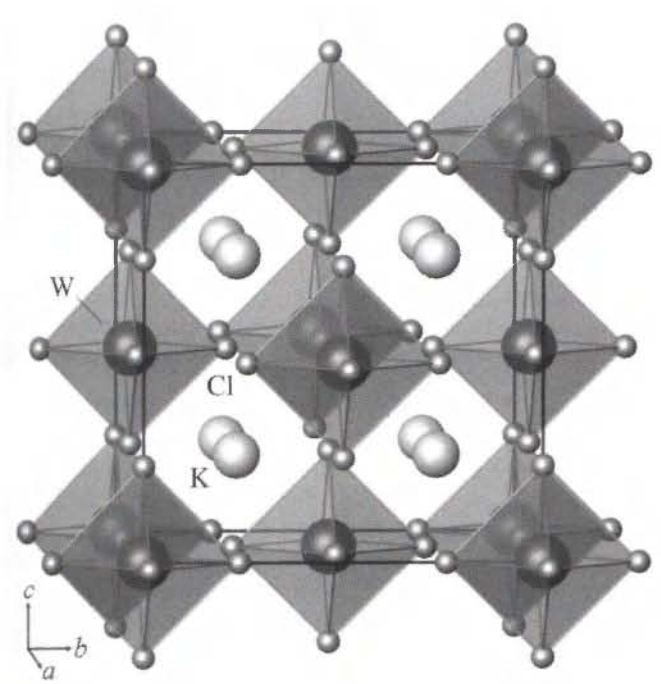
Crystal structure of dipotassium hexachlorotungstate(IV), $K_2[WCl_6]$

W. Xu and Y.-Q. Zheng*

Ningbo University, Institute of Inorganic Chemistry, Municipal Key Laboratory of Solid Materials Chemistry, Ningbo, Zhejiang, 315211 P. R. China

Received July 11, 2005, accepted and available on-line August 29, 2005; CSD no. 409840



Abstract

Cl_6K_2W, cubic, $Fm3m$ (no. 225), $a = 9.822(1)$ Å, $V = 947.6$ Å^3, $Z = 4$, $R_{gt}(F) = 0.039$, $wR_{ref}(F^2) = 0.088$, $T = 293$ K.

Source of material

The reaction of WCl_4 (0.508 g, 1.56 mmol) and KCl (0.233 g, 3.12 mmol) in a sealed silica tube at a temperature gradient 925 K/915 K for one week afforded a small amount of dark green block-shaped crystals in the low-temperature zone.

Discussion

Consisting of K^+ cations and $[WCl_6]^{2-}$ anions, the title compound crystallizes isotypically with the previously reported ternary tungsten(IV) chlorides M_2WCl_6 (M = Rb [1], Cs [2], Tl[3]) of the well-known K_2PtCl_6 type structure [4]. The W atoms are each octahedrally coordinated by six Cl atoms with d(W—Cl) = 2.347(5) Å, which is practically identical with those observed for Rb_2WCl_6 (2.360(3) Å) and Cs_2WCl_6 (2.369(6) Å), but slightly shorter than that of 2.379(4) Å for Tl_2WCl_6. The K^+ ions are each cuboctahedrally surrounded by twelve Cl atoms, d(K—Cl) = 3.4744(4) Å.

Table 1. Data collection and handling.

Crystal:	dark green plate, size 0.18 × 0.22 × 0.33 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	146.76 cm^{-1}
Diffractometer, scan mode:	Rigaku R-AXIS RAPID, ω
$2\theta_{max}$:	54.46°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1692, 79
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 79
$N(param)_{refined}$:	7
Programs:	SHELXS-97 [5], SHELXL-97 [6]

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}
W	4*a*	0	0	0	0.047(1)	U_{11}	U_{11}	0	0	0
K	8*c*	¼	¼	¼	0.059(2)	U_{11}	U_{11}	0	0	0
Cl	24*e*	0	0	0.2389(6)	0.077(3)	U_{11}	0.032(3)	0	0	0

Acknowledgments. The project was supported by the Expert Project of Key Basic Research of the Ministry of Science and Technology of China (grant no. 2003CCA00800), the Zhejiang Provincial Natural Science Foundation (grant no. Z203067), the Ningbo Science and Technology Bureau (grant no. 2003A62026) and the Scientific Research Fund of Ningbo University (grant no. 2004624).

References

1. Wang, P.; Xu, W.; Zheng, Y.-Q.: Crystal structure of dirubidium hexachlorotungstate(IV), $Rb_2[WCl_6]$. Z. Kristallogr. NCS **217** (2002) 301.
2. Wang, P.; Xu, W.; Zheng, Y.-Q.: Crystal structure of dicaesium hexachlorotungstate(IV), $Cs_2[WCl_6]$. Z. Kristallogr. NCS **218** (2003) 25.
3. Zheng, Y.-Q.; Nuss, J.; von Schnering, H. G.: Crystal structure of dithallium hexachlorotungstate(IV), $Tl_2[WCl_6]$. Z. Kristallogr. NCS **213** (1998) 472.
4. Kennedy, C. D.; Peacock, R. D.: Complex Chlorides and Bromides of Quadrivalent Tungsten. J. Chem. Soc. (1963) 3392-3397.
5. Sheldrick, G. M.: Phase Annealing in SHELX-90: Direct Methods for Larger Structures. Acta Crystallogr. A**46** (1990) 467-473.
6. Sheldrick, G. M.: SHELXL-97. Program for the Refinement of Crystal Structures. University of Göttingen, Germany 1997.

* Correspondence author (e-mail: zhengcm@nbu.edu.cn)