

Infrared and Raman spectra of aquamolybdenum (VI) oxide hydrate ($\text{MoO}_3 \cdot 2\text{H}_2\text{O}$)

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Abstract. The infrared and Raman spectra of $\text{MoO}_3 \cdot 2\text{H}_2\text{O}$ are recorded and analysed on the basis of vibrations due to MoO_6 octahedra and H_2O molecules. Considerable changes in the frequencies of the octahedra have been observed due to strong distortion in the octahedral arrangement. The inactive ν_6 vibration of O_h symmetry became active in the Raman spectrum. Co-ordinated (aquated) and hydrated (interlayer) water molecules give rise to different frequencies.

Keywords. Raman spectrum; infrared spectrum; hydrogen bond; anisotropic crystal field effect.

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1. Introduction

The structural investigation of hydrates of molybdenum trioxide (molybdic acids) has been reported earlier (Lindquist 1950; Asbrink and Brandt 1971; Guntur 1972; Krebs 1972; Boschen and Krebs 1974; Oswald *et al* 1975; Crouch Baker and Dickens 1984a, b, 1986). The dihydrate consists of infinite layers of vertex sharing $\text{MoO}_5\text{-H}_2\text{O}$ octahedra. Every octahedron shares a corner with each of the four neighbouring octahedra within the layers (Krebs 1972). The remaining water molecule assumes the interlayer position and the layers are linked by a system of hydrogen bonds involving all the four hydrogen atoms. Three H atoms participate in the normal H bonds whereas the fourth enters into bifurcated ones (Asbrink and Brandt 1971). Vibrational spectrum of the α form of the monohydrate was studied by Saleem and Aruldas (1983) assuming Mo-O co-ordination to be tetrahedral. The present investigation deals with vibrational spectroscopic studies of molybdenum trioxide dihydrate, $\text{MoO}_3 \cdot 2\text{H}_2\text{O}$.

2. Experimental

Analar grade $\text{H}_2\text{MoO}_4 \cdot \text{H}_2\text{O}$ was used for the investigation. The Raman spectrum (figure 1) of the powder sample was recorded in the Stokes region of the green line 5145 \AA (laser power, 50 mW) using a double monochromator (Spex Ramalog 1401

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