行政院國家科學委員會專題研究計畫　成果報告

單獨分子至固態晶體之鍵性分析(3/3)

計畫類別：個別型計畫
計畫編號：NSC91-2119-M-002-017-
執行期間：91 年 08 月 01 日至 92 年 10 月 31 日
執行單位：國立臺灣大學化學系暨研究所

計畫主持人：王瑜

報告類型：完整報告
報告附件：國外研究心得報告
出席國際會議研究心得報告及發表論文
處理方式：本計畫可公開查詢

中　華　民　國 93 年 3 月 1 日

Abstract

This is the report of a three-year project. Bond characterizations based on the topological analysis are applied not only to the intra-molecular chemical bonding but also to the weak intermolecular interactions. In the following publications, the intermolecular interactions in the solid are specially emphasized.

(1) **Theoretical and Experimental Characterization of Cr-L Multiple Bonds (L = O, N, and C), *J. Phys. Chem. A*, 2000, 104, 9566-9572.** The paper is mainly concerned on the covalent characters of the metal-ligand multiple bond, namely bond characterization of Cr≡O; Cr≡N; Cr≡C triple bonds.

(2) **Charge Density Distribution and Bond Characterization of Metal Dialkyldithiocarbamate Complexes (M= Co, Ni) *J. Phys. Chem. Solids*, 2001, *62*, 1613-1628.** The paper illustrates the bond characters of M-S bond in a coordinated complex.

(3) **Topological Analysis and Charge Density Studies of an α -Diimine Macrocyclic Complex of Cobalt(II)- A Combined Experimental and Theoretical Study, *Chem Eur. J. 2002, 8, 1821-1832***. It gives the detail bond characterization of a low spin Co(II) perchlorate complex. The apparent description of a coordinated bond of Co-N & Co-O bond in cation and of a normal covalent bond of Cl-O bond in anion is conclusive. In addition, the hydrogen bond between the coordinated water molecule and the perchlorate anion is strong enough to dominate the packing at low temperature**.**

(4) **A Combined Experimental and Theoretical Electron Density Study of Intra- and Inter-molecular Interactions in Thiourea S,S-Dioxide, *Chem Eur J. 2003, 9, 3112-3121*.** Here a systematic investigation on the intermolecular interactions through monomer, dimer, heptamer and finally solid. The effect of such intermolecular interaction on the chemical bonding is illustrated. There are strong H-bonds inter-connect the molecules in solid. In addition, there are weak C---S and N---O interactions as well. Such interactions are demonstrated by the polarization of the local charge density of the respective atoms.

(5) **Topological Analysis of Charge Density in Heptasulfur Imide, S_7NH, from Isolated Molecule to Solid, *J Phys & Chem in Solids*, accepted**. Here the bifurcated H-bond is illustrated, weak inter-molecular S---S & S---N interactions are also investigated. The local charge concentration and depletion are clearly shown for S and N atom as its atomic graph. The directional interaction through the solid is therefore understood.

Publication #: 243; 250; 258; 276

.

Keyword: Bond Characterization; Topological analysis, X-ray diffraction, Intermolecular interactions, Density functional calculations

摘要

本報告為三年期計劃之報告。以拓譜學為基礎的鍵性分析方法不只應用於分子內的化學鍵，也應用於較弱的分子間作用力。在以下的論文發表中，特別強調固態中的分子間作用力。

(1) **Theoretical and Experimental Characterization of Cr-L Multiple Bonds (L=O, N, and C),** ***J. Phys. Chem. A, 2000, 104, 9566-9572.*** 本篇文章主要探討金屬－配位基間的多鍵之共價性，即 Cr≡O，Cr≡N 及 Cr≡C 三重鍵之分析比較。

(2) **Charge Density Distribution and Bond Characterization of Metal Dialkyldithiocarbamate Complexs (M= Co, Ni)** ***J. Phys. Chem. Solids, 2001, 62, 1613-1628***. 本篇文章探討在配位化合物中的金屬與硫間之鍵性分析。

(3) **Topological Analysis and Charge Density Studies of an α-Diimine Macrocyclic Complex of Cobalt(Ⅱ)－A Combined Experimental and Theoretical Study,** ***Chem Eur. J. 2002, 8, 1821-1832.*** 本篇文章對低自旋的鈷二價過氯酸塩之鍵性有深入的探討。對陽離子上的 Co-N 及 Co-O 配位鍵及陰離子上的 Cl-O 一般共價鍵的描述，已有具體的結論。而且被配位的水分子及過氯酸根陰離子間的氫鍵強度足以決定在低溫下的分子堆積情況。

(4) **A Combined Experimental and Theoretical Electron Density Study of Intra- and Inter-molecular Interactions in Thiourea S,S-Dioxide,** ***Chem Eur J. 2003, 9, 3112-3121.*** 本篇文章對分子間作用力，從單體(monomer)，雙體(dimer)，七聚體(heptamer)到固態分子，有系統性的分析，並討論分子間作用力對化學鍵的影響。在固態分子中，分子間有很強的氫鍵，而且也有弱的 C--S 及 N--O 作用力，我們以個別原子的局部電荷密度之極化程度來說明。

(5) **Topological Analysis of Charge Density in Heptasulfur Imide, S_7NH, from Isolated Molecule to Solid,** ***J Phys & Chem in Solids,*** **accepted.** 本篇文章探討分叉的氫鍵以及弱的 S--S 及 S--N 分子間作用力。硫原子及氮原子的局部電荷密度集中或煥散情況被清楚地顯示，即所謂原子圖像，由此可知固態中的方向性作用力。

Publications 編號： 243；250；258；276

關鍵字：鍵性分析；拓譜學；X 光繞射；分子間作用力；功能性密度計算