
The structure of the commensurate modulated phase IV was determined by single crystal X-ray diffractions at 446 K. Space group: P11n(No. 7), Z = 2, a = 2.157(3), b = 5.818(1), c = 43.654(3), T = 89.97(1)°, V = 21.252 Å³, D = 2.98 ± 0.03 g/cm³, R = 0.037, Rs = 0.047 for 1862 reflexions (RI0).

The fivefold superstructure parallel c is caused by the ordering of the SO₄ tetrahedra. If we designate a right-handed (left-handed) rotation around a by (+) then the sequence of the SO₄ groups in one unit cell can be described by: ++++++ (phase I''), phase III:+++, phase IV:++-++-- (phase III'), phase V:++-+- +--+ (phase IV').

To facilitate the comparison of the different phases, refinements of the high temperature phases were performed using split groups in one unit cell. The structure is characterized by tetrahedral S⁻⁺⁻⁻⁺⁻ and exhibit strong stereochemical activity of the lone 6s electron pair of univalent thallium. The compound is isostructural with Ge₂GeS₄, which contains a Ge(II) atom (mean distance Ge-S = 2.619 Å, b = 2.268(17); 3: 2.619(3), 2.231(7); 4: 2.249(12); 5: 2.607(8), 2.268(17); 6: 2.770(1), 2.218(8); 7: 2.619(3), 2.231(7); 8: 2.804(7), 2.145(34).

08.2-27 STRUCTURE AND BONDING IN URANIUM(IV) COMPLEXES CONTAINING THE UO₂X₂ (X = Cl, Br) CHROMOPHORE. By J.P de Wet and M.A Cairns, Crystallography Group, Chemistry Department, University of Port Elizabeth, Port Elizabeth, South Africa.

In octahedrally co-ordinated complexes of uranium containing the UO₂X₂ (X = Cl, Br) chromophore the bonding distances involving uranium have been observed to display a complementary axial-equatorial relationship with U-O bond lengths observed in these complexes. The structural determinations were carried out on six further U(IV) complexes of the type UO₂X₂ (Table I), with X = Cl, Br. The structure determinations were based on data in which errors due to absorption were minimized as far as possible.

The U-X and U-O bond lengths observed in these structures confirm and extend the evidence found previously for axial-equatorial relationships (loc. cit.), with mean values (in Å) for U-X and U-O in each structure, respectively: 1: 2.605(3), 2.248(16); 2: 2.604(8), 2.248(12); 3: 2.607(8), 2.268(17); 4: 2.770(1), 2.218(8); 5: 2.619(3), 2.231(7); 6: 2.804(7), 2.145(34).