



第195回触媒化学研究センター談話会

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演題: Charge Density Distribution and Bond
Characterization of 3d-Transition Metal Complexes

日時: 2005年11月7日(月) 16:00 - 17:30

会場: 創成科学研究棟
4階セミナー室 04-213・214

要旨:

Chemical bond, which makes molecules from independent atoms, is a very important concept in understanding the molecular behavior. Bond characterization is therefore becoming ever needed for predicting the physical and chemical properties of the molecule and material. Bond characterization of 3d transition metal complexes has been investigated using precise single crystal diffraction data and sophisticated molecular orbital calculations. Information such as bond order, bond type etc will be described quantitatively. Atom domain in molecule can be defined uniquely. The complexity of the 3d orbital splitting when subjected in the ligand field is interesting and challenging. Detail characterization of metal-ligand coordinated bonds and M-L covalent bonds will be given. The valence shell charge concentration (VSCC) around metal ion will be demonstrated by the Laplacian topology, which provides the physical basis for the Lewis structure and VSEPR. The electronic configuration of the metal center can be realized by complementing with x-ray absorption.

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