All bonding distances and angles are within the range normally reported.

References

ABRAHAMS, S. C. & KEVE, E. T. (1971). *Acta Cryst.* A27, 157–165.
DOYLE, P. A. & TURNER, P. S. (1968). *Acta Cryst.* A24, 390–399.
GACEK, M., UNDHEIM, K., OFTEBRO, R. & LALAND, S. G. (1979). *FEBS Lett.* 98, 355–358.
GERMAIN, G., MAIN, P. & WOOLFSON, M. M. (1971). *Acta Cryst.* A27, 368–376.
GROTH, P. (1973). *Acta Chem. Scand.* 27, 1837.
JOHNSON, C. K. (1976). *ORTEPII.* Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
NORDENSON, S. & SEMMINGSEN, D. (1988). In preparation.
RISE, F. & UNDHEIM, K. (1985). *Acta Chem. Scand. Ser. B,* 39, 195–201.
STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* 42, 3175–3187.
TAYLOR, R. & KENNARD, O. (1982). *J. Am. Chem. Soc.* 104, 3209–3212.
WILLIS, B. T. & PRYOR, A. W. (1975). *Thermal Vibrations in Crystallography,* p. 102. Cambridge Univ. Press.

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Structure of Dicaesium Sodium Uranium Hexachloride

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Abstract. Cs_2NaUCl_6, $M_r = 739.55$, cubic, *Fm3m*, $a = 10.937 (1)$ Å, $V = 1308.3 (5)$ Å^3, $Z = 4$, $D_x = 3.754$ g cm^{-3}, $\lambda(Mo\ K\bar{\alpha}) = 0.71073$ Å, $\mu = 184.331$ cm^{-1}, $F(000) = 1260$, $T = 295 (1)$ K, $R = 0.039$ for 79 observed reflections. Cs_2NaUCl_6 crystallizes with the 'ideal cryolite' arrangement. The trivalent uranium (site symmetry O_h) is octahedrally coordinated to six chloride ions, each at a distance of 2.723 (9) Å. The sodium (O_h) and the caesium (T_d) ions are respectively surrounded by six and twelve equidistant chloride ions.

Experimental. The compound was obtained by heating, under a high vacuum, stoichiometric amounts of the binary halides CsCl, NaCl and UCl_3 in a quartz tube (1070–1170 K). The UCl_3 used was prepared from metal by hydriding it at 470 K, converting it to trichloride with HCl (g) at 470 K and subliming it at *ca*

1170 K. CsCl and NaCl (Merck, > 99.5% purity) were dried under vacuum at 770 K. Gradient solidification from the melt (Morss, Siegal, Stenger & Edelstein, 1970) was used to grow the single crystal (~0.25 × 0.25 × 0.25 mm) used in this study. Enraf–Nonius CAD-4 X-ray diffractometer, graphite-monochromated Mo $K\bar{\alpha}$ radiation. Cell parameters refined by least squares from angle data of 25 reflections in range 17–25° (2θ). Space group unequivocally established from systematic absences. 2569 reflections collected (θ–2θ scan mode) in range $4 \le 2\theta \le 50°$, $h\ -15/15$, $k\ -15/15$, $l\ -15/0$; 1767 reflections considered observed [$I \ge 2\sigma(I)$], averaged to 126 unique reflections ($R_{int} = 0.06$), 79 reflections with $I > 3\sigma(I)$ used in refinement. Intensities of three standard reflections measured at 30 min intervals, anisotropic decay correction applied (total decay 3.1%). Lorentz and polarization corrections. Empirical absorption corrections (trans-

Table 1. *Atomic positional and thermal parameters* (Å^2) *with e.s.d.'s in parentheses*

	x	y	z	$B(1,1)^*$ $B(2,2)$ $B(3,3)$
U	0·0	0·0	0·0	1·02 (5) 1·02 (5) 1·02 (5)
Na	0·5	0·5	0·5	1·7 (6) 1·7 (6) 1·7 (6)
Cs	0·25	0·25	0·25	3·5 (1) 3·5 (1) 3·5 (1)
Cl	0·2490 (7)	0·0	0·0	1·1 (3) 5·6 (3) 5·6 (3)

* The form of the anisotropic thermal parameter is $\exp\{-0\cdot25[h^2a^2B(1,1) + k^2b^2B(2,2) + l^2c^2B(3,3)]\}$.

mission factors range from 46·12 to 99·75%). Structure solved by Patterson method for U, remaining atoms located by difference Fourier technique; full-matrix least-squares refinement minimizing $\sum w(\Delta F)^2$. All atoms treated anisotropically. Weighting scheme based on counting statistics: $w = 1/[\sigma(F_o)]^2$, $\sigma(F_o) = \sigma(F_o)^2/2F_o$, $\sigma(F_o^2) = [\sigma^2(I) + (PI)^2]^{1/2}/\text{Lp}$, P(ignorance factor used to downweight intense reflections) $= 0\cdot05$. A secondary-extinction coefficient refined to $g = 2\cdot05 \times 10^{-7}$ $\{F_c = F_c/[1 + g(F_c)^2\text{Lp}]\}$. $R = 0\cdot039$, $wR = 0\cdot045$, $S = 1\cdot38$. Final $(\Delta/\sigma)_{\text{max}} < 0\cdot01$. Maximum and minimum heights in final difference Fourier map $+1\cdot1$ and $-0\cdot9$ e Å^{-3}. Atomic scattering factors and anomalous-dispersion terms from *International Tables for X-ray Crystallography* (1974). Enraf–Nonius (1983) *SDP* programs. Atomic coordinates and temperature factors are given in Table 1.*

Bond distances are reported in Table 2. An *ORTEP* illustration (Johnson, 1976) of the structure is given in Fig. 1.

Related literature. From X-ray powder data it is known that Cs_2NaUCl_6 (Aurov, Volkov & Chirkst, 1983; Schoebrechts, Gens, Fuger & Morss, 1988) is isostructural with other actinide analogues (Np: Schoebrechts, Gens, Fuger & Morss, 1988; Pu: Morss, Siegal, Stenger & Edelstein, 1970; Am: Morss, Siegal, Stenger & Edelstein, 1970; Bagnall, Laidler & Stewart, 1968; Soderholm, Edelstein, Morss & Shalimoff, 1986; Schoebrechts, Gens, Fuger & Morss, 1988; Bk: Morss & Fuger, 1969; Cf: Schoebrechts, Gens, Fuger & Morss, 1988), as with all similar compounds of empirical formula Cs_2NaMCl_6 for which M is a trivalent cation of ionic size within 0·6 and 1·2 Å

Table 2. *Interatomic distances* (Å)

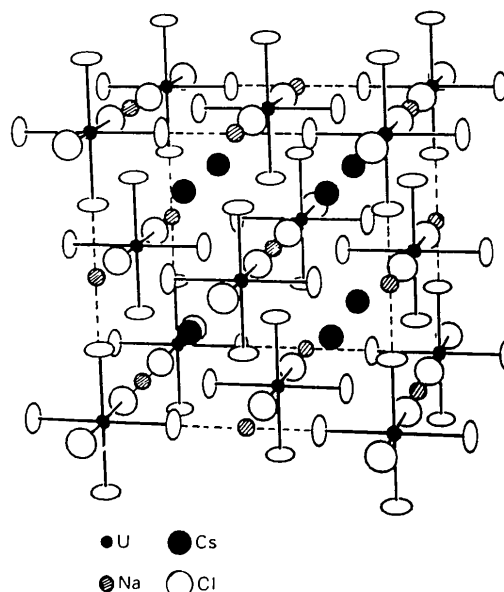| U–Cl	2·723 (9)	Cs–Cl	3·867 (8)
Na–Cl	2·746 (9)	U–U	7·734

Fig. 1. Perspective view of the crystal structure of Cs_2NaUCl_6. The thermal ellipsoids are drawn at the 50% probability level.

(Morss, Siegal, Stenger & Edelstein, 1970). The structure presents the 'ideal cryolite' arrangement described by Wells (1962) and by Cotton & Wilkinson (1966). It has been previously established for $Cs_2NaBkCl_6$ from X-ray powder pattern analysis (Morss & Fuger, 1969). The present study is the first structure analysis of a Cs_2NaMCl_6 series complex based on single-crystal X-ray data.

References

AUROV, N. A., VOLKOV, V. A. & CHIRKST, D. E. (1983). *Sov. Radiochem.* **25**, 348–353.
BAGNALL, K. W., LAIDLER, J. B. & STEWART, M. A. A. (1968). *J. Chem. Soc. A*, pp. 133–136.
COTTON, F. A. & WILKINSON, G. (1966). *Advanced Inorganic Chemistry*, pp. 443–446. New York: Interscience.
Enraf–Nonius (1983). *Structure Determination Package*. Enraf–Nonius, Delft, The Netherlands.
International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
JOHNSON, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
MORSS, L. R. & FUGER, J. (1969). *Inorg. Chem.* **8**, 1433–1439.
MORSS, L. R., SIEGAL, M., STENGER, L. & EDELSTEIN, N. (1970). *Inorg. Chem.* **9**, 1771–1775.
SCHOEBRECHTS, J. P., GENS, R., FUGER, J. & MORSS, L. R. (1988). *J. Phys. Chem.* In the press.
SODERHOLM, L., EDELSTEIN, N., MORSS, L. R. & SHALIMOFF, G. V. (1986). *J. Magn. Magn. Materials*, **54–57**, 597–598.
WELLS, A. F. (1962). *Structural Inorganic Chemistry*, pp. 369–370. Oxford Univ. Press.