

incommensurate vector  $\pm(0.5, 0.3, 0.2)$  has been observed and studied.

[1] Fourmigue M., Batail P., *Chem. Rev.*, 2004, **104**, 5379. [2] Shibaeva R., Khasanov S., Zorina L., et al., *J. Phys. IV France*, 2004, **114**, 481.

**Keywords:** X-ray analysis, organic conductors, layered structures

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#### Family of Organic Layered Salts Based on BEDT-TTF with the $[\text{OsNOCl}_5]^{2-}$ Anion

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Four new BEDT-TTF radical cation salts with the  $[\text{OsNOCl}_5]^{2-}$  anion have been synthesized:  $\alpha'$ -(BEDT-TTF)<sub>4</sub> $[\text{OsNOCl}_5]^{2-}$ NB (**1**),  $\delta$ -(BEDT-TTF)<sub>4</sub> $[\text{OsNOCl}_5]^{2-}$ 1.33NB<sub>0.67</sub> (**2**),  $\kappa$ -(BEDT-TTF)<sub>4</sub> $[\text{OsNOCl}_5]^{2-}$ BN (**3**) and  $\beta$ -(BEDT-TTF)<sub>2</sub> $[\text{OsNOCl}_5]^{2-}$  (**4**) [1]. The salts were characterized by single crystal X-ray diffraction, electrical resistance measurements, and electronic band structure calculations. Evidence for commensurate structural modulations was found for **2** and **3**. The crystals of **1**, **3** and **4** are semiconductors while those of **2** exhibit a M-I transition around 160 K. Analysis of the correlation between the crystal structure, transport properties and electronic structure of this and related salts suggests the possibility of smoothly changing the conductivity of  $\kappa$ -phases with two donors and two dimers from semiconducting to metallic as well as the need to reconsider the origin of the metal-to-insulator transitions of  $\delta$ -type salts.

[1] Simonov S.V., Shevyakova I.Yu., Zorina L.V., Khasanov S.S., Buravov L.I., Emel'yanov V.A., Canadell E., Shibaeva R.P., Yagubskii E.B., *J. Mater. Chem.*, in press.

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#### Factors Determining Polymorphism of Leflunomide

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Leflunomide is a medicament for the treatment of rheumatoid arthritis. The aim of this work was to explore its properties in the crystalline state. Single crystals of the two polymorphic modifications of leflunomide were grown by slow evaporation techniques from different solvents. The X-ray diffraction analysis revealed that forms I and II of leflunomide belong to space group P2<sub>1</sub>/c with two and one independent molecules per asymmetric unit, respectively. Two out of the three molecules are very similar in conformation whereas the third one differs in the orientation of the amide group. The molecules arrange in a chain which in the form I is organized by N-H...O and N-H...N hydrogen bonds, while that in the form II shows just the N-H...N interaction. This way, the choice of the solvent of crystallization appeared to be decisive to obtain the desired polymorphic modifications of the compound.

**Keywords:** leflunomide, polymorphism, crystal structure

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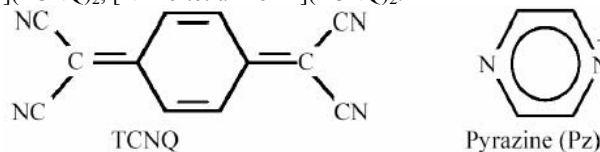
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#### New Electroconducting Radical Anion Salts Based on TCNQ with Organic Cations

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X-ray study of the first molecular semiconductors based on TCNQ  $\pi$ -acceptor with pyrazine derivatives has been carried out: (N-Et-Pz)(TCNQ)<sub>3</sub> [1], [N-Et-2,5-di-Me-Pz](TCNQ)<sub>2</sub>, [N-Me-2,5-di-Me-Pz](TCNQ)<sub>2</sub>, [N-Me-tetra-Me-Pz](TCNQ)<sub>2</sub>.



It has been established that the salts have a layered structure where conducting TCNQ layers alternate with non-conducting cationic layers. Lately organic and metal-containing TCNQ complexes have been gaining increased scientific interest since they can be used as organic sensors, high-speed optical memory devices, photo-switches, organic light emitting diodes, bio-sensors etc. [2]. Among them the so called hybrid materials were revealed that combine magnetism and electroconductivity and even superconductivity [3,4].

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**Keywords:** structure-properties relationships, TCNQ compounds, X-ray crystal structure analysis

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#### Haem-binding Properties and Crystallisation of the Bacterial Protein HemS

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Iron is one of the most important nutrients for the majority of living organisms due to its essential role in many biological processes like respiration and oxygen transport. Despite being one of the most abundant chemical elements, iron is scarcely available under physiological conditions, because of its insolubility and toxicity.

Pathogenic bacteria rely on their host as source of iron and have evolved several strategies to circumvent their iron dependency. One mechanism relies on "stealing" iron in the form of haem from host's haem proteins through a set of inter-linked haem transporters [1]. These unique systems have intriguing molecular biology mechanisms.

The haem uptake system of the gastrointestinal pathogen *Yersinia enterocolitica* consists of 5 proteins. Located on the outer membrane, the receptor HemR sequesters haem from host haem proteins or directly binds free haem. When internalised, the ligand is taken up by the periplasmic carrier HemT and passed onto the hetero-dimer HemUV, an integral inner membrane permease. In the cytosol, haem is held by the soluble protein HemS [1,2,3].

HemS purifies red from *E. coli*, has a solet peak at 412 nm and binds haem in vitro in a pH- and buffer-dependent manner. Homologues of HemS can only be found in the phylum of the Proteobacteria, with a sequence identity greater than 30%. Sequence alignments show three conserved histidine and one conserved methionine residues which might be involved in haem-iron coordination. Since tertiary structure predictions showed no significant similarity to any known structure, HemS could adopt a novel fold.

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