

energies of the halide salts; optimization of their geometrical parameters; the prediction of their thermochemical properties, and the resulting comparison to the experimental energy values and optimized parameters obtained from their structures determined by single-crystal X-ray diffraction. Similar work has been carried out on 1,6-hexanediamine hybrid semiconductors to predict their optical and electric properties [5].

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Structural study of amine and amino acid salts consisting nitrate anions. Nouredine BENALICHERIF, *Laboratoire des Structures, Propriétés et Interactions Inter Atomiques, Institut des Sciences et Technologie. Centre Universitaire Abbes Laghrour Khenchela 40000, Algeria.*

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Amine and amino acids salts are interesting for NLO applications. Their importance is due to the fact that all the amino acids have chiral symmetry and several compounds crystallize in noncentro-symmetric space groups [1].

Thus, salts of amine and amino acids with different organic/inorganic acids have been explored.

Several new complexes incorporating natural amino acids and nitrate anions have been recently crystallized [2] and their structural, optical [3], thermal properties and structural phase transitions [4] have been investigated.

In this present work, which is part of project of searching for potential new hybrid compounds obtained by the addition of amino acids with nitric acid, we will discuss crystalline structures of new salts rich in hydrogen bonding, based on nitrate anions, amine and amino acids, published by our research team during the last ten years.

All materials of this type are characterized by the presence of strong N–H...O and O–H...O hydrogen bonds connecting anionic and cationic entities together which participate in the stability and cohesion of crystal structures.

In these compounds intramolecular bond lengths in nitrate anions depend closely to 3D intermolecular interactions.

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Asymmetrically Substituted Distyrylbenzenes and Their Polar Crystal Structures. Frank Blockhuys, Roeland De Borger, Alain Collas, Christophe M.L. Vande Velde, *Department of Chemistry, University of Antwerp, Universiteitsplein 1, B-2610 Wilrijk, Belgium*
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Oligomeric organic semiconductors possess a number of intrinsic advantages over their polymeric counterparts as well as over inorganic (CMOS) materials, the most important being the straightforward molecular tunability and the fact that they can be obtained as crystalline solids [1,2]. Indeed, the supramolecular structure of these materials becomes important when they are applied in optical devices [3,4] or various types of sensors [5,6]. More so, when applications are envisaged which require a polar bulk, such as non-linear optical (NLO) or switchable memory devices, avoiding the anti-parallel orientation of the molecular dipoles in the crystal is of supreme importance. Twelve asymmetric donor-acceptor distyrylbenzenes with either one nitrile group or one, two or three nitro groups as electron acceptors, and one, two or three methoxy groups as electron donors were prepared. The electronic structures of the new materials were studied using peak potentials obtained from cyclic voltammetry, UV/Vis data and molecular dipole moments obtained from quantum chemical calculations. The supramolecular structures of five of these compounds were studied using single-crystal X-ray diffraction to monitor the influence of the positions of donor and acceptor groups on the organisation of the molecules in the solid state, and three polar crystal structures have been identified in which the molecular dipoles do *not* organize themselves in a centrosymmetric lattice. Analysis of the solid-state structures in function of the substitution pattern of the DSB scaffold leads to the conclusion that, in general, the oligomers organise themselves in a head-to-tail fashion and generate CH...O networks involving mainly the different methoxy groups. Preliminary results on the NLO properties of these new materials are also presented.

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Ionic and Neutral Forms of Ibuprofen within a Co-crystal. Petra Bombicz^a, Péter Molnár^b, Edit Székely^b, Béla Simándi^b, *^aInstitute of Structural Chemistry, Chemical Research Center, Hungarian Academy of Sciences, Hungary* *^bDepartment of Chemical and Environmental Process Engineering, Budapest University of Technology and Economics, Hungary*