Theoretical Study of the Laplacian of the Spin Density in Metal Complexes.

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Components α and β of charge density $\rho(r)$ (equation 1), define spin density, $\rho_S(r)$, as the difference between total charge density of α electrons and total charge density of β electrons (equation 2).

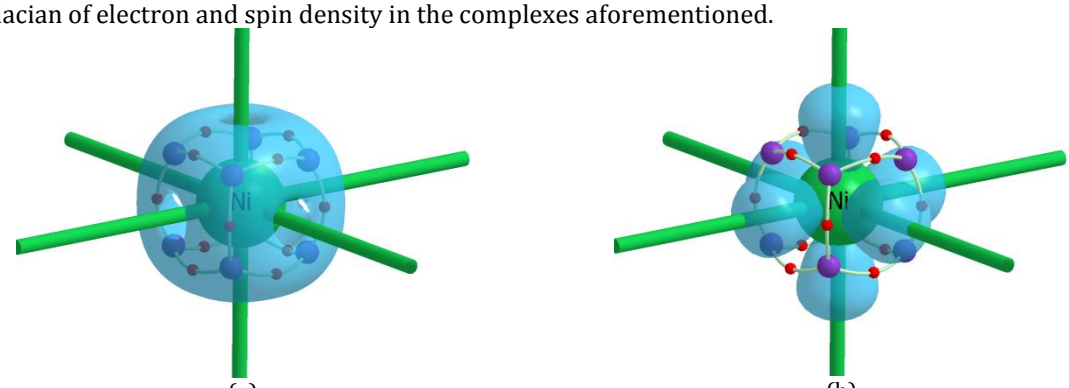
$$\rho(r) = \rho_\alpha(r) + \rho_\beta(r) \quad (1)$$
$$\rho_S(r) = \rho_\alpha(r) - \rho_\beta(r) \quad (2)$$

Using the Laplacian operator in the charge and spin density and separating again in the components α and β, we have the equations (3) and (4)

$$\nabla^2\rho(r) = \nabla^2\rho_\alpha(r) + \nabla^2\rho_\beta(r) \quad (3)$$
$$\nabla^2\rho_S(r) = \nabla^2\rho_\alpha(r) - \nabla^2\rho_\beta(r) \quad (4)$$

The Laplacian of electron and spin density are a scalar field with the property of locating where the density is locally concentrated, negative values, and locally depleted, positive values. The arrangement of charge concentration (CC) and charge depletion (CD) in metal complexes provides physical support to model donor-acceptor with the CC of ligands in direction to CD of metals.[1] From the topological perspective, the critical points (CP) occur where $\nabla^2\rho(r)=0$. A local maximum in $\nabla^2\rho(r)$, a (3,-3) and (3,+1) critical points will denote a local concentration in electronic charge and a local minimum in $\nabla^2\rho(r)$, (3,+1) and (3,+3) critical points will denote a local depletion in electronic charge.[2] A special case of Euler relationship, V-E+F=2, relates the elements of the $\nabla^2\rho(r)$ graph where the vertices (V) correspond to the (3,-3) CPs, the edges (E) to the (3,-1) CPs, and the faces (F) to the (3,+1) CPs. Each $\nabla^2\rho(r)$ graph is characterized by the set [V,E,F] when the relationship is satisfied.[3]

The principal aim of this job is a topological analysis of the Laplacian of electron density in the complexes $M[tpen]^{2+}$ and $M[(H_2O)_6]^{m+}$, where M are atoms of the first raw of "d" block with different charges m+ and the corresponding multiplicity. We found periodical trends in the behavior of the Laplacian of electron and spin density in the complexes aforementioned.



(a) (b)

Figure 1. (a) $\nabla^2\rho(r)$ and (b) $\nabla^2\rho_S(r)$ of $Ni[(H_2O)_6]^{2+}$, Multiplicity: 3, Molecular graph of $\nabla^2\rho(r)$ [8,12,6].

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