

# Bifurcated CN Group in Hexacyanometallates, the Case of $\text{Cd}_2[\text{Fe}(\text{CN})_6]$ . Structure Determination from a Combination of RDF and Direct Methods

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The crystal structure of anhydrous cadmium hexacyanoferrate (II),  $\text{Cd}_2[\text{Fe}(\text{CN})_6]$ , has been solved from powder diffraction data using information extracted from low resolution radial distribution function. Such anhydrous solid is obtained by soft heating of its parent octahydrate. The radial distribution function proves to be useful for observing changes in heavy atoms interatomic distances in the structure during phase transition related to the material dehydration process. These distances were then used for guessing the heavy atom positions from the direct methods results.  $\text{Cd}_2[\text{Fe}(\text{CN})_6]$  crystallizes in the hexagonal system, space group  $P-3$  (147) and cell parameters:  $a = 6.32046(5)$  and  $c = 6.33786(10)$  Å. The structure was refined to final agreement factors of  $R_{\text{wp}} = 6.26\%$  and  $S = 1.99$ . The proposed structural model is supported by the obtained information from Mössbauer, IR and Raman spectra.

## 1. Introduction

Much work has been devoted in the last few years to the structure and physical properties of transition metal hexacyanometallates, mainly as prototype of molecular magnet where the most interesting effects have been observed, *e.g.* high Curie temperature ( $T_c$ ) magnets [1–3], photo-induced magnetism [4], spin-glass behavior [5], among others. This family of molecular materials has also been studied in connection with their porous framework ability for small

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