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The structure of thianthrene.

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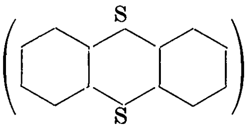
The molecular structure of thianthrene



has been determined. The unit cell is monoclinic with

$$a = 11{\cdot}97,\ b = 6{\cdot}14,\ c = 14{\cdot}53\ \text{Å}\ \text{(all } \pm 0{\cdot}3\%),$$
$$\beta = 110{\cdot}0 \pm 0{\cdot}5^\circ\ .$$

The space group is $P2_1/c$ and the unit cell contains four molecules.

The approximate structure was determined from Patterson sections and electron-density projections computed on X-RAC. At this stage of the structure determination, agreement between calculated and 'observed' structure factors was poor; for the 1700 independent reflections R was 45%. The large value of R reflected primarily uncertainties in the locations of carbon atoms which were not clearly resolved in the projections. Refinement of the structure by least-squares, using the IBM 704 computer, was therefore undertaken. The value of R dropped rapidly, in a few cycles of refinement, from 45% to 17·5%. Final refinements are still in progress to determine the extent to which variations of individual C–C bond lengths from the mean value (1·393 Å) are real, but some interesting features of the structure have been established with some certainty. The molecule is folded about the S–S axis; the dihedral angle is 127·5±0·5°. The C–S–C angle is 99·7±0·5°. The mean C–S bond length is 1·77 Å, indicating about 25% double-bond character. In the least-squares refinement, separate temperature factors were computed for each atom; the temperature factors of the carbon atoms furthest removed from the sulfur atoms were significantly greater than those computed for carbon atoms nearest the sulfur atoms.

A detailed discussion of the structure will be published shortly.

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The structures of Cs_2ThCl_6 and Cs_2UCl_6*.

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Cs_2UCl_6 and one form of Cs_2ThCl_6 are isostructural with Cs_2PuCl_5 (Zachariasen, 1948). The symmetry is trigonal and the assigned space group is D^3_{3d}–$C\bar{3}m$. Cell dimensions are given in Table 1. The observed density leads to one molecule per cell, with atoms in the following positions:

$$1\ \text{Th or U in}\ (0, 0, 0)\ ,$$
$$2\ \text{Cs in}\ \pm(\tfrac{1}{3}, \tfrac{2}{3}, u)\ ,$$
$$6\ \text{Cl in}\ \pm(x, \bar{x}, z);\ \pm(2\bar{x}, \bar{x}, z);\ \pm(x, 2x, z)\ .$$

Table 1. *Cell dimensions*

	Cs_2ThCl_6	Cs_2UCl_6
a (kX.)	7·614±0·007	7·492±0·003
c (kX.)	6·038±0·007	6·038±0·003

The coordinates, which have been deduced from the intensities of powder patterns, are shown in Table 2. These values lead to structures in which each heavy atom is bonded to 6 chlorines at the corners of slightly distorted octahedra, with Th–6Cl = 2·81 Å (2·80 Å) and U–6Cl = 2·75 Å (2·74 Å). Values given in parentheses correspond to ionic radii sums for sixfold coordination, using recent values for the Th^{+4} and U^{+4} radii (Seaborg & Katz, 1954). For the thorium salt, each cesium is bonded to 12 chlorines, with 3 chlorines at distances of 3·63 Å, 3 at 3·69 Å, and 6 at 3·82 Å, giving a weighted average of 3·74 Å. For Cs_2UCl_6, the twelvefold distribution is similar with 3 chlorines at 3·62 Å, 3 at 3·64 Å, and 6 at 3·76 Å, giving a weighted average of 3·70 Å. The average values may be compared with the ionic radii sum of 3·67 Å for exact twelvefold coordination in the Cs^+–12 Cl^- bond.

Table 2. *Coordinates for chlorine and cesium*

	Cs_2ThCl_6	Cs_2UCl_6
x	0·178±0·007	0·179±0·009
z	0·256±0·006	0·24 ±0·01
u	0·750±0·006	0·743±0·006

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* Based on work performed under the auspices of the U.S. Atomic Energy Commission.