



Existence and characterization of HOO–HOOH radical-molecule complexes: A computational study

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ARTICLE INFO

Article history:

Received 14 May 2009

Received in revised form 12 June 2009

Accepted 9 July 2009

Available online 15 July 2009

ABSTRACT

Ab initio calculations at the UMP2/6-311++G(2d,2p) and CCSD(T) levels are used to analyze the interactions in complexes pairing the hydroperoxyl radical (HOO) with dihydrogen trioxide (HOOH). The structures obtained are analyzed by the Atoms in Molecules (AIM) and Natural Bond Orbital (NBO) methodologies. Six minima were located on the potential energy surface, with stabilization energies in the range between 12 and 26 kJ mol⁻¹. Red shifts of OH bonds in HOO and HOOH moieties upon complex formation lie in the ranges between 90–330 cm⁻¹ and 90–270 cm⁻¹, respectively.

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1. Introduction

Hydrogen bonding is the strongest noncovalent intermolecular interaction and governs many chemical and biological processes in nature [1–3]. Due to this importance, many theoretical and experimental studies have been carried out to characterize the nature of the hydrogen bond. Most of the investigations carried out refer to hydrogen-bonded complexes formed between a pair of neutral molecules or between a neutral molecule and an ion. However, in recent years there has been increased interest in the study of radical-molecule hydrogen-bonded complexes, because of their importance in the chemistry of the atmosphere [4–16] and in biological [17–20] systems as well. They have been shown to play an important role in the kinetic behavior of many atmospheric reactions, but additionally, they can contribute to the spread of contamination through the atmosphere or to formation of aerosols [5,16].

The hydroperoxyl OOH radical participates in numerous oxidation reactions [21]. Its interaction with various molecules influences the stabilization of newly formed hot radicals and may affect their reactivity. One of the more intriguing areas of radical-molecule complex studies arises from the discovery of the formation of surprisingly stable OOH complexes [22]. A number of systems combining OOH with H₂O [23], CH₃OH [24], H₂O₂ [25], HNO₃ [26], H₂SO₄ [11], HC(O)OH [27], RC(O)OH (R=H, CH₃, CF₃) [12], HOC(O)OH [28], HOOCHO [29], RC(O)NH₂ (R=H, CH₃, NH₂) [30], SO₃ [31], (CH₃)₂O [32], CH₃X (X = F, Cl, Br) [33], aliphatic amines [34], NH₃ [35], HF [36], HCl [37], and O₃ [38] have been reported in the literature.

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The existence of dihydrogen trioxide (HOOH) has been confirmed in recent years [39–42]. Giguère et al. first reported IR and Raman spectroscopic evidence for the involvement of HOOH in electrically dissociated mixture of water, hydrogen peroxide and oxygen [43]. Bielski and Schwartz provided the first UV spectroscopic evidence for the existence of HOOH in solution [44]. Finally, the ground-state geometry of HOOH was reported by Fourier transform microwave (FTMW) spectroscopy and FTMWmm-wave double resonance and triple resonance spectroscopy [42]. In the gas phase, dihydrogen trioxide is a zigzag skew-chain structure with C₂ symmetry in that both HOOO dihedral angles are equal and opposite. Very recently, dihydrogen trioxide clusters, (HOOH)_n (n = 2–4), and the hydrogen-bonded complexes of HOOH with acetone and dimethyl ether have been investigated using DFT (B3LYP/6-311++G(3df,3pd)) and MP2/6-311++G(3df,3pd) methods [45].

Despite the potential importance of hydroperoxyl radical and dihydrogen trioxide in atmospheric chemistry, there is available in the literature neither theoretical nor experimental study of complexes pairing them together. In the absence of experimental information, a theoretical analysis of the potential existence of such complexes and their properties is in order. This complex is of fundamental interest not only in that it pairs a radical with a neutral, but also that it is a highly oxygen-enriched system which presents a multitude of H-bonding options. Analysis will permit a careful comparison of the H-bonding capabilities of O in various bonding situations, both with and without an unpaired electron. Moreover, the HOO–HOOH system represents a natural extension of earlier work with HOO–HOH [46], enabling the extraction of information as to just how the extra O atom affects the interaction. The present work reports for the first time a detailed examination of the stabilities, electronic structure, and vibrational frequencies of HOO–HOOH complexes.

2. Computational details

Calculations were performed using the Gaussian 03 system of codes [47]. The geometries of the isolated HOO and HOOOH species and their dimer complexes were fully optimized at the UMP2/6-311++G(2d,2p) [48] and M05-2x/6-311++G(2d,2p) [49] computational levels. Harmonic vibrational frequency calculations confirmed the structures as minima and enabled the evaluation of vibrational frequencies. The counterpoise (CP) procedure [50], was used to correct this quantity for basis set superposition error (BSSE). Additional calculations were carried out at the CCSD(T) level, using a cc-pVTZ basis set.

The Atoms in Molecules (AIM) methodology [51] was used to analyze the electron density of the systems considered at the UMP2/6-311++G(2d,2p) computational level. The topological analysis was carried out with the AIM 2000 program [52]. The Natural Energy Decomposition Analysis (NEDA) [53,54] within the Natural Bond Orbital methodology [55] have been performed to obtain insight of the source of the interaction energy. This methodology divides the interaction energy in several attractive components as orbital charge transfer that arises from the delocalization of electron from one monomer to the other, electrostatic interaction of the monomers, polarization and exchange-correlation terms. Finally, a repulsive component is considered which takes into account the electronic deformation due to the complex formation in each monomer. These calculations have been performed at the M05-2x/6-311++G(2d,2p) computational level with the NBO-5G [56] on the GAMESS program [57].

3. Results and discussion

The HOOOH molecule can occur in two different conformations. In the *trans* conformer, the two hydrogen atoms lie in opposite directions with identical $\varphi(\text{HOOO})$ dihedral angles of $+80.3^\circ$. In the *cis* conformer, the two H atoms lie in the same direction with HOOO dihedral angles $+94.4^\circ$ and -94.4° . The more stable conformer is the *trans* which is lower in energy by some 11 kJ mol^{-1} at the MP2/6-311++G(2d,2p) computational level. Each of these two configurations can form a complex with the HOO radical, in several different structures. Three minima, designated S1, S2 and S4, were identified for the *trans* HOOOH conformer, and are illustrated in Fig. 1. The *cis* conformer also coupled with HOO in three different minima (S3, S5, and S6). The numbering refers to relative stabilities as described below.

Most minima may be categorized as cyclic in that each contains a pair of H-bonds connecting the two molecules. The binding energies of these complexes are reported in Table 1. Binding energies of the HOO–HOOOH dimers, including zero-point vibrational and BSSE corrections, lie in the range of $12\text{--}26 \text{ kJ mol}^{-1}$ at UMP2/6-311++G(2d,2p) computational level. M05-2x/6-311++G(2d,2p) calculations provide similar results to the uncorrected interaction energies at the UMP2 level. The high level of agreement between this variant of DFT (M05-2x) and MP2 conforms with our recent study concerning HNO clusters [58] in which MP2 and M05-2x stabilization energies were also found to be quite similar. Additional calculations were carried out using the CCSD(T) method to consider electron correlation, with a cc-pVTZ basis set, and the

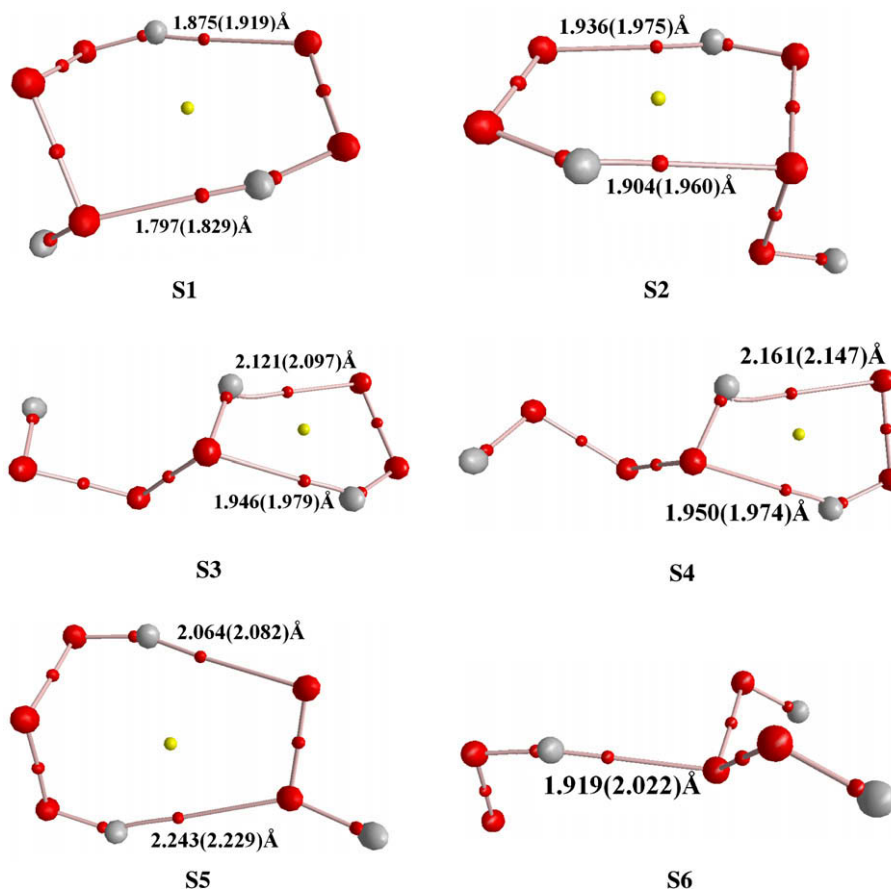


Fig. 1. Molecular graph of the dimer minima obtained at the UMP2/6-311++G(2d,2p) computational level. The red and yellow dots represent the position of the bond and ring critical points, respectively. The interatomic distances (Å) of those atoms that shows intermolecular interactions calculated at M05-2x/6-311++G(2d,2p) are shown in parenthesis.

Table 1
Interaction energies of HOO–HOOH complexes (kJ mol^{-1}).

| Complex | UMP2/6-311++G(2d,2p) | | | | M05-2x/6-311++G(2d,2p) | CCSD(T)/cc-pVTZ //UMP2/6-311++G(2d,2p) |
|-----------------|----------------------|------|-----------|-----------------|------------------------|--|
| | EI | BSSE | EI + BSSE | EI + BSSE + ZPE | EI | EI |
| S1 | –46.07 | 9.02 | –37.05 | –26.43 | –45.91 | –49.59 |
| S2 | –40.14 | 8.93 | –31.20 | –21.09 | –40.48 | –42.09 |
| S3 | –33.23 | 6.40 | –26.83 | –17.59 | –35.09 | –35.69 |
| S4 | –30.31 | 6.15 | –24.17 | –15.63 | –32.04 | –32.91 |
| S5 | –26.28 | 5.79 | –20.49 | –12.35 | –27.05 | –28.06 |
| S6 [*] | –25.48 | 6.69 | –18.79 | –12.37 | – | –24.49 |

* There is one imaginary frequency at M05-2x/6-311++G(2d,2p) level.

geometries optimized by the UMP2/6-311++G(2d,2p) procedure. The interaction energies, reported in the last column of Table 1, mimic precisely the order of both the UMP2/6-311++G(2d,2p) and M05-2x/6-311++G(2d,2p) procedures. The CCSD(T) EI interaction energies tend to be slightly more negative than either of the others, possibly reflecting a more complete treatment of correlation.

At any level of theory, S1 is clearly the most strongly bound of the studied complexes, with a binding energy of 37 kJ mol^{-1} after correction of basis set superposition error. The principal intermolecular interaction within the most stable minimum S1 corresponds to a cyclic structure with a pair of OH...O interactions. The hydrogen bonds are both about 1.8 \AA in length. Perhaps more importantly, there is little strain in these bonds, with both $\theta(\text{OH}\cdots\text{O})$ angles within 13° – 23° of linearity. Such linearity has been shown to be an important component in the strength of such H-bonds [2,3,59–61]. The two covalent O–H bonds that are involved in the H-bonds are both stretched, one by nearly 20 m\AA and the other by 17 m\AA (Table 2), with the bond in HOO stretching a bit more than its cousin in HOOOH. Also reported in Table 2 are the frequency shifts of the two O–H covalent bonds, resulting from the complexation. Both shifts are to the red, as normally anticipated for O–H bonds. They are rather large around 300 cm^{-1} , reiterating the strength of these two H-bonds.

All three S1, S2, and S4 complexes containing *trans* HOOOH involve the donation of one HOOOH proton to the terminal O atom of HOO. Where they differ is related to the second H-bond. HOO donates a proton to the terminal O atom of HOOOH in S1, to the central O atom in S2, and to the first O in S4, the O atom that is also the proton donor in the other H-bond. This distinction introduces progressively larger degrees of strain into the H-bonded ring. The two $\theta(\text{OH}\cdots\text{O})$ angles are 6° and 16° further from linearity in S2 as compared to those of S1. The complexation energy in S2 is reduced by 6 kJ mol^{-1} , compared to that of S1. The weaker H-bonds are indicated also by reductions in the O–H covalent bond stretches as shown in Table 2. The corresponding O–H stretching frequency red shifts are consequently also lowered by considerably smaller amounts in S2 as compared to S1. Further reductions are noted in going to S4, particularly the second H-bond, involving HOOOH as donor. The latter observation is not surprising, in that this H-

Table 2
Variation (red shifts) of the OH bond stretching frequencies (cm^{-1}) upon complexation and elongation of the same bond (mÅ) at UMP2/6-311++G(2d,2p) level.

| | $\Delta r(\text{O–H})$ | | $\Delta \nu(\text{O–H})$ | |
|----|------------------------|-------|--------------------------|-------|
| | HOO | HOOOH | HOO | HOOOH |
| S1 | 20 | 17 | –329 | –267 |
| S2 | 10 | 9 | –178 | –165 |
| S3 | 11 | 7 | –186 | –93 |
| S4 | 10 | 7 | –170 | –93 |
| S5 | 8 | 10 | –95 | –137 |
| S6 | 6 | – | –92 | – |

bond appears from Fig. 1 to have a very highly distorted OH...O geometry.

Pairing of the *cis* conformer of HOOOH with HOO leads to formation of S3, S5, and S6 complexes. These three structures are rather distinct from one another. S3 involves a pair of H-bonds, both angularly distorted, in which each molecule serves simultaneously as both proton donor and acceptor. There are also two H-bonds in S5, and both fairly linear. However, HOOOH serves as double donor, and HOO as double acceptor. This sort of arrangement typically involves negative cooperativity so it is not surprising that S5 is less stable than is S3. There is only a single H-bond present in S6, accounting for its comparatively weak binding. S3, the most stable of this set, contains fairly bent H-bonds, the two $\theta(\text{OH}\cdots\text{O})$ angles lie 40° – 60° from linearity. S5 is less stable, despite the near linearity of the two H-bonds, within 20° – 30° . Whereas S6, with its single H-bond, represents a minimum on the MP2 surface, it is a transition state at the DFT level, with a single imaginary frequency.

An earlier set of computations examined complexes pairing HOO with HOH [23,46] and HOOH [25] at the same levels of theory. The binding energy of the global minimum located on the potential energy surface of HOO–HOH, including BSSE corrections, is 39.3 kJ mol^{-1} which is greater than the stability calculated for the global minimum of HOO–HOOOH by only 2.2 kJ mol^{-1} . The global minimum of the HOO–HOOH complex, calculated at UMP2/6-311++G(2d,2p) level, yielded a stability of 35.6 kJ mol^{-1} after correction for BSSE, which is less stable than S1 by roughly 1.5 kJ mol^{-1} . In summary, then, there is little difference in stability between the complexes pairing HOO with HOH, HOOH, and HOO–OH, at least as far as the global minima are concerned.

A topological analysis of the electron density within the Atoms in Molecules (AIM) framework provides a variety of graphs illustrated in Fig. 1. The small yellow sphere indicates that there is a ring critical point for all those structures that contain a pair of H-bonds. The small values of the electron density and the positive values of the Laplacian and total energy density (Table 3) indicate that these intermolecular bonds correspond to weak interactions.

In order to obtain further insights into the source of the interactions the Natural Energy Decomposition Analysis (NEDA) within the NBO methodology was carried out. The data in Table 4 indicate that charge transfer makes the largest contribution to the interaction in all cases, followed thereafter by electrostatic, and then exchange and polarization. It may be noted that this trend is characteristic of NEDA treatments of hydrogen bonded clusters [54]. Note also that each of these terms diminishes in magnitude in the same sequence as does the total interaction energy.

4. Conclusions

There are six minima on the potential energy surface of the OOH + HOOOH dimer. Three of these involve the *cis* and three the *trans* configuration of HOOOH. In four of these structures, the

Table 3

Electron density, Laplacian and total energy density (a.u.) of the intermolecular bond critical points.

| | Interaction | Distance(Å) | ρ_{BCP} | Laplacian | H(r) |
|----|-------------|-------------|--------------|-----------|---------|
| S1 | O...H | 1.797 | 0.034 | 0.107 | 0.0013 |
| | O...H | 1.875 | 0.031 | 0.095 | 0.0011 |
| S2 | O...H | 1.936 | 0.027 | 0.087 | 0.0003 |
| | O...H | 1.904 | 0.028 | 0.093 | 0.0004 |
| S3 | O...H | 2.122 | 0.020 | 0.074 | -0.001 |
| | O...H | 1.946 | 0.027 | 0.091 | 5.4E-5 |
| S4 | O...H | 2.161 | 0.019 | 0.069 | -0.001 |
| | O...H | 1.955 | 0.027 | 0.090 | -7.9E-5 |
| S5 | O...H | 2.243 | 0.011 | 0.045 | -0.0014 |
| | O...H | 2.064 | 0.019 | 0.067 | -0.0009 |
| S6 | O...H | 1.925 | 0.025 | 0.087 | -0.0003 |

Table 4

NEDA components (kJ mol⁻¹) of the interaction energy calculated at the M05-2x/6-311++G(2d,2p) computational level.

| | S1 | S2 | S3 | S4 | S5 | S6 |
|------------------------------|---------|--------|--------|--------|--------|--------|
| Charge transfer | -121.14 | -85.06 | -64.87 | -59.10 | -45.10 | -52.04 |
| Electrostatic | -69.34 | -53.21 | -51.70 | -47.73 | -32.77 | -42.26 |
| Polarization | -35.36 | -25.12 | -20.77 | -20.39 | -15.59 | -24.41 |
| Exchange | -30.93 | -28.55 | -24.70 | -23.57 | -19.10 | -25.12 |
| Total electronic deformation | 212.38 | 154.20 | 128.95 | 120.63 | 87.57 | 112.10 |

OOH radical acts as H-donor and H-acceptor simultaneously. Both molecules act simultaneously as proton donor and acceptor in the most stable dimer. Stabilization energies of studied complexes including BSSE and ZPE are in the range between 12 and 26 kJ mol⁻¹.

Acknowledgment

We would like to acknowledge Prof. Ibon Alkorta for his help in NEDA analysis.

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