24.1-20  HIGH PRESSURE X-RAY DIFFRACTION STUDY OF ACTINIDES AND ACTINIDE COMPOUNDS BY AN ENERGY-DISPERSIVE METHOD. U. Benedict, CEC Joint Research Centre, European Institute for Transuranium Elements, P.O.Box 2266, D-7500 Karlsruhe 1, and K.B. Holzapfel, University of Paderborn, Experimentalphysik, Pohlweg 53, D-4790 Paderborn, F.R.G.

Actinide metals and compounds were investigated in a Holzapfel type diamond anvil cell at pressures up to 40 GPa. Measuring time is kept within the range of ten minutes to some hours by the use of a conical slit for the diffracted radiation which makes use of the complete diffraction cone. The pressures were determined from the lattice parameters of the marker substances NaCl and CsCl or with the ruby fluorescence monometer.

Studies of thorium metal (G. Bellussi, U. Benedict, W.B. Holzapfel, J. Less Common Metals 74(1981)147-153) and of stoichiometric uranium dioxide were completed. Investigation of uranium metal (together with I. Sirkel) and of other actinide materials is under way. Uranium dioxide gradually transforms to a low symmetry high pressure phase in the range 29 to 38 GPa. On release of pressure, a marked hysteresis to transformation is observed, but complete retransformation to the fluorite type occurs between 15 and 5 GPa. Among the known high density Ab structure types, the lead chloride type gives the best match with the observed high pressure phase, using the atom coordinates of thorium disulfide in the L23 PULVERIX program. Lattice parameters a=859, b=390, c=676 (pm; Pnma setting) are obtained when approximate lattice parameters estimated from the volume compression on transformation are refined by Taupin's indexing program.

Single-peak fitting of the data obtained for uranium metal up to 6.6 GPa gives a bulk modulus B=126.6 GPa and the elastic constants e11=3.627, e22=2.191, e33=1.956 (10 TPa-1).

24.1-22  ON THE RELATION OF BINARY SYSTEM DIAGRAMS. By L.I. Salipuz, E.M. Benzon, Yu.S. Ikonyayev and N.V. Belov, NII, The Institute of High Pressure Physics, Moscow, USSR.

One of the most important problems in chemistry and crystal chemistry is the establishment of compositions and structures for all possible phases. In regard to this problem, all diagrams of e-elements and d-elements of the Mendeleev table were observed, and all phases from these diagrams were systematized. In the 350 diagrams researched there are 882 phases differing in composition and structure. These phases were divided into two groups: basic and supplementary.

The compositions of basic phases correspond with the simple component ratios A:B = 3:1, 2:1, 1:1, 1:2, 1:3, supplying 386 basic phases from a total of 882. In the sequence of basic phases A2B-2A-B-AB-PB2 found in the diagrams, for each phase was shown all neighboring phases into which it transforms (reconstructs) when its composition changes. In this way all basic phase groupings (BPG) were illustrated. It was shown to which ST these phases correspond, so that the two basic phases enter into the BPG with their corresponding ST. Complete groupings of all five basic phases (CBF5) are found only in some diagrams. In most cases there are incomplete basic phase groupings (BFG). BFG from individual diagrams and BFG common to many diagrams permit the establishment of a system of phase interrelationships for all observed diagrams. This system shows groupings of coexisting neighbour phases (CEC). The existence of CEC shows that the transformations of ST are limited in direction and number. This system of phase interrelationships, representing a composite of all ST and their interrelations, ensures easy access to and easy handling of the given material. Because the CEC is shown for each phase, the system is more informative than individual diagrams - it shows not only existing, but also potential relationships between phases. This system, therefore, can be used in the prediction of phases in the diagrams, where new phases are possible along with those already known. With the help of the known composition of new phases, it is possible to predict ST.