Crystal structure of copper(I) chromium(III) oxide, 3*R*-$CuCrO_2$

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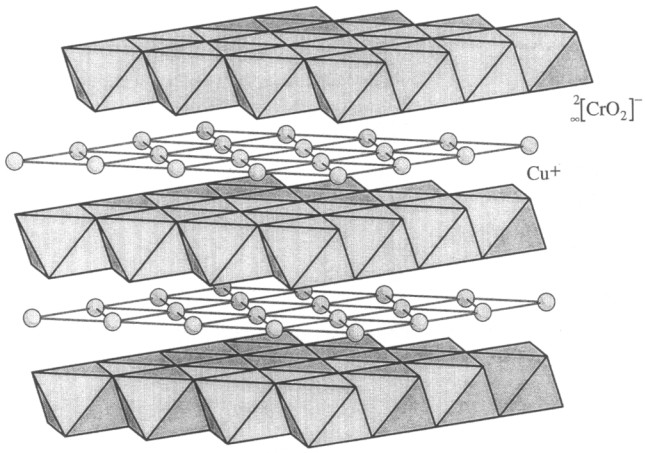
Received October 11, 1995, transferred to database ICSD September 1996, CSD-No. 402290



Source of material: The compound is synthesized by flux growth from a mixture of $K_2Cr_2O_7$ and CuO (weight ratio 4:1) in a platinum crucible at 1133 K.
3*R*-$CuCrO_2$ is the stable form of $CuCrO_2$. It is isostructural with 3*R*-$CuFeO_2$ (see ref. 1). The structure is characterized by an AABBCC stacking of close packed oxygen layers, with chromium atoms in octahedral sites. The copper atoms are in linear coordination between directly superposed oxygen layers.

$CrCuO_2$, trigonal, $R\bar{3}m$ (No. 166), a =2.9734(3) Å, c =17.100(4) Å, V =130.9 Å^3, Z =3, $R(F)$ =0.025, $R_w(F)$ =0.025.

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 $K\alpha$ radiation (0.71073 Å)
μ:	179.3 cm^{-1}
Diffractometer:	Stoe Stadi 4
Scan mode:	ω-θ
$T_{measurement}$:	293 K
$2\theta_{max}$:	49.9°
N(hkl)$_{unique}$:	212
Criterion for F_o:	$F_o > 3\,\sigma(F_o)$
N($param$)$_{refined}$:	9
Program:	Xtal 3.2

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	3*a*	0	0	0	0.0143(1)	U_{11}	0.0073(1)	$U_{11}/2$	0	0
Cr	3*b*	0	0	1/2	0.0059(1)	U_{11}	0.0069(1)	$U_{11}/2$	0	0
O	6*c*	0	0	0.10792(8)	0.008(4)	U_{11}	0.008(8)	$U_{11}/2$	0	0

Reference

1. Prewitt, C.; Shanon, R. D.; Rogers, D. B.: Chemistry of nobles metal oxides. II. Crystal Structure of $PtCoO_2$, $PdCoO_2$, $CuFeO_2$, and $AgFeO_2$. Inorg. Chem. **10** (1971) 719-723.