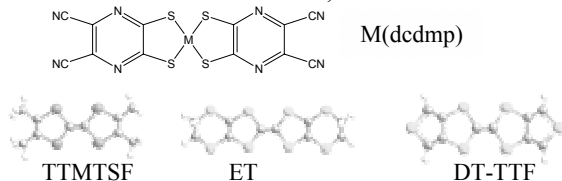


P.08.14.46*Acta Cryst.* (2005). A61, C351**The Role of Cation on the Crystal Packing of the Molecular Conductors Based on Ni(dcdmp)₂**

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Square planar dithiolates have for long been appealing candidates as building blocks for molecular based conductors. Such transitions metal complexes can be used as simple counter-anions in charge transfer with other widely known planar species as TTF, BET-TTF, TMTSF or ET^{1,2,3}. Here we report the crystal structures as well as the role of cationic spacers on the crystal packing of the charge transfer salts. Using electrocrystallisation techniques was possible to obtain crystals of several charge transfer salts combining the [Ni(dcdmp)₂] anion with different π donors: TMTSF, ET and DT-TTF.



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[1] Tomura M., Tanaka S., Yamashita Y., *Synthetic Metals*, 1994, **24**,197. [2] Belo D., Morgado J., Rabaça S., Duarte M.T., Lopes E. B., Santos I. C., Gama V., Henriques R. T., Almeida M., *Synthetic Metals*, 1999, **102**, 751. [3] Belo D., Santos I.C., Almeida M., *Polyhedron*, 2004, **23**, 1351.

Keywords: molecular compounds, intermolecular interactions, conductors

P.08.14.47*Acta Cryst.* (2005). A61, C351**Structure and Emission Properties of Erbium Quinolinolate Complexes**

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We have recently reported the first combined optical and structural investigation of the water free Er-quinolinolate complex [1], a prototype organo-lanthanide system for 1.5- μm telecom applications. The complex has a trinuclear structure (Er₃Q₉) which provides the Er metals with an octa-coordination by the organic ligand and prevents solvent and water molecules from entering the lanthanide coordination sphere. By using the 5,7-dichloro-8-hydroxyquinoline (ClQH) the new [ErCl(ClQ)₂(ClQH)₂] compound has been obtained. The Er intrinsic deactivation occurs in this case with a time constant which is approximately twice the value obtained for Er₃Q₉ (4.0 vs 2.2 μs) but still three orders of magnitude faster than the erbium radiative lifetime. Structural data have been used to calculate the transfer time from the Er ions to the C-H groups of the ligand in the framework of the Förster's theory and the obtained decay times are in agreement with those experimentally found. Thus the C-H groups sitting in the Er inner coordination sphere represent a very severe limit to the IR emission yield of organo-Er complexes. Ligands which do not bear CH or OH groups appear to be promising to prepare complexes with enhanced emission efficiency.

[1] Artizzu F., et al., *Inorg. Chem*, 2005, **44**, 840-842.

Keywords: luminescent compound, structure, lanthanides

P.08.15.1*Acta Cryst.* (2005). A61, C351**Approximate Reduced Density Matrix for Bioactive Systems: an Ab-initio Approach**

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Modelling complex systems such as bioactive molecules in their real environment implies two notions : accuracy and robustness of the results, reasonable computation time. Usual ab initio methods or MD simulations do not fulfil those two conditions. Decreasing the computation time and keeping the reliability of an Hartree-Fock approach is possible through the 1-Particule Reduced Density Matrix which can be approximated as a sum of molecular fragments obtained from finite clusters simulating the local environment [1]. This method is a useful tool to go beyond the mere electrostatic properties and to obtain more precise and more sensitive information about interaction mechanisms and reactivity.

After its validation for simple periodic systems, the method was adapted and implemented for complex systems. We report our results obtained on some pharmaceutical compounds, such as busulphan and styrylquinolines.

[1] Ragot S, Gillet J.M., Becker P., *Physical Review B*, 2002, **65**, 235115.

Keywords: ab-initio calculations, density matrices, environment

P.08.15.2*Acta Cryst.* (2005). A61, C351-C352**Hydroxyapatite-bisphosphonate Nanocrystals**

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Bone resorption is strongly inhibited by bisphosphonates [1], a family of compounds with physicochemical properties and structure very similar to those of pyrophosphates, which are widely used to treat a variety of diseases with excess bone resorption [2].

Although the mode of action has yet to be fully elucidated, it is known that bisphosphonates bind very strongly to hydroxyapatite (HA), and as a result are taken up by bone [3]. We have investigated the interaction of hydroxyapatite with alendronate, a bisphosphonate used for treatment of various diseases of bone metabolism. Hydroxyapatite nanocrystals with an alendronate content up to about 7% wt have been prepared through direct synthesis in aqueous solution. The results of TEM investigation indicate that alendronate affects the morphology of the hybrid crystals, which exhibit much smaller dimensions than HA crystals. On the other hand, the values of the lattice constants of the apatitic phase, as well as the coherence lengths of the perfect crystalline domains, evaluated by the line broadening of the 002 and 310 reflections, are not significantly affected by alendronate incorporation. These composite materials can be suitable for potential application as a local bisphosphonate delivery system.

[1] Russell R.G.G., Rogers M.J., *Bone*, 1999, **25**, 97-106. [2] Fleisch H., *Bisphosphonates in bone disease, from the laboratory to the patients*, Academic Press, San Francisco, 2000. [3] Lin J.H., *Bone*, 1996, **18**, 75-85.

Keywords: bone, calcium phosphate, biomaterials design