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Effect of Copper on 1,1-Diamino-2,2-dinitroethene - A DFT Treatment

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Abstract

Interaction of 1,1-diamino-2,2-dinitroethene which is a well known explosive called FOX-7 and copper atom is investigated computationally in the form of 1:1 composite, at the levels of UB3LYP/6-31++G(d,p) and UB3LYP/LANL2DZ within the restrictions of density functional theory. Some geometrical, spectral and quantum chemical data have been obtained and discussed. The both levels of computational approach yield geometries in accord with each other but LANL2DZ basis set produced unreasonable charges for the atoms of the composite. However, both of the methods indicate that copper atom donates some electron population to the organic component meantime the nitro groups change their conformation by twisting about the C-NO_2 bonds. Thus, the push-pull character of the system varies which should affect some of the explosive properties, beside the others.

1. Introduction

1,1-Diamino-2,2-dinitroethene ($C_2H_4N_4O_4$), *geminal* DADNE, also known as FOX-7 (preferred name in the present study) is commonly expected to be a promising explosive, combining comparatively high performance and low sensitivity. It has a push-pull type structure which is beneficial for the creation of strong inter- and intra-molecular hydrogen bonds for stabilizing the molecule. Since 1998, when FOX-7 was first synthesized by Latypov *et al.* [1], it has been the subject of many experimental investigations [2-15]. FOX-7 has a favorable oxygen balance and its decomposition produces some gaseous products (CO, H_2O, N_2). Also it is far less sensitive to impact

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and shock than RDX (1,3,5-trinitro-1,3,5-triazinane), but its explosive properties are comparable to those of RDX. For these reasons FOX-7 has been accepted as very useful for systems in which insensitivity is more important than maximum performance [16]. A review by Bellamy includes routes for the synthesis of FOX-7, together with its structural, spectroscopic, and explosive properties [17]. Kretschmer *et al.* investigated the chemical stability, sensitivity and mechanical and explosive properties of mixtures of FOX-7 with paraffin, ethylene-propylene rubber (EPM) and the polyacrylate elastomer (Hy Temp) [18]. Interactions of FOX-7 with various elements are found in the literature [19-21].

In the present study, interaction of copper with FOX-7 structure has been investigated quantum chemically in the realm of density functional theory (DFT).

2. Method of Calculation

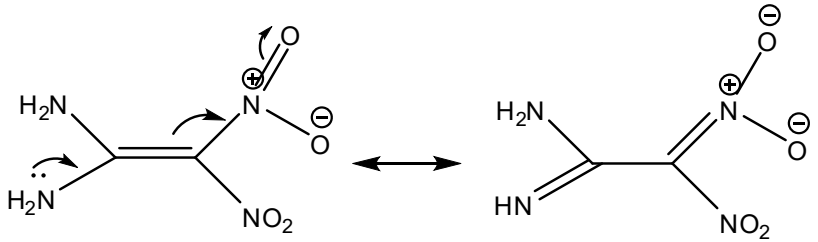
In the present study, the initial structural optimizations of all the structures leading to energy minima have been achieved by using MM2 method followed by semi-empirical PM3 self-consistent fields molecular orbital (SCF MO) method [22, 23] at the restricted level [24, 25]. Subsequent optimizations were achieved at Hartree-Fock level using various basis sets. Then, the structural optimizations were managed within the framework of density functional theory (DFT) [26, 27] at the levels of UB3LYP/6-31++G(d,p) [25, 28] and UB3LYP/LANL2DZ [29] both of which are suitable for copper atom. Note that in the ground state copper atom possesses an unpaired electron thus the calculations have been performed employing the unrestricted methodology. The exchange term of B3LYP consists of hybrid Hartree-Fock and local spin density (LSD) exchange functions with Becke's gradient correlation to LSD exchange [27, 30]. The correlation term of B3LYP consists of the Vosko, Wilk, Nusair (VWN3) local correlation functional [31] and Lee, Yang, Parr (LYP) correlation correction functional [32]. Also, the vibrational analyses have been done. The total electronic energies are corrected for the zero point vibrational energy (ZPE). The normal mode analysis for each structure yielded no imaginary frequencies for the $3N–6$ vibrational degrees of freedom, where N is the number of atoms in the system. This indicates that the structure of each molecule corresponds to at least a local minimum on the potential energy surface. All these calculations were done by using the Spartan 06 package program [33].

3. Results and Discussion

Copper in the field of explosives emerges mainly in the structures of primary explosives as copper salts of certain explosives, such as azides [34]. It has some subsidiary applications in the ammunition compositions or in the construction of shaped charge devices [35]. Interaction of it with explosives, at least with FOX-7 has not been studied yet up to the best knowledge of the author.

In the ground state, copper has $[Ar]3d^{10}4s^1$ electronic configuration. Copper interacts with ammonia to some extent [36, 37].

FOX-7 being a push-pull type structure, the electron density on the amino nitrogens is expected to be low in contrast to density on oxygen atoms of NO_2 groups.



Therefore, more than one site happens to undergo interactions with copper atom, with its empty atomic orbitals or its unshared electron in attractive or repulsive manner.

Figure 1 shows the optimized structures of FOX-7 and the composite considered. It also shows the direction of the dipole moment vectors. FOX-7 molecule is nearly coplanar at the amino side but has inclined at the nitro side having N2C2C1N4 and N1C2C1N3 dihedral angles of 13.16º and 13.19º (see Figure 2 for numbering of the atoms). The same angles in the composite have the values of 2.72º and 5.70º. The O4N4C1C2 and O2N3C1C2 dihedral angles are in FOX-7 are -23.15º and 154.93º, whereas in the composite -42.57º and 174.52º, respectively.

The NH_2-C bond lengths in FOX-7 are 1.34 Å whereas in the composite 1.35 Å and 1.34 Å. The C=C bond in FOX-7 is 1.42 Å but in the composite it is 1.41 Å. The C-NO_2 bond lengths in FOX-7 are 1.43 Å but in the composite 1.40 Å. Therefore the presence of copper atom slightly affects the bond lengths.

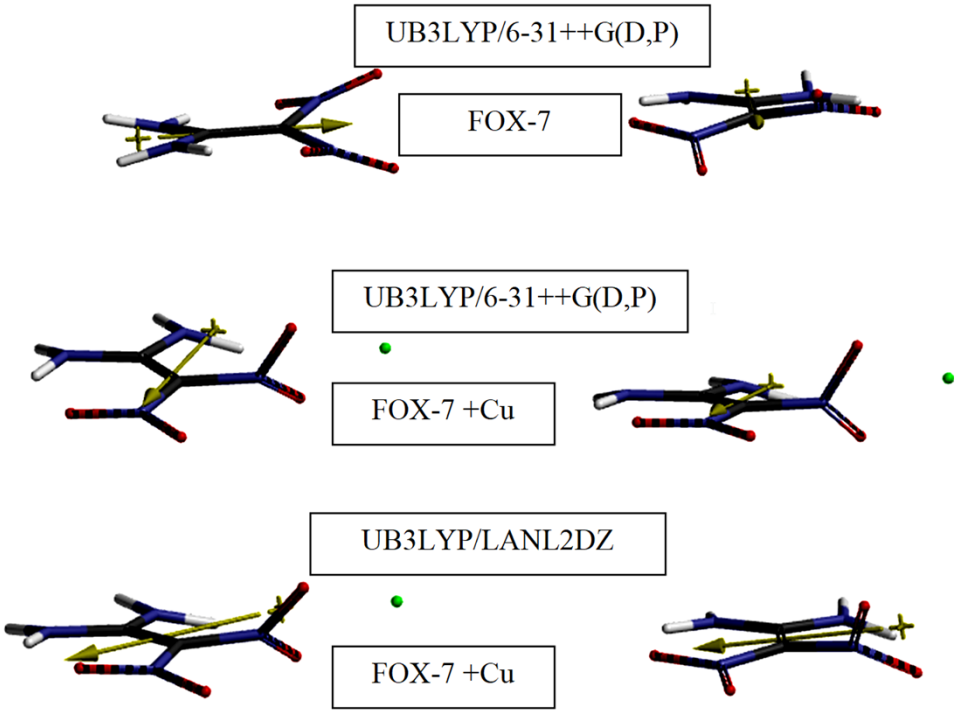


Figure 1. Optimized structures of FOX-7 and the composite considered (from different angles of view).

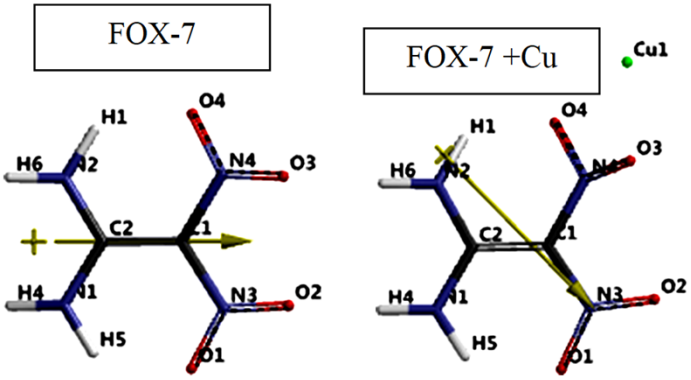


Figure 2. Numbering of the atoms in the structures considered.

Figure 3 shows the electrostatic charges (ESP) on the atoms of FOX-7 and its copper composite. Note that the ESP charges are obtained by the program based on a numerical method that generates charges that reproduce the electrostatic potential field from the entire wavefunction [33].

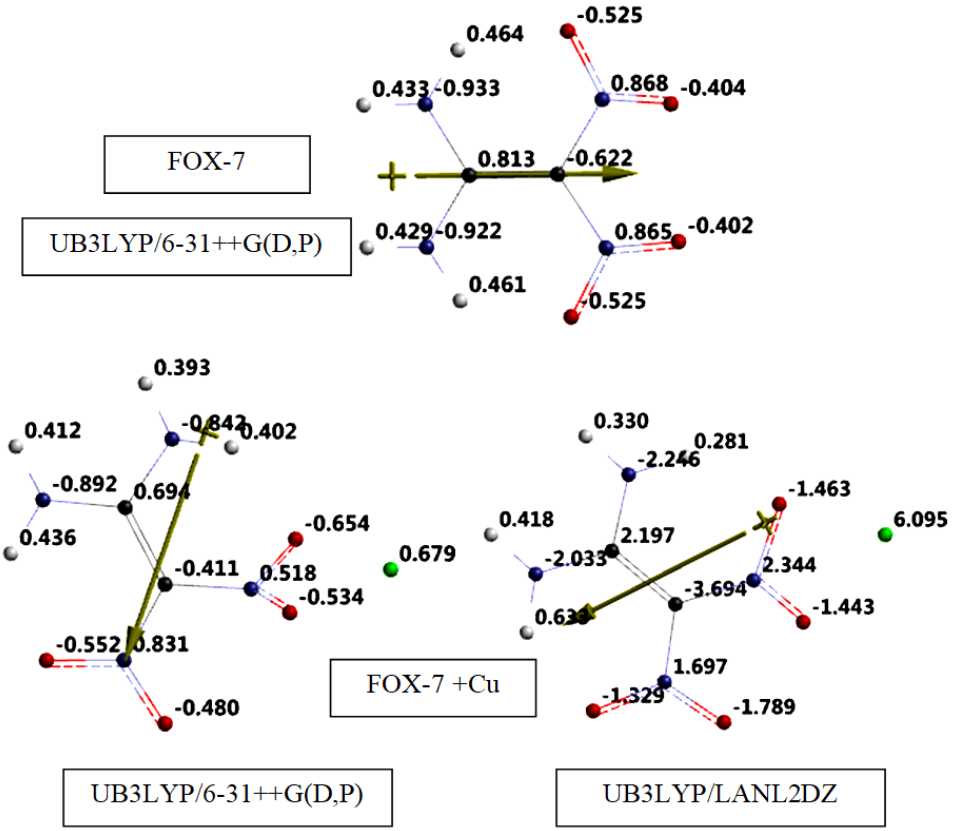


Figure 3. ESP charges on the atoms of FOX-7 and the composite considered.

The UB3LYP/LANL2DZ level of calculation predicts rather unreasonable positive charge development on the copper atom in the composite, so do the charges on the other atoms. The UB3LYP/6-31++G(d,p) level of calculation yields a reasonable positive charge for the copper atom. By comparing the magnitudes of charges on FOX-7 and the composite, one observes that the copper atom transfers some electron population into the organic component so that less amount of charges (absolutely) emerge on the carbon atoms, thus push-pull character of the system is highly affected. The positive charge on N4 has been decreased compared to the charge of the respective atom in FOX-7 whereas the negative charges on O3 and O4 are increased. The dipole moment values (UB3LYP/6-31++G(D,P)) are 8.68 and 8.40 debye, respectively for FOX-7 and FOX-7+Cu. The UB3LYP/LANL2DZ level of calculation on the composite yields the dipole moment as 60.86 debye. One should observe the direction of the dipole moment vectors in the composite case by the two methods of calculations performed.

Figure 4 shows the IR spectra of the species considered (UB3LYP/6-31++G(d,p)). The presence of copper atom affects N-H stretching and bending frequencies as well as C=C and C-NO_2 stretchings. Symmetric and asymmetrical N-H stretchings in FOX-7 occur at 3468 cm^{-1} and 3693 cm^{-1}, respectively. Whereas in the composite they are at 3422 cm^{-1} and 3694 cm^{-1}, respectively. The NH_2 scissoring of FOX-7 occurs at 1645 cm^{-1} whereas at 1663 cm^{-1} in the composite. The C-NH_2 and C-NO_2 stretchings strongly appear in the case of the composite in the range of 1569-1324 cm^{-1}.

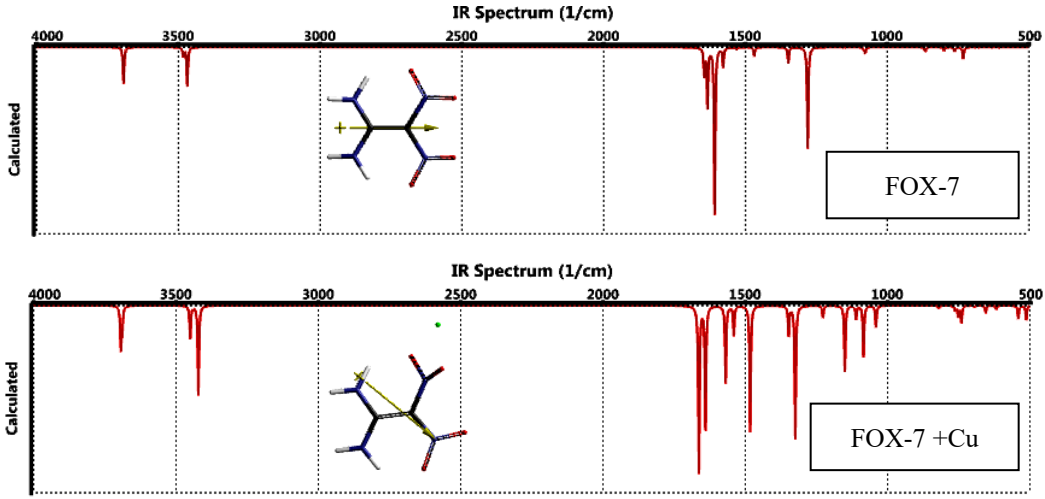


Figure 4. IR spectra of the structures considered (UB3LYP/6-31++G(d,p)).

Figure 5 displays the electrostatic potential maps of FOX-7 and its copper composite

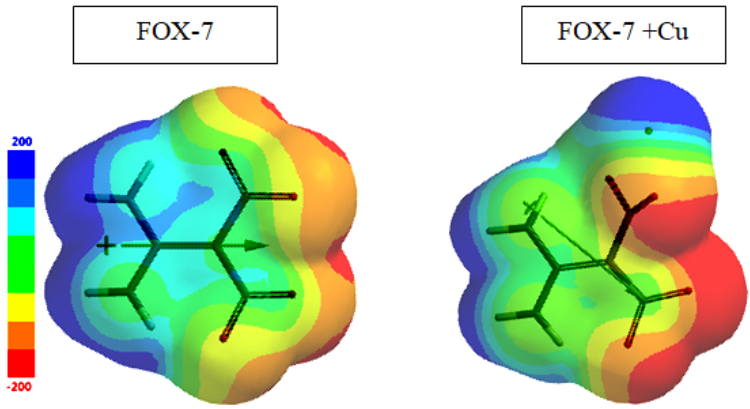


Figure 5. Electrostatic potential maps of the structures considered (UB3LYP/6-31++G(D,P)).

(UB3LYP/6-31++G(d,p)). In the figure red/reddish and blue/ green regions stand for negative and positive potential fields, respectively. The presence of copper atom enhances the negative potential around the NO_2 oxygens as compared to FOX-7 case while decreasing the positive potential around the NH_2 groups. A very pronounced positive potential field exists around the copper atom.

Table 1 shows the HOMO, LUMO energies and the interfrontier molecular orbital energy gap (Δε) values of the structures considered. As seen in the table the incorporation of copper atom in the structure raises up the HOMO and LUMO energy levels of FOX-7. This is usually the case whenever some electron donating group(s) linked to the conjugated system. In the present case the copper atom takes the role of electron donor group. These changes affect the Δε values in the order of FOX-7 > FOX-7+Cu. Since Δε value of an explosive is associated with its sensitivity to impact [38, 39], such that as Δε decreases the impact sensitivity increases, the copper composite of FOX-7 is expected to be more sensitive than the parent explosive. Structurally, NH_2 groups (electron donors) in FOX-7 raise up the HOMO and LUMO energy levels as compared to ethylene case whereas the nitro groups (electron acceptors) lower those energy levels [40, 41]. Normally, twistings of the NO_2 groups about the C-NO_2 bonds decrease the extended conjugation thus those energy levels are expected to be raised in the composite. However, donation of some electron population from the copper atom, in which case it takes the role of an electron donor group, raises up the energies of the frontier molecular orbitals to yield the values shown in Table 1.

Table 1. The HOMO, LUMO energies and Δε values of the structures considered.

Structure	**HOMO**	**LUMO**	**Δε**
FOX-7	-722.34	-276.03	446.31
FOX-7 +Cu	-506.97	-271.66	235.31

Energies in kJ/mol. UB3LYP/6-31++G(d,p) level of calculations.

Tables 2 and 3 show the Mulliken bond orders and lengths in FOX-7 and the composite both calculated at the UB3LYP/6-31++G(d,p) level whereas Table 4 contains Löwdin bond orders and lengths of the composite.

Table 2. Mulliken bond orders of FOX-7.

Bond	Bond order	Length (Å)	Remark
C1 C2	1.404	1.4279	[deloc]
C1 N3	0.790	1.4319	[single]
C1 N4	0.789	1.4322	[single]
C2 N1	1.310	1.345	[deloc]
C2 N2	1.309	1.3451	[deloc]
N1 H4	0.824	1.0083	[sing-H]
N1 H5	0.727	1.0173	[sing-H]
H5 O1	0.081	1.8074	[Hbond]
N2 H1	0.727	1.0171	[sing-H]
N2 H6	0.824	1.0083	[sing-H]
H1 O4	0.081	1.8069	[Hbond]
N3 O1	1.807	1.2573	[double]
N3 O2	2.145	1.2252	[double]
N4 O3	2.144	1.2252	[double]
N4 O4	1.807	1.2571	[double]

UB3LYP/6-31++G(d,p) level of calculations. Refer Figure 2 for numbering of the atoms.

Comparison of the data in the tables indicates some changes in the bond orders and bond lengths. The data in Table 4 shows that some interactions, almost equal, take place between the copper atom and the nearby oxygen atoms of the NO_2 group.

Table 3. Mulliken bond orders of the composite.

Bond	Bond order	Length (Å)	Remark
C1 C2	1.435	1.4104	[deloc]
C1 N3	0.905	1.4041	[single]
C1 N4	0.525	1.4054	[single]
C2 N1	1.281	1.3464	[deloc]
C2 N2	1.270	1.3541	[deloc]
N1 H4	0.822	1.008	[sing-H]
N1 H5	0.725	1.0192	[sing-H]
H5 O1	0.084	1.8373	[Hbond]
N2 H1	0.742	1.0203	[sing-H]
N2 H6	0.815	1.0077	[sing-H]
H1 O4	0.102	1.8582	[Hbond]
N3 O1	1.818	1.2645	[double]
N3 O2	2.149	1.2355	[double]
N4 O3	1.396	1.3225	[deloc]
N4 O4	0.982	1.3501	[single]
N4 Cu	1.127	2.3144	[single]

UB3LYP/6-31++G(d,p) level of calculations. Refer Figure 2 for numbering of the atoms.

Table 3 shows the Löwdin bond orders and lengths in the composite.

Table 4. Löwdin bond orders of the composite.

Bond	Bond order	Length (Å)	Remark
C1 C2	1.236	1.4104	[single]
C1 N3	1.135	1.4041	[single]
C1 N4	1.075	1.4054	[single]
C2 N1	1.442	1.3464	[deloc]
C2 H4	0.052	2.0516	[Hbond]
C2 N2	1.407	1.3541	[deloc]
N1 H4	0.891	1.008	[sing-H]
N1 H5	0.833	1.0192	[sing-H]
H5 O1	0.087	1.8373	[Hbond]
N2 H1	0.835	1.0203	[sing-H]
N2 H6	0.896	1.0077	[sing-H]
H1 O4	0.079	1.8582	[Hbond]
N3 O1	1.797	1.2645	[double]
N3 O2	1.924	1.2355	[double]
N4 O3	1.529	1.3225	[deloc]
N4 O4	1.436	1.3501	[deloc]
O3 Cu	0.551	1.9529	[single]
O4 Cu	0.545	1.9713	[single

UB3LYP/6-31++G(d,p) level of calculations. Refer Figure 2 for numbering of the atoms.

Figure 6 shows some of the molecular orbital energies of FOX-7 and the composite. Since copper atom has an unpaired electron in its ground electronic state, the composite has α- and β-orbitals. In the figure those orbitals are designated as a- and b-orbitals. As seen in the figure UB3LYP/6-31++G(D,P) level of calculations yield almost nearly degenerate α- and β-HOMOs (also LUMO energy levels) for the composite. As for the

UB3LYP/LANL2DZ level of calculations, the frontier molecular orbital energy levels are to be noticed that they have positive energy values and the HOMO-LUMO energy differences (either α- or β-type) are about 1eV.

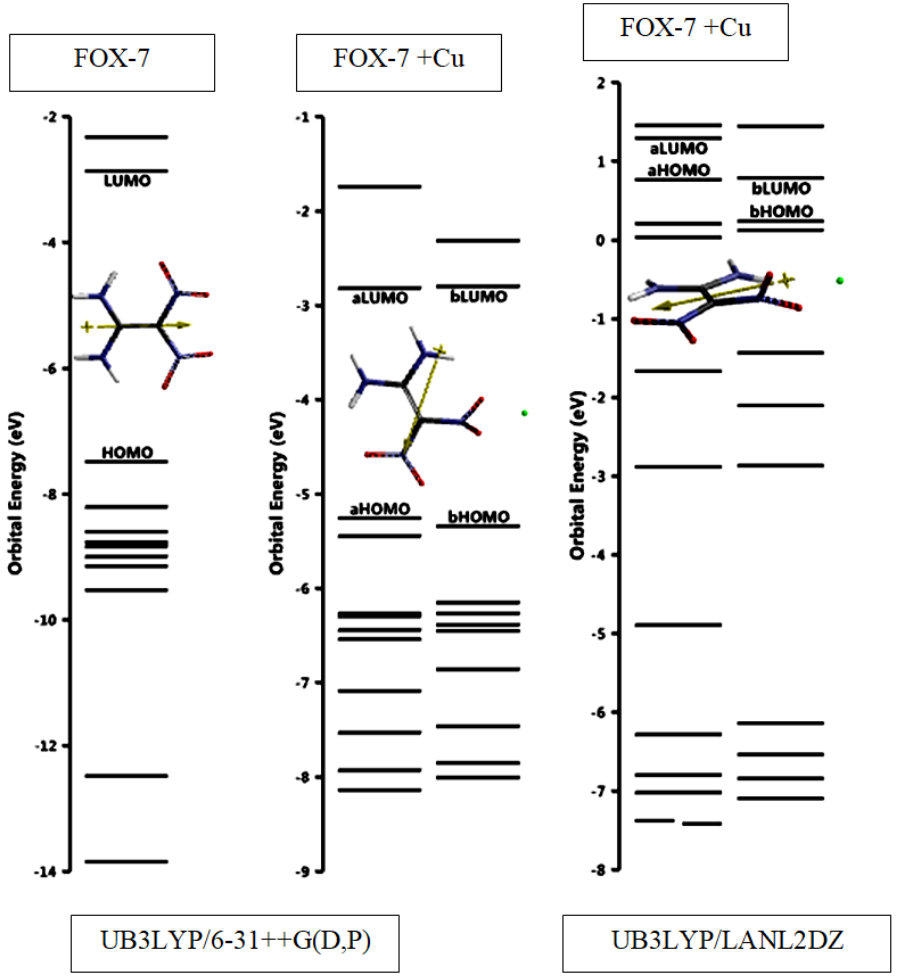


Figure 6. Some of the molecular orbital energies of FOX-7 and the composite.

Figures 7 and 8 show the HOMO and LUMO patterns of FOX-7 and the composite (UB3LYP/6-31++G(D,P)), respectively. In the case of FOX-7 the frontier molecular orbitals exhibit some sort of π-symmetry. In the composite case, α- and β-HOMO exhibit different patterns. In each case some contribution from d-atomic orbitals of the copper atom is discernable. On the other hand, α- and β-LUMO show the same pattern. Note that they are (almost) degenerate (see Figure 6).

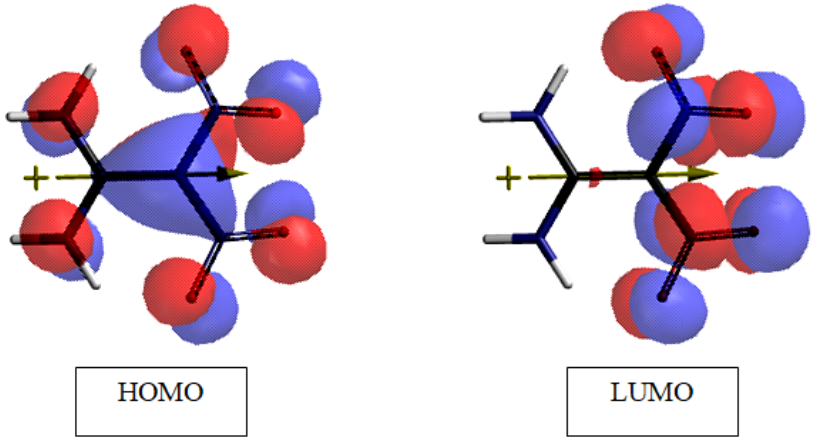


Figure 7. The HOMO and LUMO patterns of FOX-7 (UB3LYP/6-31++G(D,P)).

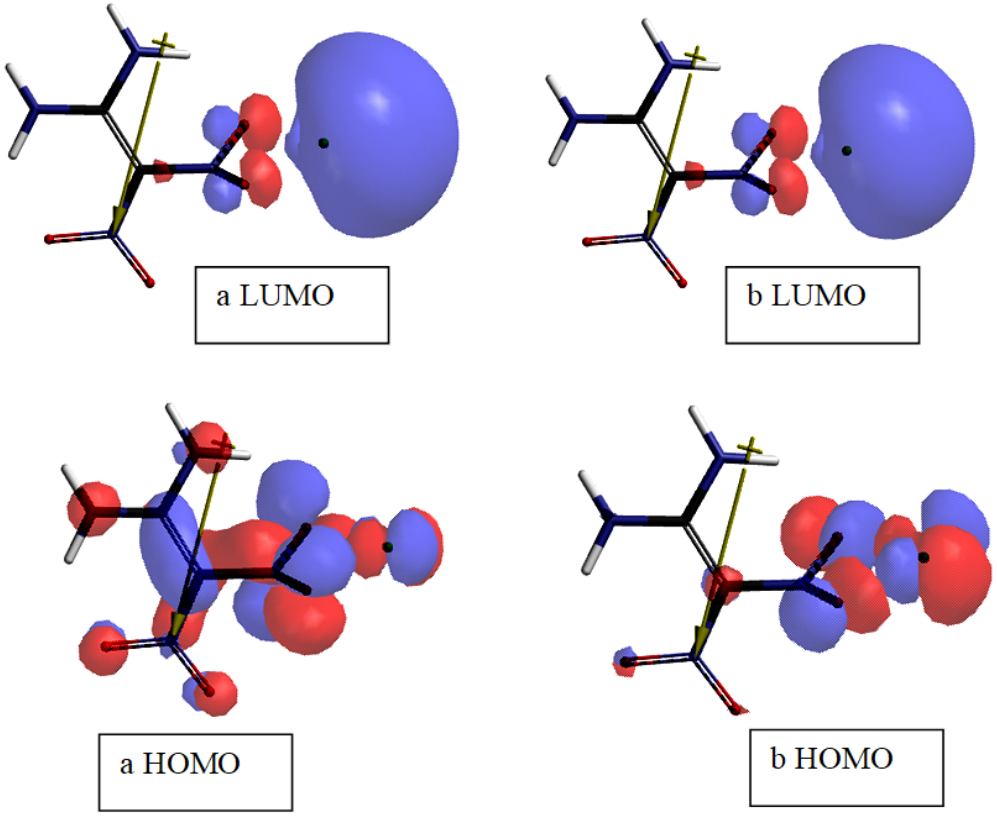


Figure 8. The HOMO and LUMO patterns of the composite (UB3LYP/6-31++G(d,p)).

Figure 9 shows the local ionization maps of the structures considered. In a local ionization potential map conventionally red regions on the density surface indicate areas from which electron removal is relatively easy, meaning that they are subject to electrophilic attack.

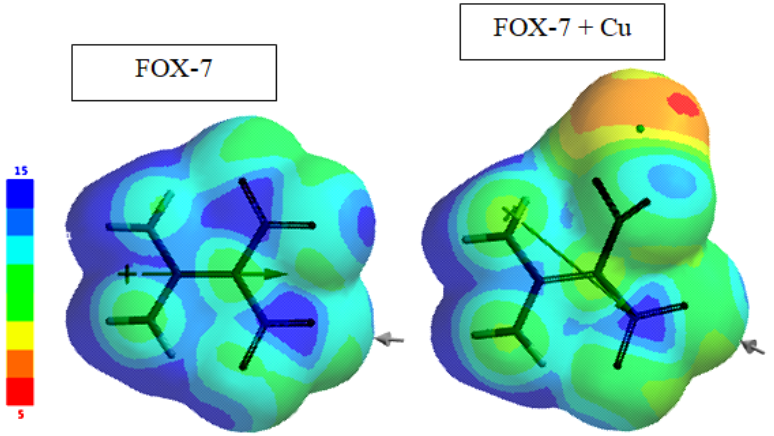


Figure 9. The local ionization maps of the structures considered **(**UB3LYP/6-31++G(d,p)).

Comparison of FOX-7 and the composite local ionization maps reveals that the electron population donated by the copper atom is widely distributed over the organic component of the composite. Therefore, blue/bluish regions of FOX-7 turn into greenish.

Figure 10 shows the spin density map of the composite which indicates the distribution of the unpaired electron over the system.

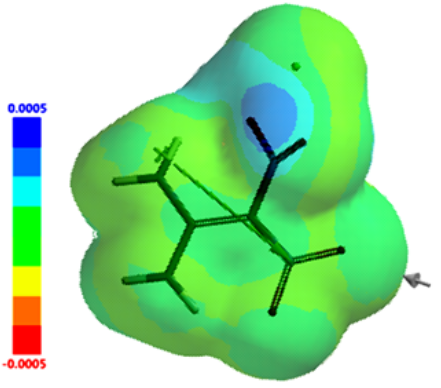


Figure 10. Spin density map of the composite **(**UB3LYP/6-31++G(d,p)).

4. Conclusion

The effect of copper atom on FOX-7 has been investigated within the constraints of DFT. Two different basis sets were employed using the UB3LYP functional. Both of the basis sets predicted the similar geometries. The FOX-7 structure/bonding remained intact in the composite but some conformational changes occurred in the C-NO_2 bonds in such a way that the HOMO-LUMO energy gap decreased compared to FOX-7 case. This outcome is not only due to the indicated conformational changes but also because of the copper atom which donates some electron population to the organic component. All those changes occurring in the composite with respect to FOX-7 should affect ballistic properties as well, such as the impact sensitivity.

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