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Crystal structure of copper(I) chromium(III) oxide, 3R-CuCrO₂

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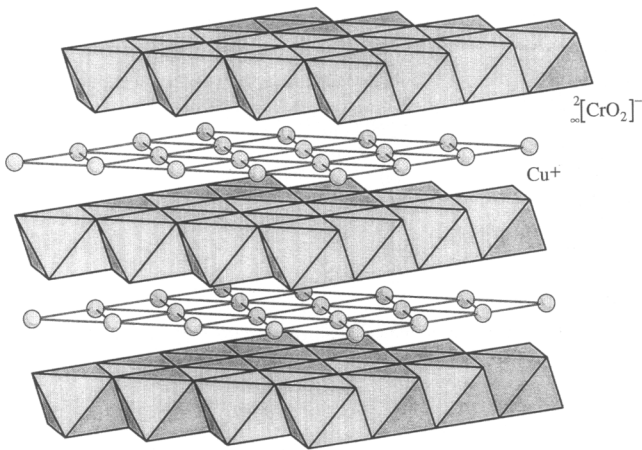


Table 1. Parameters used for the X-ray data collection

Crystal:	plate shaped, size 0.18 x 0.15 x 0.04 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	179.3 cm ⁻¹
Diffractometer:	Stoe Stadi 4
Scan mode:	ω - θ
T _{measurement} :	293 K
2 θ _{max} :	49.9°
N(hkl) _{unique} :	212
Criterion for F _o :	F _o > 3 σ (F _o)
N(param) _{refined} :	9
Program:	Xtal 3.2

Source of material: The compound is synthesized by flux growth from a mixture of K₂Cr₂O₇ and CuO (weight ratio 4:1) in a platinum crucible at 1133 K.

3R-CuCrO₂ is the stable form of CuCrO₂. It is isostructural with 3R-CuFeO₂ (see ref. 1). The structure is characterized by an AABBC 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, trigonal, $R\bar{3}m$ (No. 166), $a=2.9734(3)$ Å, $c=17.100(4)$ Å, $V=130.9$ Å³, $Z=3$, $R(F)=0.025$, $R_w(F)=0.025$.

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

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Cu	3a	0	0	0	0.0143(1)	U ₁₁	0.0073(1)	U ₁₁ /2	0	0
Cr	3b	0	0	1/2	0.0059(1)	U ₁₁	0.0069(1)	U ₁₁ /2	0	0
O	6c	0	0	0.10792(8)	0.008(4)	U ₁₁	0.008(8)	U ₁₁ /2	0	0

Reference

I. Prewitt, C.; Shanon, R. D.; Rogers, D. B.: Chemistry of nobles metal oxides.
II. Crystal Structure of PtCoO₂, PdCoO₂, CuFeO₂, and AgFeO₂. Inorg. Chem. **10** (1971) 719-723.