

Crystal engineering of non-centrosymmetric systems

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Organometallic crystals lacking of inversion center were synthesized starting from acentric reagents following two different approaches: asymmetric metal center or asymmetric ligand.

The former is a mixed halide of mercury (II), HgBrI, crystallizing in the space group Cmc2(1) [1], which was prepared by a completely new solid state reaction. The latter is 2-(2'-pyridyl)-1,8-naphthyridine (pyNP) whose crystalline structure was first determined by our research group and results in space group P2(1).

A series of organometallic compounds were synthesized and their crystalline structure verified by single crystal X-ray diffraction, Raman, IR and UV-VIS electronic spectroscopies. Complexes with mixed salt and aromatic heterocyclic ligands drift to a non-centrosymmetry crystalline structure while those with pyNP tend to be centrosymmetric. From results obtaining we deduced the crystalline packing was mainly influenced by metal center respect to ligand. *Crystals of mixed salt have a structural disorder due to Iodide-Bromide VICARIANZA facilitating non-centrosymmetry.*

These systems could present NLO properties and could be employed in optical and optoelectronic application. [2]

[1] Wu Q., Li Y., Chen H. et al., *Inorg. Chem. Comm.* 34 (2013) 1.

[2] Long N. J. , *Angew.Chem. Int. Ed. Engl.*, 34 (1995) 21