



Article scientifique

Article

1996

Published version

Open Access

This is the published version of the publication, made available in accordance with the publisher's policy.

Crystal structure of copper(I) chromium(III) oxide, $2H-CuCrO_2$

Crottaz, Olivier; Kubel, Frank

How to cite

CROTTAZ, Olivier, KUBEL, Frank. Crystal structure of copper(I) chromium(III) oxide, $2H-CuCrO_2$. In: Zeitschrift für Kristallographie. Crystalline materials, 1996, vol. 211, n° 7, p. 481. doi: 10.1524/zkri.1996.211.7.481

This publication URL: <https://archive-ouverte.unige.ch/unige:175914>

Publication DOI: [10.1524/zkri.1996.211.7.481](https://doi.org/10.1524/zkri.1996.211.7.481)

Crystal structure of copper(I) chromium(III) oxide, 2H-CuCrO₂

O. Crottaz

University of Geneva, Department of Applied Chemistry, 30 quai Ernest Ansermet, CH-1211 Geneva 4, Switzerland

and F. Kubel

University of Geneva, Department of Physical Chemistry, 30 quai Ernest Ansermet, CH-1211 Geneva 4, Switzerland

Received October 11, 1995, transferred to database ICSD September 1996, CSD-No. 402289

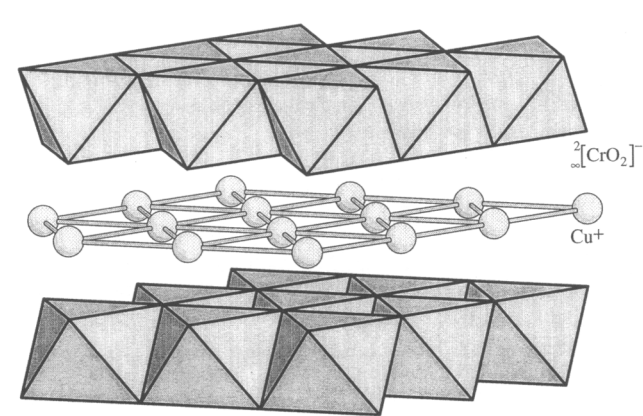


Table 1. Parameters used for the X-ray data collection

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 θ _{max} :	49.8°
N(hkl) _{unique} :	204
Criterion for F _o :	F _o > 3 σ (F _o)
N(param) _{refined} :	9
Program:	Xtal 3.2

Source of material: The compound is prepared by quenching trigonal CuCrO₂ crystals at 1373 K. 2H-CuCrO₂ is the metastable form of CuCrO₂. It is isostructural with 2H-CuFeO₂ (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.

CrCuO₂, hexagonal, *P*6₃/*mmc* (No. 194), *a* = 2.9740(3) Å, *c* = 11.400(1) Å, *V* = 87.3 Å³, *Z* = 2, *R*(*F*) = 0.035, *R*_w(*F*) = 0.029.

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
Cu	2 <i>c</i>	1/3	2/3	1/4	0.0127(1)	<i>U</i> ₁₁	0.0043(2)	<i>U</i> ₁₁ /2	0	0
Cr	2 <i>a</i>	0	0	0	0.0046(1)	<i>U</i> ₁₁	0.0044(2)	<i>U</i> ₁₁ /2	0	0
O	4 <i>f</i>	1/3	2/3	0.0881(2)	0.007(3)	<i>U</i> ₁₁	0.004(7)	<i>U</i> ₁₁ /2	0	0

Reference

1. Effenberger H.: Structure of hexagonal copper(I)ferrite. Acta Crystallogr. C47 (1991) 2644-2646.