Crystal structure of dicaesium hexachlorotungstate(IV), $\text{Cs}_2[\text{WCl}_6]$

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Abstract

$\text{Cl}_6\text{Cs}_2\text{W}$, cubic, $Fm\bar{3}m$ (No. 225), $a = 10.245(1) \text{ \AA}$, $V = 1075.3 \text{ \AA}^3$, $Z = 4$, $R_{\text{gt}}(F) = 0.060$, $wR_{\text{ref}}(F^2) = 0.139$, $T = 293 \text{ K}$.

Source of material

The reaction of CsCl (0.3 g, 1.78 mmol), WCl_4 (0.3 g, 0.92 mmol) and W powder (0.15 g, 0.82 mmol) in a sealed silica tube at a temperature gradient of 925 K/915 K for 1 week afforded a small amount of red octahedral crystals in the lower temperature zone.

Discussion

The title compound crystallizes with the well-known K_2PtCl_6 type structure, consisting of Cs^+ cations and the $[\text{WCl}_6]^{2-}$ anions. The W atoms are each octahedrally coordinated by six Cl atoms, $d(\text{W}-\text{Cl}) = 2.369(6) \text{ \AA}$, and the Cs^+ cations are each cuboctahedrally surrounded by twelve Cl atoms, $d(\text{Cs}-\text{Cl}) = 3.6273(5) \text{ \AA}$.

Table 1. Data collection and handling.

Crystal:	red octahedron, size $0.19 \times 0.19 \times 0.20 \text{ mm}$
Wavelength:	Mo K_{α} radiation ($0.71073 \text{ \AA}$)
μ :	188.33 cm^{-1}
Diffractometer, scan mode:	Bruker P4, $\theta/2\theta$
$2\theta_{\text{max}}$:	54.8°
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$:	488, 90
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 83
$N(\text{param})_{\text{refined}}$:	7
Program:	SHELXL-97 [1]

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References

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Table 2. Atomic coordinates and displacement parameters (in $\text{\AA}^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
W	4a	0	0	0	0.058(1)	U_{11}	U_{11}	0	0	0
Cs	8c	1/4	1/4	1/4	0.054(1)	U_{11}	U_{11}	0	0	0
Cl	24e	$-0.2312(6)$	0	0	0.055(3)	0.062(3)	U_{22}	0	0	0

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