

for silver atoms. Accuracy of QTAIM analysis was checked by keeping the integral of Laplacian for each atomic basin below 10^{-4} au that demonstrates a weak bond connects two silver nuclei which is in the normal range of metal-metal bonds in binuclear complexes.

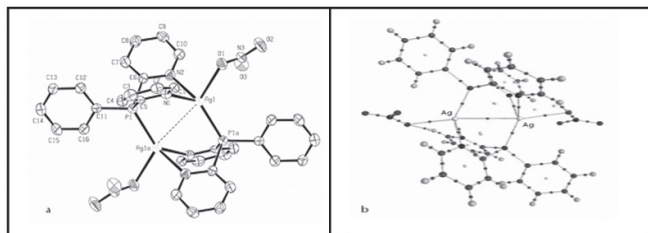


Figure 1. a) ORTEP view b) Molecular graph of synthesized complex

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Keywords: binuclear Ag (I) complex, metal-metal interaction, QTAIM analysis

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Structures, thermal behaviors and magnetic properties of two fumarato-bridged lanthanides

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$\{[Ln_2(C_4H_2O_4)_3(H_2O)_4] \cdot 3H_2O\}_n$ with $Ln=Ho^{3+}$; Gd^{3+} , are two isostructural coordination polymers belonging to $P2_1/n$ space group, which have been prepared *via* two different synthetic routes, and structurally studied at room temperature^[1] and 100 K, respectively. Single crystal structures reveal that the materials are 3D frameworks built up from corrugated layers containing noncentrosymmetric double oxo-bridged binuclear entities. In the extended network, the basic building block corresponds to the bi-polyhedra sharing one edge $Ln_2O_{12}(H_2O)_4$. Each metal is nine-coordinate and surrounded by the same number of ligands. Two independent ligands are pentadentate, in a *syn-anti* conformation, acting as bridging-chelating, and moreover, one is carboxylato-bridging and the other a chelate. The third ligand is tetradentate, in a *syn-syn* conformation, and involves its two terminal groups respectively in a chelate and a conventional carboxylate-bridge.

ATG/ATD analyses show that the dehydrated solids $[Ln_2(C_4H_2O_4)_3(H_2O)_4]$ nor $[Ln_2(C_4H_2O_4)_3]$ cannot be obtained, all the water molecules being released at the same time. This behavior indicates the great effect of the lattice water upon the crystallinity, and the role of the strong H-bonds among the coordinated and uncoordinated water molecules, in coordination polymer's stability. After dehydration, the decomposition process involves intermediate compounds as Ho acrylate^[2] and complex Gd oxide respectively. Variable-temperature magnetic measurements in the range (0-300) K, obey the Curie-Weiss law, and reveal the occurrence of very weak antiferromagnetic coupling between the lanthanide ions. In the light of the XRD structures, the possible exchange pathways could be responsible for the magnetic coupling through $\mu-1,1$ and $\mu-1,3$ bridges within the binuclear entity, or

across the backbone of the ligand. However, the shorter Ln-Ln distances are observed through μ bridges (4.143(2) Å and 4.113(2) Å for Gd and Ho compound respectively). In the resulting modeling of the magnetic data, although J values are negative, they are very small if compared to other lanthanide coordination polymers containing binuclear entities.^[3] This might be due to the relatively great values^[4] of Ln-O-Ln angles (111.57(6)° and 110.24(6)° for Gd and Ho compound respectively).

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Key-words: binuclear entities, antiferromagnetic coupling, coordination polymers

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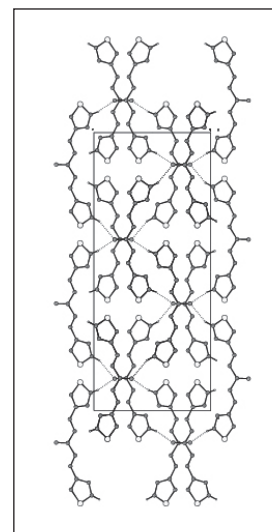
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Crystal structure and semi-empirical quantum chemical calculation of 1,5-Bis (3-thiophenyl)-1,4-pentadiene-3-one

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The chalcones are important chemical intermediates used in the synthesis of various organic compounds containing five and seven-membered heterocycles. The study of such compounds have attracted considerable interest as they possess wide spectrum of biological activities such as anti-oxidant, neuroprotective, anti-miotic and anti-malarial etc. Moreover, they have significant contribution in the production of photochemical materials through the solid-state photo cycloaddition process. In view of the importance of these factors, the title compound is synthesized and its crystal structure is studied. The compound crystallizes in orthorhombic space group $Pbca$ with the crystal parameters as: $a=11.8908(3)$ Å, $b=7.18070(10)$ Å, $c=28.3004(6)$ Å $V=2416.41(9)$ Å³, $Z=8$ and $\mu=0.415$ mm⁻¹. The structure is solved by direct method using SIR-97 program and refined by full matrix least square on F^2 using SHELXL-97 program to a final value 0.0443 for 3671 reflections with $I > 2 \sigma(I)$. The crystal structure is stabilized by intra- and intermolecular C-H...O interactions, as well as weak C-H... π interactions. The thiophene rings are planar within themselves and are oriented at an angle of 5.60(15)° and 14.26(15)° with the mean plane passing through 1,4-pentadiene-3-one moiety.

Semi-empirical Quantum Chemical Calculations were performed on the refined parameters using MOPAC2009 program to optimize the structure with Parametrization Model 6 (PM6) approximation together with the



Molecular Packing viewed down the 'b' axis