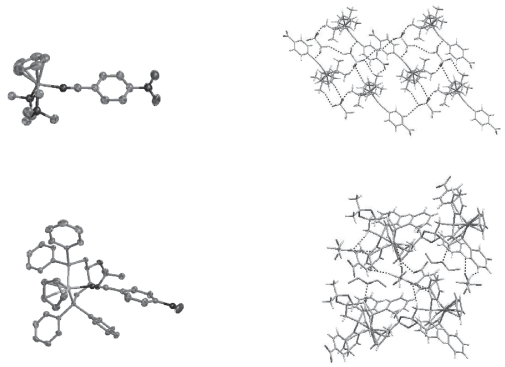
s13.m42.p9 **Molecular Structure and Crystal Packing of CpMR Isonitriles (M= Ru, Fe; R = Phosphines and TMEDA). How to Obtain New Solids for NLO.** M. F. M. da Piedade[a,b], A. R. Dias[a], M. T. Duarte[a], P. Florindo[b], M. H. Garcia[a,b], J. C. Rodrigues[c], M. P. Robalo[a,d], [a]*Centro de Química Estrutural, I.S:T., Av. Rovisco Pais, 1096-001 Lisboa, Portugal.* [b]*Departamento de Química e Bioquímica da FCUL, Campo Grande, 1749-016 Lisboa, Portugal.* [c]*Departamento de Química Universidade da Madeira, Campus Universitário da Penteada 9000-390 Funchal, Portugal.* [d]*Departamento de Engenharia de Química do ISEL, 1950-062 Lisboa, Portugal. E-mail: mdpiedade@fc.ul.pt*

Keywords: NLO materials; Crystal packing; Crystal engineering

Organometallic compounds have found great importance in the area of non linear optical materials, due to their significant values of second and third harmonic generation. This has been possible owing to the diversity of metal centres, oxidation states, ligands and geometries.

We present here a systematic study on Fe and Ru isonitrile derivatives, where we try to emphasize the relationship between molecular design and crystal engineering: the metal centers have been enriched and depleted by changing the type and number of ligands, the p systems have been extended and different counter ions have been used. The effects that this diversity has promoted in the 3D crystal packing will be discussed and compared.



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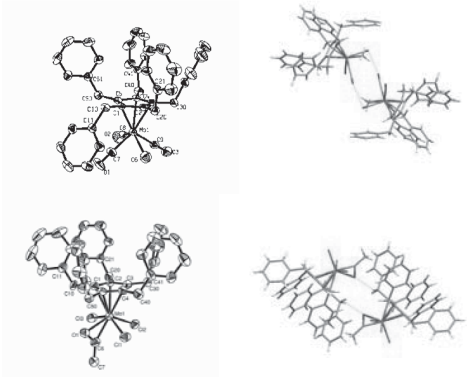
s13.m42.p10 **Crystal Packing Studies on $C_5(CH_2Ph)_5M$ (M=Mo,W) Derivatives. Conformational Behaviour of the $C_5(CH_2Ph)_5$ Moiety.** M. Teresa Duarte, Ana M. Martins, Rita Branquinho, Jinlan Cui, José Fernandes, Sandra S. Rodrigues, Alberto R. Dias, *Centro de Química Estrutural, Instituto Superior Técnico, Av. Rovisco Pais no 1, 1049-001 Lisboa, Portugal. E-mail: teresa.duarte@ist.utl.pt*

Keywords: Crystal packing; Conformation; Systematic study

Besides decreasing the relative air and moisture sensitivity, the introduction of the bulky pentabenzylcyclopentadienyl ligand (CpBz) in organometallic systems has also led to the synthesis of compounds where the ligand shows a high degree of conformational flexibility. It has been shown that two to five benzyl substituents can be accommodate in the same side of the planar Cp ring without any apparent strain.

Several effects can be taken into account: bulkiness of the CpBz ligand; number of different ligands in the coordination sphere; electronic effects; steric effects; and packing effects.

Trying to understand the effects that determine the different conformations adopted, we present here a systematic study on the packing versus steric effects in the conformation of the bulky ligand CpBz in organometallic compounds. The Mo and W structures, all new, will be compared with data from the CCDC on both transition and main group metal derivatives.



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