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MS16 O4

Single-Crystal to Single-Crystal Photochemical Reactions in Inclusion Compounds.

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Keywords: Photochemistry, Inclusion Compounds, Solid-State Reaction

We have found that single-crystal to single-crystal photochemical reaction takes place when we irradiated inclusion compounds with a regular mercury lamp.

Photochemical reaction of reactant guest molecules in inclusion compounds results in changes in the volume of the product guest molecules. In cases where the size of the reaction core is large enough to accommodate the substrate and the product (not simultaneously), the reaction is expected to be homogeneous (single-crystal to single-crystal) [1]. Voids are expected to be created if the volume of the product is significantly smaller than that of the pre-reacted guest molecules. In such cases either the single crystal will be destructed or?

In this paper we describe the photodimerization of two compounds 2(1H)-pyridone or 6-methyl-2-(1H)-pyridone, present as guest molecules in inclusion compounds. In each of these compounds, the volume of the dimer is smaller than the volume of the separated monomers, and as a result voids are created. In both cases water molecules that penetrate into the crystal occupy these voids in an ordered fashion. It was found that the water penetration occurs only at a late stages of the conversion suggesting that a critical amount of voids are necessary for the penetration to take place. After dimerization, voids are generated forming discontinuous channels. The discontinuity comes about from plugs of unreacted monomers. Only when all the monomers have dimerized the pieces of channels can merge to become continuous allowing for the penetration of water. After a period of several months the water diffuses out leaving single crystals. In both cases significant rotation induced by the dimerization occurs and is in association with hydrogen bond breakage and formation. [2]

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MS16 O5

Novel Acetylpentanedionato Complexes for MOF Construction

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Keywords: Metal-Organic Complexes; Structure Analysis of small Molecules; Framework Structures

Symmetrically functionalized β-diketonate complexes, bearing linkable terminal substituents like the acetylpentanedionato complexes presented herein, hold the potential for the synthesis of new coordination polymers, namely metal-organic frameworks (MOFs). This class of porous materials is attracting continuous attention due to their large and adjustable cavities, high apparent surface areas, and selective uptake of small molecules. Acetylpentanedionate as a ligand forms exceptionally stable complexes and allows for a wide variety of linkable terminal substituents. It thus represents an inviting challenge to investigate its use in secondary building units. The novel compounds based on this complex and presented herein encompass four- and bi-ligand complexes and a variety of linear ligand-forming molecules.

The crystal structures of the complexes were determined from laboratory X-ray powder diffraction data. A comprehensive characterisation by a variety of spectroscopic and physico-chemical methods reflects the molecular and crystallographic differences between the compounds. The divalent metals palladium and magnesium both form linear bi-ligand complexes with plane-square coordination of the central cation. The Pd(II) complex forms a crystal structure of isolated molecules, in which the molecular conformation does not show any significant deviation from the expected ideal state. The use of this complex in MOF construction is promising for catalytic applications. In contrast, the Mg(II) complex crystallises in a way to complete the octahedral coordination of the central cation, resulting in strong inter-molecular bonds and a significant distortion of the ligands. This is reflected by vibrational band shifts and low solubility of the compound. Zr(IV) is coordinated by four chelating ligands [2], forming a square-antiprismatic oxygen coordination polyhedron. The geometry of this complex makes it capable to form network nodes. High pseudo-symmetry of the complexes is observed in all cases. The oxygen coordination polyhedron of the central metal in all cases is of very high regularity. The molecules symmetry is generally broken by orientational order of the free acetyl groups only. In $[Zr(C_4H_9O_3)_4]$ and $[Pd(C_4H_9O_3)_2]$ the symmetry of the molecule is retained on Wyckoff positions of lower site symmetry, indicating the absence of any significant inter-molecular forces.

From these components, a large variety of MOFs could be constructed. Experiments to this end are in progress.

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