Acta Cryst. (1966). **21**, 1011

The crystal structure of the compound Cs_2CeCl_6.

By T. Kaatz and M. Marcovich, *Israel Atomic Energy Commission*

(*Received* 23 *August* 1965 *and in revised form* 3 *August* 1966)

The compound Cs_2CeCl_6 was recently prepared by the authors (Marcovich & Kaatz, 1966) as a finely divided yellow powder.

Diffraction patterns were obtained with a Philips X-ray powder diffractometer with filtered Cu $K\alpha$ radiation, $\lambda = 1{\cdot}5418$ Å. Unit-cell dimensions were determined by an extrapolation procedure which eliminated errors due to specimen displacement, as described by Wilson (1950). A hexagonal cell with the following dimensions was obtained: $a = 7{\cdot}476 \pm 0{\cdot}002$, $c = 6{\cdot}039 \pm 0{\cdot}002$ Å, $c/a = 0{\cdot}808$. Considering known interionic distances, it appeared that this cell could contain only *one* Cs_2CeCl_6 molecule, giving a calculated density of 3·52 g.cm^{-3}.

On the basis of the well-known structural similarity of the lanthanides and the actinides, the structure was assumed to be the same as that of Cs_2PuCl_6 (Zachariasen, 1948), Cs_2ThCl_6 and Cs_2UCl_6 (Siegel, 1948), with the space group $P\bar{3}m$ and the following atomic positions:

1 Ce in (a), $(0,0,0)$
2 Cs in $(d) \pm (\frac{1}{3}, \frac{2}{3}, u)$
6 Cl in $(1) \pm (x, \bar{x}, z)$ *etc.*

The structure is of the K_2GeF_6 type, as established by Hoard & Vincent (1939) from single-crystal studies.

The parameters of Zachariasen (1948) were used as the starting point in a least-squares treatment, in which three positional parameters, an overall isotropic thermal parameter, and a scale factor were refined. The function minimized was $\Sigma\, w(F_o^2 - F_c^2)$, where F_o^2 and F_c^2 represent the observed and calculated values of the quantity $F_{khl}^2 + F^2_{\overline{hkl}}$. The weights are based on counting statistics as described by Evans (1961), giving zero weight to unobserved reflections. F values were obtained by correcting the observed intensities with the Lorentz-polarization factor, and making allowance for multiplicity. The absorption factor was assumed constant for the flat powder sample used. Atomic scattering factors for Cl^- were taken from Dawson (1960), and those for Cs^+ and Ce^{4+} from Thomas & Umeda (1957). Corrections for anomalous dispersion were made with the values given by Cromer (1965). The final parameters obtained were: $x = 0{\cdot}171 \pm 0{\cdot}003$, $z = 0{\cdot}259 \pm 0{\cdot}009$, $u = 0{\cdot}255 \pm 0{\cdot}005$; $B = 2{\cdot}3$ Å^2. Final values of the observed and calculated structure factors are given in Table 1. The conventional R index, omitting unobserved F values, is 8·5%.

In this structure each cerium atom is bonded to six chlorine atoms at the interatomic distance Ce–Cl = 2·71 Å. Each cesium atom is bonded to twelve chlorine atoms, three of them at a distance 3·61 Å, three at 3·75 Å and six at 3·74 Å, giving a weighted average of 3·71 Å.

Table 1. *Observed and calculated structure factors for the powder lines of* Cs_2CeCl_6

hkl	$(F_{hkl}^2 + F_{hk\bar{l}}^2)^{\frac{1}{2}}_{\text{obs}}$	$(F_{hkl}^2 + F_{hk\bar{l}}^2)_{\text{calc}}^{\frac{1}{2}}$
100	8	7
001	19	21
101	50	52
110	61	56
200	23	19
111	13	22
002	61	60
201	101	103
102	52	53
210	—	8
112	—	8
211	44	46
202	73	76
300	52	47
301	18	26
003	22	27
103	31	39
212	41	41
220	83	78
310	—	4
221	—	15
113	15	19
302	—	10
311	38	37

The interatomic distances obtained from the sum of the ionic radii and by employing the appropriate coordination number correction (Seabord & Katz, 1954) are Ce^{4+}–$6Cl^- = 2{\cdot}73$ Å and Cs^+–$12Cl^- = 3{\cdot}67$ Å, in fair agreement with the above values.

The authors wish to thank Prof. E. D. Bergmann and Dr B. Gina for their interest in this study.

References

Cromer, D. T. (1965). *Acta Cryst.* **18**, 17.
Dawson, B. (1960). *Acta Cryst.* **13**, 403.
Evans, H. T. (1961). *Acta Cryst.* **14**, 689.
Hoard, J. L. & Vincent, W. B. (1939). *J. Amer. Chem. Soc.* **61**, 2849–2852.
Marcovitch, M. & Kaatz, T. (1966). *The Preparation and Properties of Dicesium Hexachlorocerate.* To be published.
Seaborg, G. T. & Katz, T. T. (1954). *The Actinide Elements.* Ch. 18, p. 769. New York: McGraw-Hill.
Siegel, S. (1956). *Acta Cryst.* **9**, 827.
Thomas, L. H. & Umeda, K. (1957). *J. Chem. Phys.* **26**, 293.
Wilson, A. J. C. (1950). *J. Sci. Instrum.* **27**, 321.
Zachariasen, W. H. (1948). *Acta Cryst.* **1**, 268.