

Hydrogen Storage in Metal-Organic Frameworks

Omar M. Yaghi, *Department of Chemistry, University of Michigan, Ann Arbor, Michigan.* E-mail: oyaghi@umich.edu

Reticular synthesis (logical construction of networks from molecular building blocks) has yielded a new class of crystalline porous materials commonly referred to as metal-organic frameworks (MOFs) in which metal ions and clusters are linked by organic units. The ability to prepare MOFs in high yield and with adjustable pore size, shape and functionality has led to their study as gas sorption materials. We have demonstrated that systematic variation of the organic component in isorecticular metal-organic frameworks (IRMOFs) has a marked effect on their capacities for methane. More recently, we discovered that IRMOFs are also capable of storing significant amounts of H₂, and inelastic neutron scattering studies of molecular hydrogen adsorbed in IRMOF-1 pointed to the organic unit as one of the important adsorption sites. Thus, there is an acute need to collect and analyze more hydrogen uptake measurements on such materials in order to establish the favorable factors for its storage. Hydrogen adsorption isotherms measured at 77 K show a distinct dependence of uptake on the nature of the link for a set of five MOF materials containing the Zn₄O(CO₂)₆ cluster. At 1 atm, the materials sorb between 4.2 and 9.3 molecules of H₂ per formula unit. The results imply a trend in hydrogen capacity with the number of rings in the organic moiety. Additionally, the significant influence of the inorganic unit, namely when open metal sites are present, on hydrogen uptake will be presented.

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