

Charge Density and Electrostatic Potential in Octa-Nuclear Chromium Complexes

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Beamline(s): X3A1

We are investigating host-guest compounds consisting of the big octa-nuclear "chrome-wheel", $[\text{Cr}_8\text{F}_8(\text{O}_2\text{CC}(\text{CH}_3)_3)_{16}]$ molecules intercalated with various smaller molecules – e.g. C_6H_6 , FeCp_2 and Bu_2NH . In this molecule, each chromium atom is coordinated to two neighbor chromium atoms through the carboxylate part of two pivalate groups and a fluorine atom, as shown in **Figure 1**. The superior combination of high flux, short wave-length, area detection and very low-temperature capability, offered by beamline X3A1, was used to collect an extensive data set from a tiny crystal of the "empty" compound, the naked chromium wheel. **Figure 1** indicates that there is a trace of dynamical/rotational disorder still present in three of the 16 t-butyl groups at 28K. The aim of the study is to establish the charge density distribution and the electrostatic potential of the naked compound, and to gain insight into the nature of the interactions between guest and host molecules by subsequent comparisons with similar studies of the intercalated compounds.

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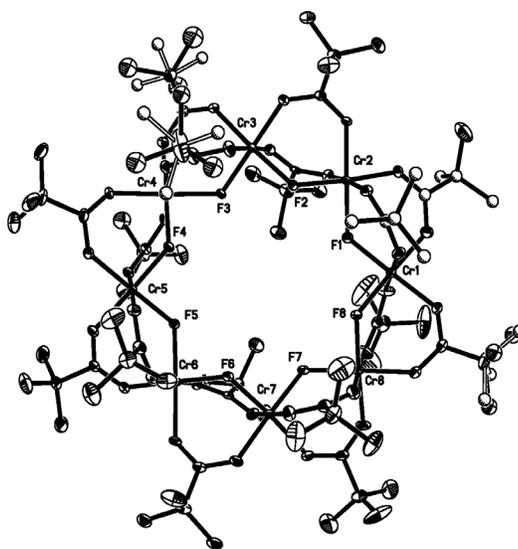


Figure 1. Octa-nuclear "chrome-wheel", $[\text{Cr}_8\text{F}_8(\text{O}_2\text{CC}(\text{CH}_3)_3)_{16}]$ molecule.