

AN EPR AND ESEEM STUDY OF $\text{Fe}(\text{CN})_6^{3-}$ IN KCl SINGLE CRYSTALS

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An EPR and ESEEM study was made at $\sim 15\text{K}$ on the ferricyanide complex in KCl lattice for a further investigation of the large compensation mechanism of trivalent impurity ions in alkali-metal halides [1,2]. A large number of $\text{Fe}(\text{CN})_6^{3-}$ centres were found through EPR spectra. Due to the complexity of the spectra, detailed analysis only was possible for three centres. They are all at the low spin state, i.e., $S=1/2$. The dominant centre, which makes more than 60% of the total occupancy, has an orthorhombic symmetry. The three principal g -values, $g_z=0.4$, $g_x=2.079$ and $g_y=3.056$, are found when B [100], [011], and $[0\bar{1}\bar{1}]$, respectively. A second centre is very similar to the dominant centre, having the same symmetry, but possessing a different set of g -values. The third centre has monoclinic

symmetry with the symmetry determined principal axis along $\langle 110 \rangle$. These centres are due to the $\text{Fe}(\text{CN})_6^{3-}$ complex with different configurations of the local charge compensating cation vacancies. Models are proposed for the three identified centres and a comparison is made between $\text{Fe}(\text{CN})_6^{3-}$ in KCl and the $\text{Cr}(\text{CN})_6^{3-}$ complex in both KCl and NaCl. The relaxation times, both T_1 and T_2 were measured as a function of orientation and temperature by the Electron Spin Echo (ESE) technique. The Electron Spin Echo Envelope Modulation (ESEEM) was used to study the interaction with the nitrogen nuclei of the CN ligands.

[1] D.M. Wang, D.R. Hutton and J.R. Pilbrow, J. Phys. C. 19 (1986) 789

[2] D.M. Wang and E. de Boer, Phys. Rev. B 39 (1989)