

# On the structure and Mössbauer spectra of ferrous nitroprusside

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Monoclinic ferrous nitroprusside trihydrate and its dehydration products have Mössbauer spectra composed of two quadrupole doublets. The quadrupole splitting of the high-spin ferrous cation decreases stepwise as the compound loses water up to the anhydrous state. Cubic ferrous nitroprusside has a complex Mössbauer spectrum with three quadrupole doublets for high-spin ferrous cations, which are determined by the number of water molecules in its environment. The Mössbauer parameters of low-spin ferrous cations in ferrous nitroprusside are practically independent of its hydration degree and crystalline structure.

## 1. Introduction

When ferrous nitroprusside (FeNP),  $\text{Fe}[\text{Fe}(\text{CN})_5\text{NO}] \cdot x\text{H}_2\text{O}$ , is precipitated by mixing solutions of a soluble  $\text{Fe}^{2+}$  salt and sodium nitroprusside (NaNP), it adopts an fcc structure analogous to Prussian Blue [1–5], but when the crystal growth is controlled by slow diffusion, single crystals of a monoclinic phase are obtained [6]. The Mössbauer spectrum of the polycrystalline material has been studied by several authors [3, 7, 8]. Garg and Goel [3] and Fung and Drickamer [7] report a simple spectrum with two quadrupole doublets assignable to low-spin  $\text{Fe}^{\text{II}}$  and high-spin  $\text{Fe}^{2+}$  in unique crystallographic sites. Long et al. [8] found a more complex spectrum with eight dips. The two strongest dips belong to the low-spin  $\text{Fe}^{\text{II}}$  from the complex nitroprusside anion with about 50% of the total intensity. The remaining six dips, grouped into three doublets, indicate the presence of different sites for high-spin  $\text{Fe}^{2+}$  nuclei.

In this paper, we report a spectroscopic and crystallographic study using Mössbauer, infrared (IR) and XRD techniques of the monoclinic single crystals and their dehydration products, whose Mössbauer spectra have not been previously reported, and of polycrystalline material obtained by different procedures. A spectrum–structure correlation is presented which sheds light on the origin of the complex Mössbauer spectra.