

EXCHANGE INTERACTION IN DIMER METALLOORGANIC MAGNETICS IN THE BROKEN SYMMETRY APPROXIMATION

Sheka E.F., Zayets V.A.

Russian Peoples' Friendship University, Moscow

Sheka E.F.
Zayets V.A.
¹Russian Peoples'
Friendship University

Transition metal atoms embedded into organic molecular structures are source of odd, or magnetic, electrons which do not participate in the covalent interatomic bonding. Forming a set of weakly bound spins, the atoms provide magnetic properties of the substances. Theoretical description of the phenomenon concerns the interaction between the odd electrons leading to superexchange characterized by exchange integral J . The paper presents results of the integral determination for two dimer complexes, containing either two cobalt or two nickel atoms surrounded by amidine ligands [1]. J values were calculated in the broken symmetry approximation [2] by using semiempirical quantum-chemical technique NDDO-WF [3] implemented in the program CLUSTER-Z2 [4]. The integrals J are determined as [2]

$$J = \frac{E_{S=0}^{UHF} - E_{S_{max}}^{UHF}}{S_{max}^2}, \quad \text{where } E_{S=0}^{UHF} \quad \text{and} \quad E_{S_{max}}^{UHF}$$

are the complex energies in the broken symmetry singlet state and in the state with the highest multiplicity $2S_{max}+1$ related to spin $S_{max}=n$. The number of non-paired odd electrons in the complexes $2n$ constitutes 4 and 6 for the nickel and cobalt species, respectively. The calculations have been performed for the complex structures determined by X-ray measurements [1]. The obtained J values are of +0.146 (Ni complex) and -1.269 kcal/mol (Co complex). A weak ferromagnetic exchange in the first case and rather big antiferromagnetic exchange in the second undoubtedly point out to the difference in magnetic properties of the studied complexes. Shown as well, changing in the ligand structure, say, optimization of the hydrogen atom positions, results in considerable changing of the obtained values.

Литература

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