

Optical absorption spectrum of Ni^{2+} ion doped in synthetic lecontite

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Abstract. The optical absorption spectrum of Ni^{2+} ion doped in lecontite (sodium ammonium sulphate dihydrate) single crystal has been studied at room and liquid air temperatures. All the bands could be assigned assuming O_h symmetry for the Ni^{2+} ion in the crystal. The splitting of ${}^3T_{1g}(F)$ band at liquid air temperature has been attributed to spin-orbit interaction. The crystal field and spin-orbit parameters derived are $Dq = 1000 \text{ cm}^{-1}$; $B = 740 \text{ cm}^{-1}$; $C/B = 4.27$ and $\zeta = 600 \text{ cm}^{-1}$. All the bands observed show a blue shift when the crystal was cooled to liquid air temperature.

Keywords. Optical absorption spectrum; lecontite; spin-orbit interaction; crystal field; Racah parameters.

1. Introduction

The optical absorption spectrum of Ni^{2+} ion doped in several host lattices has been extensively studied (Piper and Koentge 1960; Pryce *et al* 1964; Solomon and Ballhausen 1975; Datta and Debabala 1976; Lakshman and Janardhanam 1978; and Lakshmana Rao and Purandar 1981). The present investigation reports the optical absorption spectrum of Ni^{2+} ion doped in sodium ammonium sulphate dihydrate, $\text{NaNH}_4\text{SO}_4 \cdot 2\text{H}_2\text{O}$ single crystal. This synthetic crystal is identical with natural lecontite as reported by Faust and Bloss (1963). The crystal structure of synthetic lecontite has been determined by Corazza *et al* (1967). The unit cell is orthorhombic with $a = 8.216$, $b = 12.854$ and $c = 6.232 \text{ \AA}$ and space group $P 2_1 2_1 2_1$. The structure shows chains of Na octahedra sharing one face with each other (Na–Na distance is 3.15 \AA). The SO_4 tetrahedron is regular. The NH_4^+ ion coordinates seven oxygen atoms forming an irregular polyhedron.

2. Experimental

Single crystals of sodium ammonium sulphate dihydrate doped with Ni^{2+} were grown by slow evaporation of equimolar solution of sodium sulphate and ammonium sulphate to which nickel sulphate (1 mole % by wt) was added as an impurity. The crystals were clear, transparent and green in colour. A crystal of 2.5 mm thickness was found suitable in the present work.

The optical absorption spectrum was recorded on a Hilger medium quartz spectrograph both at room and liquid air temperatures in the wavelength region λ 300 to