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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Keywords: *n*-alkylammonium halide salts, single-crystal X-ray diffraction, DFT calculations

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Structural study of amine and amino acid salts consisting nitrate anions. Nourredine BENALI-CHERIF, *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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Keywords: amino acids, hydrogen bonds, hybrid compounds, x-ray diffraction

FA4-MS26-P06

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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Keywords: organic semiconductors, crystal packing, polar crystals

FA4-MS26-P07

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

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The aim of the study of optical resolution processes is to achieve a more efficient and less time consuming way of enantiomer separation. Supercritical fluid extraction as an alternative green technology for optical isomer separation was applied for the resolution of ibuprofen. Ibuprofen is widely used as non-steroidal anti-inflammatory drug. The resolution of ibuprofen (**1**) with the mixture of (+)-*(R)*-phenylethylamine (**2**) and benzylamine (**3**) was compared to the results obtained without the achiral additive [1]. Single crystal X-ray studies were performed on the salts of (+)-*(R)*-phenylethylamine crystallized with (-)-*(R)*-ibuprofen (**4**) and (+)-*(S)*-ibuprofen (**5**) as well as on the co-crystal resulted from the crystallisation of the racemic ibuprofen with the achiral benzylamine (**6**) in order to study the influence of the structurally similar achiral additive. (+)-*(R)*-phenylethylamine crystallises with (-)-*(R)*-ibuprofen and (+)-*(S)*-ibuprofen, respectively with 1:1 stoichiometry. Unexpectedly, the crystal of the benzylamine – ibuprofen salt contains an additional neutral ibuprofen molecule thus having 1:2 stoichiometry obtaining both from solution crystallisation and by mass balance calculation of the supercritical fluid CO_2 extraction. The lack of the methyl moiety in the benzylamine in structure (**6**) compared to the (+)-*(R)*-phenylethylamine molecule in structures (**4**) and (**5**) results a sterically favourable closer packing, higher crystal density. There is enough space in crystal (**6**) close to the ladder like hydrogen bond column to bond a neutral ibuprofen molecule as end group in the low acidity medium.

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Keywords: co-crystal, crystal packing, chiral separation

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p-Toluidinium nitrate.

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P-toluidine is an organic benzene derivative with a methyl substituent and an amino group, the name is derived from toluene and aniline. P-toluidine can cause anoxia due to formation of methemoglobin and hematuria in man [1].

The crystal structure of *p*-methylanilinium nitrate was determined as part of our investigations on the structural characteristics of organic-inorganic layered compounds and an ongoing study on *D*—*H*···A hydrogen-bonding in systems of hybrid materials including anilinium derivatives such as, 3-hydroxyanilinium hydrogensulfate [2], *o*-methylanilinium nitrate [3], 2-carboxyanilinium dihydrogenphosphite [4] and 2-carboxyanilinium nitrate [5].

The asymmetric unit of the title compound, *p*-toluidinium nitrate or *p*-methylanilinium nitrate, $C_7H_{10}N^+$. NO_3^- contains a monoprotonated p-methylanilinium cation and nitrated anion. The crystal of the title compound, $C_7H_{10}N^+$. NO_3^- consists of anionic- cationic layers linked by a complex three-dimensional hydrogen-bond network. The structure is stabilized by anion-cation N—H···O hydrogen-bonding.

The structure of ($C_7H_{10}N^+$. NO_3^-) is composed of cationic($C_7H_{10}N^+$.) and anionic (NO_3^-) linked through N-H…O hydrogen bonds and building up a corrugated layers parallel to the (001) plane

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Hydrogen bonding in Anilinium hydrogensulfate.

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The main purpose of this structural study was a determination of the arrangement of the cations and anions which are held together by two-dimensional hydrogen-bond networks.

Hydrogen bonding is one of the most versatile noncovalent forces in supramolecular chemistry and crystal engineering [1]. Therefore, in the past decades assessment of discrete hydrogen bonding patterns had received great attention [2] because of its widespread occurrence in biological systems.

The aim of this paper is to discuss hydrogen patterns assuring the connection between anilinium and hydrogensulfate entities and to establish their different graph-set motifs [3].

Bis (anilinium hydrogensulfate) is one of the hybrid compounds, rich in H-bonds [4-5], which could have potential importance in constructing sophisticated assemblies from discrete ionic or molecular building blocks due to the strength and the directionality of hydrogen bonds [6].

Recently, similar structures containing anilinium cations have been reported. Among examples, can be named the fo-lowing ones: anilinium nitrate [7], , anilinium hydrogenphosphite and anilinium hydrogenoxalate [8].

The structure of may be described as formed by alternating sheets of cations and anions which are held together with four five centered N-H…O bonds to form $C_4^4(10)$ infinite chains running through the c direction. Moreover, strong O-H…O hydrogen bonds observed between bisulfate anions generate $C_2^2(8)$ chains in the *a* axis direction. The infinite chains resulting from anion-anion and anion-cation interactions can be described as zigzag layers parallel (ac) plans. The crossing of these chains builds up different rings with $R_3^3(10)$ and $R_5^4(16)$ graph set motifs [9].

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