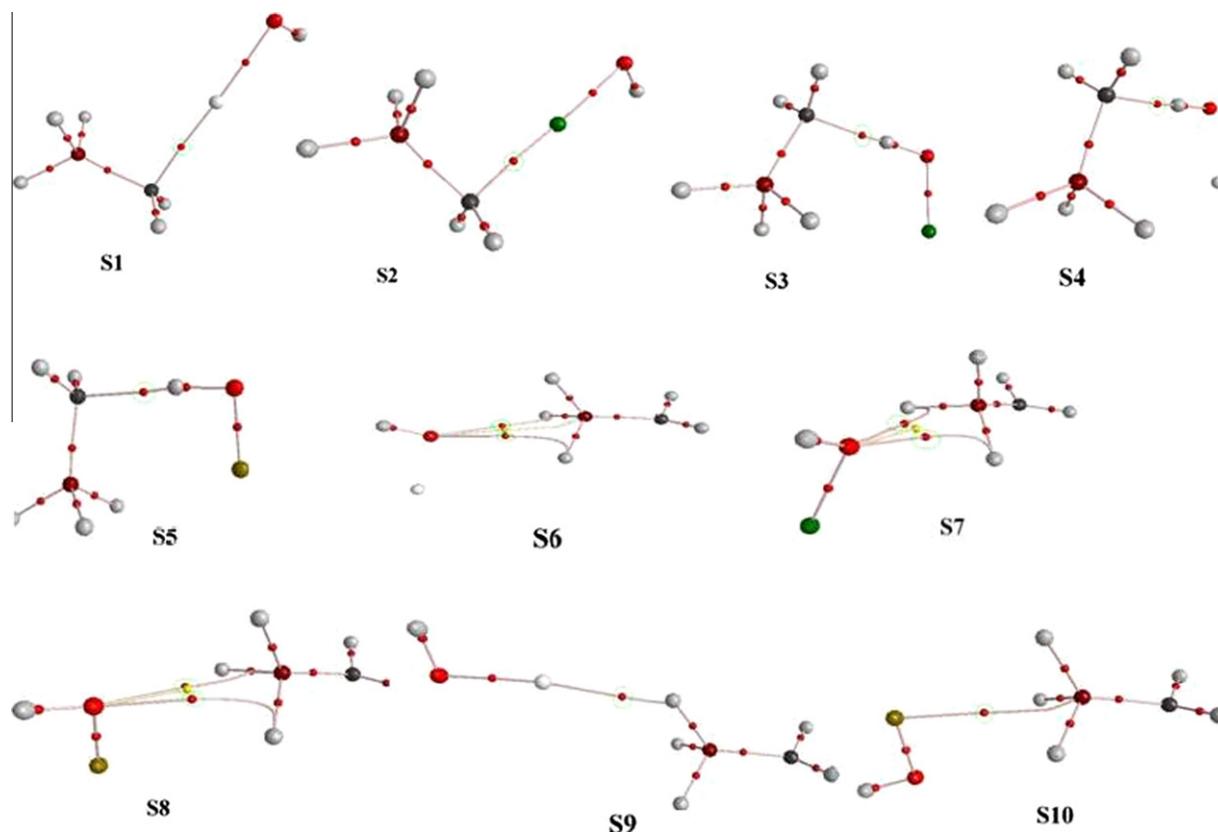


Fig. 2. Molecular graphs of PY...HOX complexes at MP2/6-311++G(2d,2p).

in studied complexes. The parameters ( $\rho$  the electronic density,  $\nabla^2_{\rho_{BCP}}$  is Laplacian of electron density at BCP and  $H_C$  is the electron density at BCP and is the sum of the kinetic electron energy density ( $G_C$ ) and the potential electron density ( $V_C$ ),  $H_C = G_C + V_C$ ) derived from the Bader theory also indicate the type of interaction. The negative value of the Laplacian of the electron density at BCP ( $\nabla^2_{\rho_{BCP}} < 0$ ) designates the concentration of the electron charge in the region between the nuclei of the interacting atoms and is typical of covalent bonds-shared interactions. In the case of the  $\nabla^2_{\rho_{BCP}} > 0$ , there is a depletion of the electron charge between atoms, indicating that there is an interaction of closed-shell systems like ions, van der Waals interactions, or H-bonds. Hence one can see that the Bader theory arbitrarily provides the characteristics of BCPs based on whether the interaction is covalent in nature. For a negative value of a Laplacian, there is no doubt about its covalency (from the AIM theory point of view). When  $H_C < 0$ , we have an H-bond or van der Waals interaction while  $H_C > 0$  returns to bonds with covalent in character.

The molecular graphs and values of topological parameters for each intermolecular BCPs of complexes are given in Table 6 and Fig. 2. The H...C type complexes S1–S5 have  $\nabla^2_{\rho_{BCP}} > 0$ ,  $-G_C/V_C < 1$  and  $H_C > 0$  thus they could be considered as interactions with partially covalent character in their natures. On the other hand, the rest of complexes, S6–S10, have  $\nabla^2_{\rho_{BCP}} > 0$ ,  $-G_C/V_C > 1$  and  $H_C < 0$  and they are interactions with noncovalent character in their nature.

Topological parameters  $\rho$  and  $\nabla^2_{\rho_{BCP}}$ , also describe the stability of complexes through the identification of charge density centers within the intermolecular bonds. Considering the results of the topological analysis presented in Table 6 a good agreement could be found between the values of the electronic density ( $\rho$ ) and stabilization energy (SE) of HB complexes. Except to S1 and S9 (contain Br...C and Br...H interactions) that AIM2000 did not support the Br atom, in the other cases the electronic density for intermolecular BCPs confirms the trend obtained for SE of optimized complexes.

## 5. Natural bond orbital analysis

Natural bond orbital (NBO) analysis [24] was performed for the minima found on the studied HOX–PY complexes, to derive conclusions about the direction and magnitude of the charge-transfer (CT) interactions. The results from this analysis at HF/6-311++G(2d,2p)//MP2/6-311++G(2d,2p) level of theory for the minima on the corresponding PESs are summarized in Table 5.

These complex formations are associated with an orbital interaction between the lone pairs in the electron donor and the antibonding orbital in the electron acceptor. The NBO analysis stresses the role of intermolecular orbital interaction in the complex, particularly charge transfer, the second-order perturbation energy ( $E^{(2)}$ ) can be taken as an index to judge the strength of intermolecular bonds.

Table 5 lists the quantity of charge transferred from donor to the acceptor qCT and the second-order perturbation energy ( $E^{(2)}$ ) due to the interaction of donor and acceptor orbital.  $E^{(2)}$  allow us to quantitatively evaluate the charge transfer involving the formation of the HOX–PY complexes. In general, qCT and  $E^{(2)}$  of type (I) interactions are greater than other types. In this type, the X...C complexes (S1 and S2) has greater qCT and  $E^{(2)}$  than H...C complexes (S3–S5). On the other hand, for the H...C complexes

(S3–S5) the qCT and  $E^{(2)}$  decrease in the order: C...H–OF, C...H–OCl and C...H–OBr. For the O...H complexes (S6–S8) qCT and  $E^{(2)}$  of HOBr are greater than HOCl and HOF. The S10 has the least  $E^{(2)}$  between these complexes.

From the results given in Tables 1 and 5, one can conclude that there is a positive relationship among the interaction energies SE, the second-order perturbation energy lowering  $E^{(2)}$  and the charge transfer qCT in the studied systems.

## 6. Concluding remarks

The phosphorous ylide could interact with HOX molecules. The different patterns including non-classical hydrogen bond H...C, halogen bond X...C, classical hydrogen bonds H...X and H...O, and F...P interactions were found for complex formation between phosphorous ylide and hypohalous acids molecules. From these models, the X...C type complexes are more stable than other types. Good correlations have been found between the interaction energies SE, the second-order perturbation energy  $E^{(2)}$  and the charge transfer qCT in the studied systems.

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