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A redetermination of the crystal structure of cupric chloride dihydrate

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Crystal structure / Cupric chloride dihydrate

Abstract. Cupric chloride dihydrate $CuCl_2 \cdot 2\ H_2O$ crystals are in the space group *Pbmn* with $a = 7.4141(4)$, $b = 8.0886(5)$, $c = 3.7458(3)$ Å and $z = 2$. The O–H bond lengths of 0.82(4) and the hydrogen positions are consistent with neutron diffraction, and infrared determinations but not the proton resonance interpretation.

Introduction

The crystal structure of cupric chloride dihydrate and the positions of the copper, chlorine and oxygen atoms were first obtained by X-ray diffraction (Harker, 1936). Subsequently the parameters were refined somewhat and the positions of the hydrogen atoms determined by neutron diffraction (Peterson et al., 1957). Calculations of hydrogen atom positions were also made from infrared (Rundle et al., 1955) and proton resonance results (Poulis et al., 1953). Since we obtained high quality crystals of this compound in the course of another investigation (Brownstein et al., 1989), it seemed worthwhile to obtain hydrogen atom positions and more accurate structure parameters by current X-ray procedures.

Experimental methods and structure determination

The crystals were grown by hydrolysis from an acetone solution of hexakis(benzonitrile)copper(II) bis[hexachloroantimonate(V)] (Brownstein et al., 1989). X-ray diffraction intensities were collected at room temperature

Table 1. Atom positions.

Atom	x	y	z	B_{iso} [a]
Cu	0	0	0	1.67(4)
Cl	0.23998(20)	0	0.3798(4)	1.79(6)
O	0	0.2402(5)	0	2.52(19)
H	0.099(5)	0.275(7)	0.064(14)	5.4(16)

[a] B_{iso} is the mean of the principal axes of the thermal ellipsoid.

Table 2. Bond distances and angles

Cu–Cl	2.2781(14)	Cl–Cu–Cl	180.0
Cu–O	1.943(4)	Cl–Cu–O	90.0
O–H	0.82(4)	O–Cu–O	180.0
H–H	1.54(7)	Cu–O–H	110(4)
		H–O–H	139(6)

on an Enraf-Nonius CAD-4 diffractometer with graphite monochromatized MoK_a radiation using the $\Theta/2\Theta$ scan technique with profile analysis (Grant, 1978). The structure was solved by direct methods and refined by full matrix least-squares techniques to $Rf = 0.030$ and $Rw = 0.032$ with weights based on counting statistics. All calculations were performed using the NRCVAX program system (Gabe, 1985).

Results and discussion

The final atomic positional parameters and the mean of the principal axes of the thermal ellipsoids are listed in Table 1. The bond distances and angles are listed in Table 2. Structure factor tables and the anisotropic temperature factors have been deposited. [1] There is no disagreement between the present data and the previous less precise X-ray values (Harker, 1936). It is worth noting that the O–H bond length determined by X-ray diffraction is significantly shorter than that determined by neutron diffraction, which is in agreement with theory. The present results are therefore in agreement with the infra-red and neutron diffraction measurements but not the proton resonance interpretation.

[1] Additional material to this paper can be ordered from the Fachinformationszentrum Energie-Physik-Mathematik, D-7514 Eggenstein-Leopoldshafen 2, FRG. Please quote reference no. CSD 53806, names of the authors and the title of the paper.

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