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X-ray study of metal-organic framework compounds

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Metal-organic frameworks (MOFs) are porous materials consisting of inorganic metal nodes, known as secondary building units, bridged together by organic linkers. In the past few decades, MOFs have attracted a great deal of attention due to their potential applications in heterogenous catalysis, controlled drug release, selective adsorption or gas storage and separation. [1]

The organic ligand 3,3,5, 5'-Tetrakis(4-carboxyphenyl)bimesityl (H_4L) used by us in the synthesis of several new MOFs was obtained through a Suzuki coupling reaction [2] between 3,3',5,5'-tetraiodobismesitylene and 4-carboxyphenylboronic acid, in the presence of tetrakis(triphenylphosphine)palladium (0) as a catalyst. The MOFs were obtained by mixing the appropriate metals salt with H_4L in DMF (Zn, Cd) or DMF/water (Mg, Ca, Na) in solvothermal conditions(heating at 80 °C for 48-72 hours).

All diffraction experiments were performed at Stoe STADIVARI diffractometer with a Dectris Pilatus 300 K detector and with an Genix3D Cu HF source (Cu-Kα, λ = 1.54186 Å). Data were collected at 100 K with the use of a nitrogen gas open-flow cooler Cobra Oxford Cryosystems. For data reduction X-Area (Stoe, 2017) software package [3] was used. The crystal structures were solved and refined in OLEX 2 software using SHELX suite of programs.

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