The crystal structure of Cs₂HfCl₆ was determined to be cubic, Fm3m, similar to K₂PtCl₆, with parameters: \( a_0 = 10.42 \pm 0.01 \) Å and \( u = 0.247 \pm 0.003 \). Powder diffraction data on which the determination was based are given.

### Origin of specimens

Crystals of Cs₂HfCl₆ were grown from the melt by lowering an evacuated quartz ampule containing Cs₂HfCl₆ through a temperature gradient (Axe, 1960). The maximum temperature of the furnace was 820°C and the lowering speed was 2 cm/d. The Cs₂HfCl₆ has to be prepared in a dry atmosphere as it will decompose in the presence of water vapour. It was prepared as follows: HfCl₄ was dissolved in methanol saturated with HCl in a three necked, round-bottom flask. A soxhlet extractor containing CsCl was inserted in one of the necks of the flask. The HfCl₄ solution was boiled and stirred. The methanol vapour gradually dissolved the CsCl also appeared. These lines were used as a standard for the determination of the effective radius of the camera. The powder data are given in Table 1.

It was assumed that Cs₂HfCl₆ has the same structure as K₂PtCl₆ (Wyckoff, 1957), and therefore space group Fm3m. According to this assumption the structure is completely determined by the size of unit cell \( a_0 \) and by the parameter \( u \) where \( a_0 \) is the Hf–Cl distance. Therefore, the observed \( d \) values were tentatively indexed with the corresponding \( hkl \)s, and the parameter \( a_0 \) was determined by least-squares fitting, i.e. \( a_0 = 10.42 \pm 0.01 \) Å. The agreement in Table 1 confirms that the crystal has indeed f.c.c. symmetry (\( hkl \)'s are either all odd or all even).

To determine the parameter \( u \) the relative intensities were calculated by the formula:

\[
I = j|F|^2g(\theta),
\]

where

\[
g(\theta) = \frac{[1 + \cos^2 \theta \cos^2 \alpha]}{[\sin^2 \theta \cos \theta \cos^2 (2\theta - 30^\circ)]},
\]

\( j \) is the multiplicity and \( \alpha = 26.5^\circ \). Atomic scattering factors were taken from International Tables for X-ray Crystallography (1967). The \( u \) parameter was determined by comparing the experimental with the calculated relative intensities as a function of \( u \). The best fit was obtained for \( u = 0.247 \pm 0.003 \); the corresponding intensities are those given in Table 1.

Measurement of X-ray Laue diffraction photographs of single crystals of Cs₂HfCl₆ showed that the mosaic structure angle of \( \theta_{e.m.} \approx 1.7^\circ \).

For the purpose of electron paramagnetic resonance and optical measurements (Maniv, 1971), the crystals were doped with paramagnetic ions of low concentration and no change in the X-ray measurements was observed.

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### References


