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.

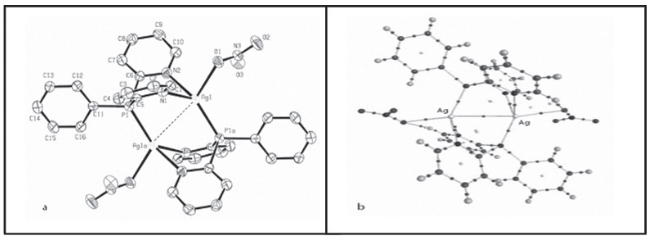

Figure 1. a) ORTEP view b) Molecular graph of synthesized complex

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

MS03.P07

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

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$\{[Ln_2(C_4H_2O_4)_3(H_2O)_4].3H_2O\}_\infty{}^3$ 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 μ-1,1 and μ-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

MS03.P08

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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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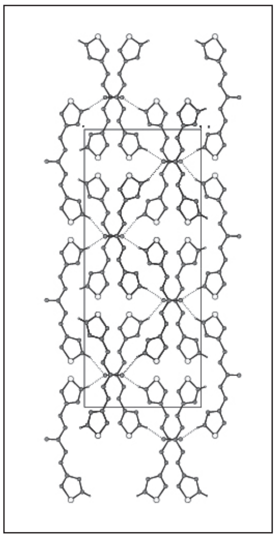
The chalcones are important chemical intermediates used in the synthesis of various organic compounds containing five and seven-membered heterocycles. The study of such compounds have attracted considerable interest as they possess wide spectrum of biological activities such as anti-oxidant, neuroprotective, 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) Å^3, Z = 8 and μ = 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 σ (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.



Molecular Packing viewed down the 'b' axis

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 restricted Hartree Fock closed- shell wave function. The minimizations were terminated at r. m. s. gradient of less than 0.01 KJ-mol^{-1} Å^{-1}. The optimized geometry of the structure displays significant change in the orientation of thiophene rings thereby resulting participation of such rings in the C-H…O and C-H… π interactions. The Semi-empirical Quantum Chemical Calculations were also performed on the analogous structure that has the substitution of two thiophene rings at position 2 to pentadiene moiety and these results will be compared with the present one and their detailed analysis will be presented later.

Keywords: bis-chalcones, hydrogen bond interactions and MOPAC 2009

MS03.P09

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Characterization of some di-block copolymers and investigation of their temperature-dependent structural behaviors

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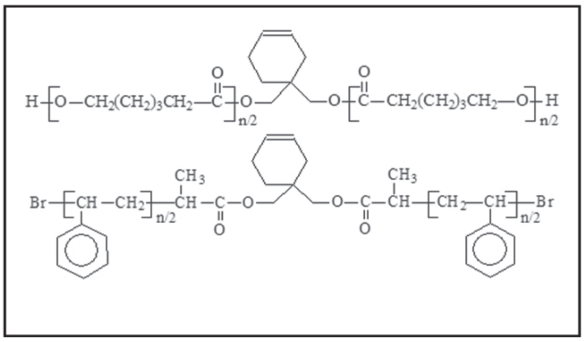
The synthesis and characterization of novel polymeric materials is crucially important for new scientific researches and technological applications. The present research is focused on Cyclohexene Mid-Chain polymers containing polystyrene (PS) and [Poly(ε- Caprolactone)] (PCL) functional groups. These polymers, because of their easily crystallization feature, can make some blends with other polymers, that have a wide technological utilization field [1]. The usage of an apolar aliphatic polyester [Poly(ε- Caprolactone)] and polystyrene which has a low melting point can cause radical polymerization controlling with light and cationic polymerization. Thus, molecular weight of the polymer and end-groups of the polymer chains can be also controlled. So, the physical properties of the polymers can be changed by adding different functional end groups (such as PS and PCL) to the Cyclohexene Mid-Chain.

In the present work, X-Ray diffraction (XRD) and X-Ray scattering methods (SAXS and WAXS) have been used to characterize these type polymeric structures (Figure 1.) in solid and solution forms. On the other hand, because of their big importance in living radical polymerization, thermo response behaviors of the novel synthesized polymers (in solution form) have been also examined.



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Keywords: SAXS, WAXS, copolymer

MS04.P01

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A SAXS Study of an enzyme-reponsive self-assembling polymer/ peptide conjugate

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Enzyme-responsive biopolymer systems are attracting considerable interest for applications in biocatalysis, drug delivery, tissue scaffolding and other applications. Recent work in our group led to the development of an enzyme-responsive nanocontainer delivery and release system [1].

The micelles are formed by PEG/peptide conjugates comprising a core of amyloid peptide βAβAKLVFF. This peptide has been the subject of recent investigation by our group, having interesting self-assembly properties [2] and the potential to develop amyloid inhibition systems with therapeutic applications [3]. In the PEG/peptide construct, the polymer-peptide linkage is selectively cleaved using the model enzyme α-chymotrypsin which cleaves between phenylalanine (F) residues. This produces products βAβAKLVF and F-PEG3000 (PEG with molar mass of 3 kDa). Remarkably, the product βAβAKLVF was found not to aggregate into amyloid fibrils, in contrast to the parent peptide βAβAKLVFF, pointing to the importance of aromatic interactions and the presence of two phenylalanine residues in driving self-assembly. The relase of unassociated non-amyloid peptide may be useful in applications.

The release of the peptide from the PEGylated nanocontainer delivery system upon enzymatic cleavage was studied by mass spectrometry, circular dichroism, SAXS, TEM (including cryo-TEM) and FTIR spectroscopy. These materials are under further study as bio-responsive self-assembling systems, with potential applications in detection and delivery.

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Keywords: peptide, enzyme, SAXS

MS04.P02

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Characterization by SAXS of lignin from modified straw and bagasse sugarcane

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A biorefinery deals with process of converting biomass like bagasse and straw sugarcane into a variety of products [1]. Different useful products derived from sugarcane bagasse and straw can be obtained via separation process of hemicellulose, cellulose and lignin matrix [2]. Separation processes consists of a pretreatment that removes hemicellulose and the remaining product is submitted to a delignification procedure leading to a final product composed of pure lignin. Lignin can be modified for generation of a variety of novel and useful chemical agents and substances.

A standardized lignin for industrial applications is required to minimize the costs of reagents and processing power. In this work the effects of different pretreatment and delignification processes