Crystal structure of copper(I) chromium(III) oxide, *2H-CuCrO$_2$*

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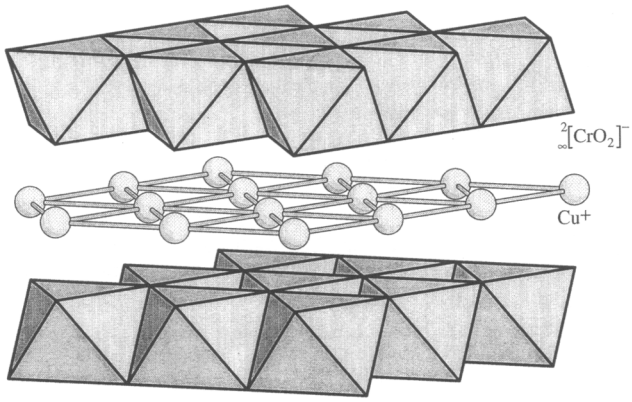

Table 1. Parameters used for the X-ray data collection

Crystal:	plate shaped, size 0.4 x 0.4 x 0.025 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	179.23 cm^{-1}
Diffractometer:	Stoe Stadi 4
Scan mode:	ω-θ
$T_{measurement}$:	293 K
$2\theta_{max}$:	49.8°
$N(hkl)_{unique}$:	204
Criterion for F_o:	$F_o > 3\,\sigma(F_o)$
$N(param)_{refined}$:	9
Program:	Xtal 3.2

Source of material: The compound is prepared by quenching trigonal $CuCrO_2$ crystals at 1373 K.
2*H*-$CuCrO_2$ is the metastable form of $CuCrO_2$. It is isostructural with 2*H*-$CuFeO_2$ (see ref. 1). The structure is characterized by an AABB stacking of close packed oxygen layers with chromium atoms in octahedral sites. The copper atoms are in linear coordination between directly superposed oxygen layers.

$CrCuO_2$, hexagonal, $P6_3/mmc$ (No. 194), a =2.9740(3) Å, c =11.400(1) Å, V =87.3 $Å^3$, Z =2, $R(F)$ =0.035, $R_w(F)$ =0.029.

Table 2. Final atomic coordinates and displacement parameters (in $Å^2$)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu	2*c*	1/3	2/3	1/4	0.0127(1)	U_{11}	0.0043(2)	$U_{11}/2$	0	0
Cr	2*a*	0	0	0	0.0046(1)	U_{11}	0.0044(2)	$U_{11}/2$	0	0
O	4*f*	1/3	2/3	0.0881(2)	0.007(3)	U_{11}	0.004(7)	$U_{11}/2$	0	0

Reference

1. Effenberger H.: Structure of hexagonal copper(I)ferrite. Acta Crystallogr. C**47** (1991) 2644-2646.