

An electron spin resonance study of Mn^{2+} doped calcium hydrazine carboxylate monohydrate

M M ABDEL GAWAD, G V MAHESH*, K C PATIL* and S V BHAT
Department of Physics, *Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560 012, India

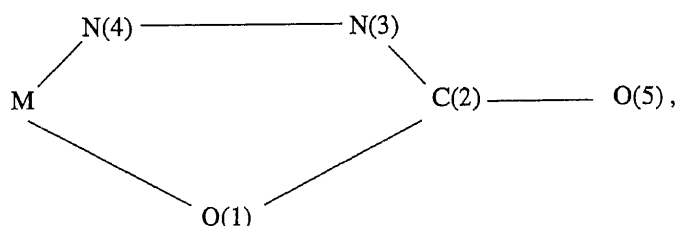
Abstract. Single crystals of calcium hydrazine carboxylate, monohydrate have been studied by ESR of Mn^{2+} doped in the calcium sites. X-band ESR indicated a large crystal field splitting necessitating experiments at Q band. The analysis shows two magnetically inequivalent (but chemically equivalent) sites with $g_{xx} = 2.0042 \pm 0.0038$, $g_{yy} = 2.0076 \pm 0.0029$, $g_{zz} = 2.0314 \pm 0.001$, $A_{zz} = 0.0099 \pm 0.0002 \text{ cm}^{-1}$, $A_{xx} = 0.0092 \pm 0.0002 \text{ cm}^{-1}$, $A_{yy} = 0.0082 \pm 0.0002 \text{ cm}^{-1}$, $D = 3/2 D_{zz} = 0.0558 \pm 0.0006 \text{ cm}^{-1}$, and $E = 1/2 (D_{xx} - D_{yy}) = 0.0127 \pm 0.0002 \text{ cm}^{-1}$.

One of the principal components of the crystal field, (D_{zz}), is found to be along the $Ca \leftrightarrow Ca$ direction in the structure and a second one, (D_{xx}), along the perpendicular to the plane of the triangle formed by three neighbouring calciums. The A tensor is found to have an orientation different from that of the g and D tensors reflecting the low symmetry of the Ca^{2+} sites.

Keywords. Electron spin resonance; Mn^{2+} ESR; low symmetry effects in ESR; $Ca(N_2H_3COO)_2 \cdot H_2O$.

1. Introduction

The hydrazine carboxylate compounds consisting of the complexes of 3d-metals, calcium and magnesium with hydrazine carboxylic acid have attracted recent scientific attention (Ravindranathan and Patil 1985). While they present various types of octahedral coordination, all of them contain pentatomic chelate rings of the type



which are similar to rings formed by α -amino acids with the same metals (Freeman 1967). Therefore, these complexes can serve as model compounds for non-crystallizable compounds of α -amino acids. Braibanti *et al* (1971) determined the crystal structure of calcium hydrazine carboxylate monohydrate, $Ca(N_2H_3COO)_2 \cdot H_2O$ and found that it belongs to the triclinic system with $Z = 2$. The two calcium ions were surrounded by six oxygens and two nitrogens forming what can be roughly