Synthesis and Structural Characterization of Novel Metal-Organic Frameworks

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Studies of structurally and chemically diverse open framework solids have been flourishing in the recent years in an attempt to increase and improve applications of such materials in areas such as catalysis, sorption and ion-exchange. Our research is aimed at finding new 3-dimensional porous frameworks, which may possess interesting physical properties. We report the hydrothermal synthesis and structural characterization of several new metal-organic hybrid frameworks constructed from various metal cations and organic ligands of different functionalities.

For example, $Zn_2(C_2H_2N_3)_2(C_8H_4O_4)\cdot H_2O$, synthesized using 1,2,4-triazole and 1,4-benzenedicarboxylic acid as organic linkers, possesses a structure (P4/ncc, a = 13.521(2) Å, c = 27.221(5) Å, Z = 8) based on the sheets containing 8-membered rings of $ZnON_3$ tetrahedra and triazole molecules along the (001) direction. The sheets are connected by benzenedicarboxylates through Zn – O – C links to produce channels which are occupied by water molecules. Its thermal behavior has also been characterized by thermogravimetric analysis. It is stable up to 300ºC before the organic molecules start to decompose, leading to the framework collapse.

Keywords: materials structure and characterization, porous materials, x-ray crystallography