

MS23-P2 Charge Density Study of Distorting Tetrahedral and Octahedral Cu(II) Complexes

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How to understand the intermolecular interactions (especially the hydrogen bond and halogen bond) in the context of crystal packing and the utilization of such understanding in the design of new solids with desired physical and chemical properties is one of the most flourishing fields in crystal engineering.^[1] Based on the high resolution X-ray data, experimental charge density provides us one perspective to study the interaction existing between two molecules. Furthermore, for those transition metal complexes, which electrons of d-orbital is not fully occupied, experimental charge density also leaves people some kind of clues, which can help to figure out how the distribution of d-orbital's configuration in different coordination situation is.^[2] In this work, we will present different charge settings for central metal and refinement strategies based on the different data banks in aspheric atomic density expansion^[3] for distorting tetrahedral and octahedral coordinating surrounding Cu²⁺.

[1]Desiraju, G. R. *Crystal Engineering: The Design of Organic Solids*, Elsevier, 1989, Amsterdam.

[2]Mallinson, P. R., Koritsanzsky, T., Elkaim, E., Li, N., and Coppens, P. *Acta Cryst.* A44, 336(1988).

[3]Hansen, N. K. & Coppens, P. *Acta Cryst.*, A34, 909-921(1978).

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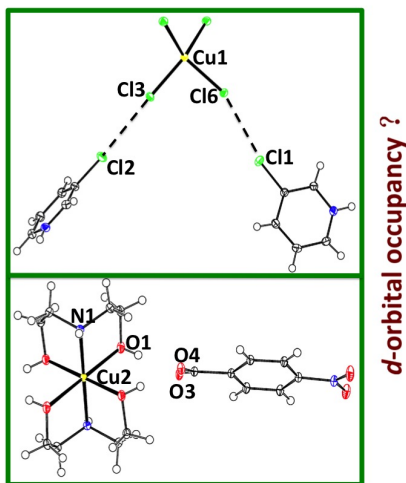


Figure 1. How are the d orbital populations distribution for distorting tetrahedral and octahedral Cu(II) complexes?