Crystal structure of silver chloride chromate (VI), Ag_3ClCrO_4

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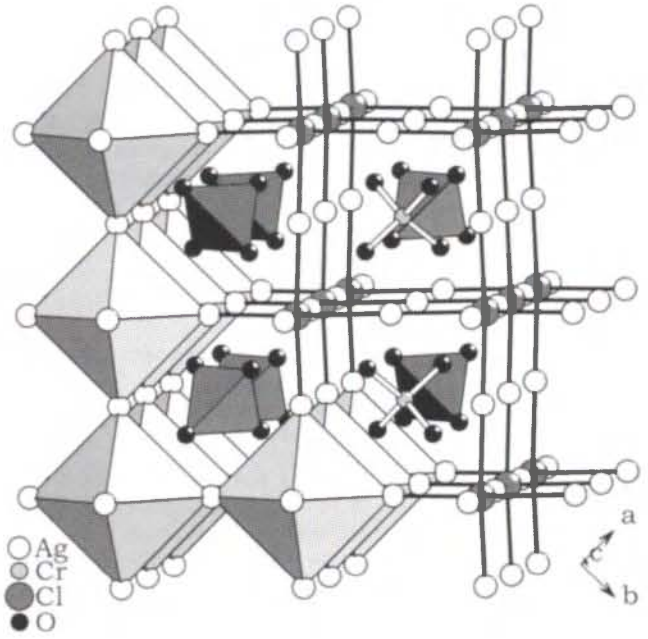

Abstract

Ag_3ClCrO_4, tetragonal, *P4/nmm* (No. 129), $a = 7.3889(5)$ Å, $c = 5.3065(3)$ Å, $V = 289.7$ Å^3, $Z = 2$, $R_{gt}(F) = 0.042$, $wR_{ref}(F^2) = 0.097$, $T = 293$ K.

Source of material

Single crystals of Ag_3CrO_4Cl have been prepared by solid state reaction of a mixture of Ag_2O and elemental Cr (molar ratio 3 : 2) under an elevated oxygen pressure. The mixture was annealed for 30 h in silver crucibles placed in stainless-steel autoclaves [1] using 2 ml of 3% $HClO_4$ as an accelerator. The reaction temperature and oxygen pressure were 753 K and 100 MPa, respectively.

Discussion

Ag_3CrO_4Cl was first obtained as a by-product of different syntheses aiming at ternary silver oxides in steel autoclaves with per-chloric acid as an accelerator. The crystal structure can be described as an anti-perowskite with CrO_4-tetrahedra at Ca-sites, Cl at Ti-sites and Ag at O-sites showing a close structural relationship to $Cd_3O(SiO_4)$ [2], which crystallizes in the same space group, and the $Cs_3Cl(CoCl_4)$ type [3, 4]. The Cl atom is displaced from the center of its surrounding Ag_6 octahedron along [001] resulting in a 5 + 1 coordination of the chlorine atom.

Table 1. Data collection and handling.

Crystal:	red cube, size 0.05 × 0.08 × 0.10 mm
Wavelength:	Mo K_α radiation (0.71069 Å)
μ:	121.97 cm^{-1}
Diffractometer, scan mode:	Bruker AXS, ω/2θ
$2\theta_{max}$:	69.96°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2887, 390
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 382
$N(param)_{refined}$:	20
Programs:	SHELXL-97 [5], DIAMOND [6]

References

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Table 2. 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}
Ag(1)	2*c*	0	1/2	0.1010(1)	0.0310(3)	U_{11}	0.0232(3)	0	0	0
Ag(2)	4*e*	1/4	1/4	1/2	0.0438(3)	U_{11}	0.0486(4)	0.0181(2)	–0.0050(1)	U_{13}
Cr(1)	2*a*	0	0	0	0.0174(3)	U_{11}	0.0246(6)	0	0	0
O(1)	8*i*	0	0.1793(5)	0.1849(8)	0.063(2)	0.023(1)	0.043(2)	0	0	–0.006(1)
Cl(1)	2*c*	0	1/2	0.6267(3)	0.0375(6)	U_{11}	0.0200(7)	0	0	0

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