

## The Interaction Strength, Frequency-shifts and Covalence of the $C_2H_4O \cdots HOCl$ and $C_2H_5N \cdots HOCl$ Heterocyclic Complexes

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Article history: Received: 11 November 2016; revised: 10 January 2017; accepted: 03 April 2017. Available online: 01 June 2017. DOI: <http://dx.doi.org/10.17807/orbital.v9i2.853>

**Abstract:** A theoretical study of the structural parameters, electronic properties and vibration modes of the  $C_2H_4O \cdots HOCl$  and  $C_2H_5N \cdots HOCl$  complexes. The great particularity of these complexes is the O–Cl  $\sigma$ -hole, which is considered a proton donor center due to the depletion of charge density along the bonding axis. The examination of the interaction strength complexes was conducted through the intermolecular length, interaction energy and charge transference. The red shifts in the stretch frequencies of the H–O and O–Cl bonds as well as the identification of the new vibration modes were also presented. Regarding the hybrid orbitals, the contributions of the *s* and *p* orbitals were used to value the red shifts in the H–O and O–Cl bonds. The covalence of the O $\cdots$ H and N $\cdots$ H hydrogen bonds was also examined.

**Keywords:** heterorings; hydrogen bonds; infrared; QTAIM; NBO

### 1. INTRODUCTION

The chemistry of small ring compounds is often recognized as a cornerstone of heterocyclic chemistry [1-2]. A wide range of properties of the heterocyclic compounds, such as the importance and application in biological processes [3], the development of polymer materials [4] as well as in the optimization of new bioactive sources to treat several diseases [5] were unveiled by research groups all over the world. In a specific point, the capability of the heterocyclic compounds to form intermolecular interactions also has been evaluated [6-8]. The recent historical background of the contemporary chemistry defines the hydrogen bond as the most important intermolecular interaction [9-11]. In terms of heterocyclic compounds, the properties of hydrogen bonding have been useful to ascribe insights about the stabilization of small rings, of which, the oxirane ( $C_2H_4O$ ) and aziridine ( $C_2H_5N$ ) are some of them [12-15].

To form these intermolecular systems, usually the standard proton donor is the hydrogen fluoride, resulting in the formation of the  $C_2H_4O \cdots HF$  and  $C_2H_5N \cdots HF$  complexes [16]. On the other hand, some works have highlighted the particularity of the proton

donor centers [17]. Besides the lone-electron pairs of halogen ( $X = Cl$  or  $F$ ), the  $HOX$  hypohalous acids [18-20] have been studied upon the formation of hydrogen-bonded complexes and other intermolecular bound systems [21], although the O–X bonds reveal the existence of a acid center, namely as  $\sigma$ -hole [22-23]. In view of this, the possibility to study hydrogen complexes formed by  $C_2H_4O$  or  $C_2H_5N$  and  $HOCl$  is the main goal of this current research, wherein the comparison between the molecular parameters of both  $C_2H_4O \cdots HOCl$  and  $C_2H_5N \cdots HOCl$  with similar systems already documented must be worthwhile. Of course, the amphoteric character of the hypochlorous acid will not be evaluated, but in addition to forming hydrogen bonds, the influence of the  $\sigma$ -hole in the O–Cl bond should be taken into account.

The selection of the theoretical approach used for hydrogen bond studies is one of the most important tasks because the intermolecular phenomenology can be poorly described whether the level of theory is inappropriate or even inaccurate. The most accurate studies of intermolecular properties for model systems often leads to the many-body perturbation theory [24], in particular, the use of second-order Møller–Plesset (MP2). It is by the reliability of the results obtained that MP2 is routinely

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applied. On the basis of the well-known intermolecular scope, some reports highlighted more efficient results obtained via Density Functional Theory (DFT) [25-26] calculations rather than MP2 [27-28]. In view of this, the B3LYP hybrid functional was chosen to be used in this current work. In line with DFT [29], the Bader's Quantum Theory of Atoms in Molecules (QTAIM) [30] was also included in our protocol of calculations. The orbital contributions of both s and p to form the chemical bond can be determined at light of the Natural Bond Orbital (NBO) [31]. However, the variations of these orbitals may be more useful, e.g., to the interpretation of some observable events, such as the frequency shifts in the bonds of the proton donors.

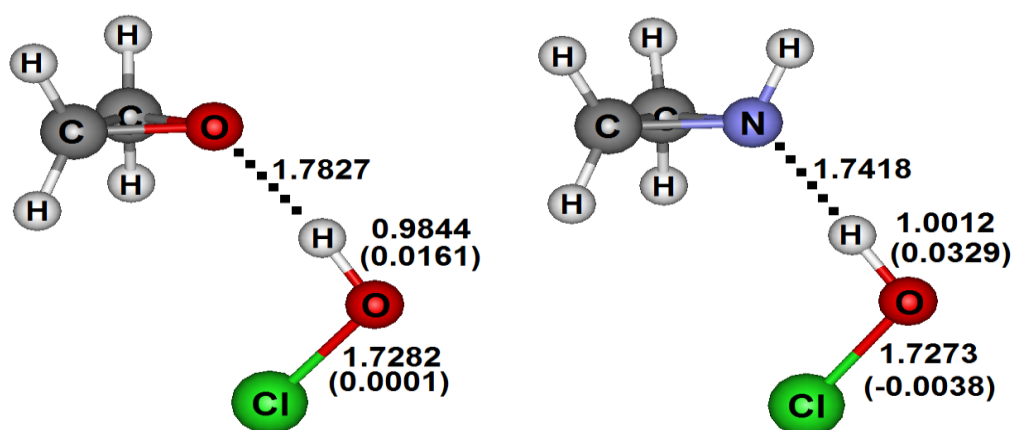
## 2. COMPUTATIONAL PROCEDURE AND DETAILS

The geometries of the  $C_2H_4O \cdots HOCl$  and  $C_2H_5N \cdots HOCl$  complexes were optimized at the B3LYP/6-311++G(d,p) theory level with all calculations performed through the GAUSSIAN 03W software [32]. The values of the hydrogen bond energies were corrected by the Zero-Point vibrational Energy (ZPE) [33] as well as by the Basis Sets Superposition Error (BSSE) [34], whose results were

determined at light of the Boys and Bernardi's Counterpoise procedure [35]. Moreover, the NBO [36] calculations were also developed by GAUSSIAN 03W at the B3LYP/6-311++G(d,p) theory level, but the QTAIM integrations were computed through the AIMAll 11.05.16 [37] quantum package.

## 3. RESULTS AND DISCUSSION

The optimized geometries of the  $C_2H_4O \cdots HOCl$  and  $C_2H_5N \cdots HOCl$  complexes are presented in Figure 1, in which are pictured the values of bond lengths (variations in parentheses) of the hydrogen bonds, H–O and O–Cl  $\sigma$ -hole. The hydrogen bond lengths of 1.7827 and 1.7418 Å indicate a more intense interaction in  $C_2H_5N \cdots HOCl$ , what corroborates fully with the  $C_2H_5N \cdots HF$  complex in which hydrogen fluoride is the proton donor. Therefore, the H–O bond length of  $C_2H_5N \cdots HOCl$  undergoes a drastic variation almost twice as large in comparison with the value of  $C_2H_4O \cdots HOCl$  complex. In opposition to these systematic tendencies, the H–O and O–Cl  $\sigma$ -hole are distinctly affected. Note that, besides the increase and reduction of 0.0001 and -0.0038 Å respectively, the second one is really a notable variation because the O–Cl bond in  $C_2H_4O \cdots HOCl$  is slightly perturbed.



**Figure 1.** Optimize geometries of the  $C_2H_4O \cdots HOCl$  and  $C_2H_5N \cdots HOCl$  complexes.

For the vibrational analysis, the values of stretch frequencies and absorption intensities are listed in Table 1. Initially for the HOCl monomer, it is worthy to announce that the theoretical values of 3776.6  $cm^{-1}$  and 700.8  $km.mol^{-1}$  are satisfactory in agreement with the experimental data [38] of stretch frequency and absorption intensity of 3609  $cm^{-1}$  and

725  $km.mol^{-1}$ , respectively. The largest frequency shifts are manifested in the H–O proton donating center, whose values are -664.1 and -310.2  $cm^{-1}$ . Otherwise, it is clearly perceived that the frequency shifts in the O–Cl  $\sigma$ -hole have identical profiles and are not affected by the interaction strength [36]. Moreover, the absorption intensity ratios of 7.2 and 10.4 are much greater than the values of 0.3 and 0.5.

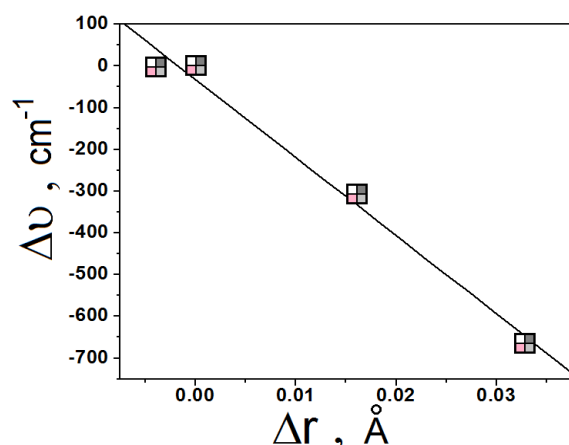
**Table 1.** Infrared vibrational modes.

IR modes	Systems		
	HOCl	C <sub>2</sub> H <sub>4</sub> O...HOCl	C <sub>2</sub> H <sub>5</sub> N...HOCl
$\nu_{\text{H-O}}$	3776.6 (3609) <sup>a</sup>	—	—
$\text{I}_{\text{H-O,m}}$	79.3	—	—
$\nu_{\text{O-Cl}}$	700.8 (725) <sup>a</sup>	—	—
$\text{I}_{\text{O-Cl,m}}$	3.2	—	—
$\Delta\nu_{\text{H-O}}$	—	3466.4 (- 310.2)	3132.5 (- 664.1)
$\text{I}_{\text{H-O,c/IH-O,m}}$	—	875.7 (7.2)	826.4 (10.4)
$\Delta\nu_{\text{O-Cl}}$	—	700.7 (-0.1)	699.0 (-1.8)
$\text{I}_{\text{O-Cl,c/I O-Cl,m}}$	—	1.2 (0.3)	1.6 (0.5)
$\nu_{\text{Y...H}}$	—	215.5	244.0
$\text{I}_{\text{Y...H}}$	—	16.8	15.5

Values of  $\nu$  and  $\text{I}$  are given in  $\text{cm}^{-1}$  and  $\text{km.mol}^{-1}$ , respectively. <sup>a</sup> Ref. [38]

In a direct comparison with the bond length variation, the Figure 2 illustrates a linear relationship with a correlation coefficient ( $r^2$ ) of 0.99:

$$\Delta\nu = -18718.7\Delta r - 32.0, r^2 = 0.99 \quad (1)$$

**Figure 2.** Relationship between the frequency shifts and variations on bond lengths.

The hydrogen bond frequencies, which are commonly named new vibration modes, and its absorption intensities are organized in Table 1. Although the values of the stretch frequencies of 215.5 and 244.0  $\text{cm}^{-1}$  are not closely located in low infrared regions, the absorption values of 16.8 and 15.5  $\text{km.mol}^{-1}$  are small. Actually, the new vibration modes agree totally with the hydrogen bond lengths, wherein the C<sub>2</sub>H<sub>5</sub>N...HOCl complex is more strongly stabilized than C<sub>2</sub>H<sub>4</sub>O...HOCl. However, in order to unveil the intermolecular stability more critically in details, in Table 2 are listed the values of the hydrogen bond energies and NBO charge transfers.

**Table 2.** Hydrogen bond energies and charge transfers of the C<sub>2</sub>H<sub>4</sub>O...HOCl and C<sub>2</sub>H<sub>5</sub>N...HOCl complexes.

Parameters	Complexes	
	C <sub>2</sub> H <sub>4</sub> O...HOCl	C <sub>2</sub> H <sub>5</sub> N...HOCl
$\Delta E$	-34.75	-51.03
$\Delta ZPE$	6.97	7.66
BSSE	4.29	5.27
$\Delta E^C$	-23.49	-38.10
$\Delta Q^{\text{NBO}}$	-0.028	-0.059

Values of  $\Delta E$ ,  $\Delta ZPE$ , BSSE and  $\Delta E^C$  are given in  $\text{kJ.mol}^{-1}$ ; Values of  $\Delta Q^{\text{NBO}}$  are given in electronic unites (e.u.).

Regardless, the BSSE corrections are smaller than the  $\Delta ZPE$  ones. In comparison with the C<sub>2</sub>H<sub>5</sub>N...HOF system [39], whose value of BSSE is 1.4  $\text{kJ.mol}^{-1}$ , the current BSSE values (Table 2) contribute much more significantly to correct the hydrogen bond energies. Ideally, the corrected values of the hydrogen bond energies and charge transfers summarize the stronger interaction profile of the C<sub>2</sub>H<sub>5</sub>N...HOCl complex. The QTAIM analysis and its topological parameters are organized in Table 3.

**Table 3.** QTAIM topological parameters of the C<sub>2</sub>H<sub>4</sub>O...HOCl and C<sub>2</sub>H<sub>5</sub>N...HOCl complexes.

BCPs	Hydrogen complexes	
	C <sub>2</sub> H <sub>4</sub> O...HOCl	C <sub>2</sub> H <sub>5</sub> N...HOCl
$\rho_{\text{H-O}}$	0.3425	0.3234
$\nabla^2\rho_{\text{H-O}}$	-2.4048	-2.1950
$U_{\text{H-O}}$	-0.7333	-0.6879
$G_{\text{H-O}}$	0.0660	0.0696
$-G/U_{\text{H-O}}$	0.0900	0.1011
$\rho_{\text{O-Cl}}$	0.1871	0.1874
$\nabla^2\rho_{\text{O-Cl}}$	-0.0261	-0.0241
$U_{\text{O-Cl}}$	-0.0261	-0.2103
$G_{\text{O-Cl}}$	0.1017	0.1021
$-G/U_{\text{O-Cl}}$	0.4842	0.4855
$\rho_{\text{Y...H}}$	0.0357	0.0487
$\nabla^2\rho_{\text{Y...H}}$	0.1215	0.1051
$U_{\text{Y...H}}$	-0.0308	-0.0430
$G_{\text{Y...H}}$	0.0306	0.0347
$-G/U_{\text{Y...H}}$	0.9935	0.8069

Values of  $\rho$  and  $\nabla^2\rho$  are given in  $\text{e.a}_0^{-3}$  and  $\text{e.a}_0^{-5}$ , respectively; Values of  $U$  and  $G$  are given in electronic unites.

Confirming the initial expectation, the H-O bonds are shared interactions due to the negative values of the Laplacian. Relatively, the electronic densities of these bonds attain the higher values. Surely, this profile is typical of covalent bonds, and as such, not only the H-O bonds, but the O-Cl  $\sigma$ -hole is also recognized as such. Regarding the covalent character, which can be total or partial, the ratio between the kinetic and potential electronic energies

reveals interesting insights in this regard [40]. As is well known, the interaction is identified as partially covalent whether the value of  $-G/U$  is ranged between 0.5 and 1.0, whereas the ratios greater than 1.0 are non-covalent [41-42]. In addition, values of  $-G/U$  smaller than 0.5 indicate that the interaction are totally covalent. As can be perceived, the H–O bond is also fully covalent, whereas the O–Cl  $\sigma$ -holes are in threshold of covalence with  $-G/U$  values of 0.4842 and 0.4855 for the  $C_2H_4O\cdots HOCl$  and  $C_2H_5N\cdots HOCl$  complexes, respectively. Even almost partially covalent, this trend agrees with the  $\sigma$ -hole feature because a depletion of charge density must weakens the O–F and O–Cl bonds. About the hydrogen bonds, the values of electronic density are smaller followed by the positive values of Laplacian, by which, it would be attributed a non-covalent character. However, the  $-G/U$  ratios of 0.9935 and 0.8069 attest that the hydrogen bonds of the  $C_2H_4O\cdots HOCl$  and  $C_2H_5N\cdots HOCl$  are partially covalent. By taking into the account the hydrogen bond lengths, whose average values is 1.7, in fact these complexes are strongly bound.

In Table 4 are listed the values of the NBO parameters, namely: percentage of the  $s$ - and  $p$ -hybrid orbitals of the H–O, O–F and O–Cl bonds. The benchmark of these hybridizations is the interpretation with justification of the frequency shifts in the proton donors. Because red shifts were the infrared effects identified in these bonds, the variations of the  $s$ - and  $p$ -orbitals should provide insights in this regard. According to the values listed in Table 4, the reductions of -5.41 and -6.93 % of the  $p$ -orbital for oxygen praise the weakening of the H–O bond, what agrees with the red shifts [41]. The other hybridizations have not significant contributions to access any interpretation to the slight red-shifts in the O–Cl  $\sigma$ -hole, and thereby, they have no influence in the interaction strength of the  $C_2H_4O\cdots HOCl$  and  $C_2H_5N\cdots HOCl$  complexes.

**Table 4.** Hybridization values.

Hybridization	Systems		
	HOCl	$C_2H_4O\cdots HOCl$	$C_2H_5N\cdots HOCl$
$s_{H-O}$	99.85	99.81 (0.00)	99.80 (-0.05)
$p_{H-O}$	0.15	0.19 (0.00)	0.20 (0.05)
$s_{O-H-O}$	21.98	26.22 (5.43)	28.93 (6.95)
$p_{O-H-O}$	77.90	73.67 (-5.41)	70.97 (-6.93)
$s_{O-Cl}$	9.83	9.04 (1.56)	8.86 (-0.97)
$p_{O-Cl}$	90.04	90.83 (-1.49)	91.02 (0.98)
$s_{Cl-O-Cl}$	6.62	7.02 (-1.39)	7.21 (0.59)
$p_{Cl-O-Cl}$	92.40	92.05 (0.57)	91.87 (-0.53)

All values are given in %.

#### 4. CONCLUSION

The theoretical study of the properties of the  $C_2H_4O\cdots HOCl$  and  $C_2H_5N\cdots HOCl$  complexes revealed interesting systematic tendencies. Firstly, it is worthy to be mentioned the stronger interaction of the  $C_2H_5N\cdots HOCl$  complex, wherein culminated with shorter hydrogen bond lengths, higher stretch frequencies and larger red shift in the H–O bond. In this context, the participation of the O–Cl  $\sigma$ -hole is shy upon complexation of both  $C_2H_4O\cdots HOCl$  and  $C_2H_5N\cdots HOCl$ , i.e., slight variations of bond lengths and stretch frequencies. Nevertheless, the partial covalent characters of the O $\cdots$ H and N $\cdots$ H hydrogen bonds were unveiled through the QTAIM protocol wherein the electronic kinetic energy is outweighed by the potential. The NBO calculations testified the most impressive red shifts are manifested in the H–O bonds due to the most drastic variations in the  $p$ -orbital of the oxygen.

#### 5. ACKNOWLEDGMENTS

FAPESB and CAPES

#### 6. REFERENCES AND NOTES

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