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 W.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 manometer.

Studies of thorium metal (G. Bellussi, U. Benedict, W.B. Holzapfel, J. Less Common Metals 78(1981)147-153) and of stoichiometric uranium dioxide were completed. Investigation of uranium metal (together with I. Birkel) 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_2 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 LAZY-PULVERIX program. Lattice parameters a=559, b=350, 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_0=128.6 GPa and the elastic constants ε_{11}=3.627, ε_{22}=2.191, ε_{33}=1.956 (in TPa^{-1}).

24.1-21 TWINNING BY PSEUDO-MEROHEDRY IN $(NH_4)_2ZnCl_4$. By H. v. Koningsveld, Lab. of Technical Physics, Delft University of Technology, Postbox 5046, 2600 GA DELFT, The Netherlands.

Some time ago we tried to refine the structure of $(NH_4)_2ZnCl_4$ in space group $P2_1cn$. Satisfactory agreement could not be achieved. Therefore the correctness of the space group was doubted. Recently, papers on the same compound were published by I. Mikhail (Acta Cryst. (1980) B36, 2126) and by J. Warczewski (Kristall u. Technik (1980), 667). Both authors adopted the orthorhombic space group $P2_1cn$. The anisotropic thermal parameters given by Mikhail show some anomalous values which do not find a reasonable explanation. Warczewski determined the space group photographically and a small difference in general (pseudo-orthorhombic) reflection intensities can easily have been overlooked. This confusion about the space group induced us to examine our data more closely. Systematic extinctions, h0ℓ for ℓ=odd, are obvious from our data set but several hk0 reflections with (h+k)=odd are significantly different from zero. Six general reflections were accurately remeasured from several crystals. The results clearly prove monoclinic symmetry. The systematic extinctions are consistent with space group P2/c or Pc. The polar space group Pc is chosen because of the pyroelectricity effect observed (J. Warczewski, Kristall u. Technik (1980), 667). In some crystals the apparent mmm symmetry, due to twinning and to the pseudo-orthorhombic lattice, can lead to an incorrect determination of the space group. All measured crystals exhibit twinning by pseudo-merohedry with obliquity (apparently) equal to zero (H. Catti and G. Ferraris, Acta Cryst. (1976) A32, 163). The twinning ranges from a small amount to nearly equal fractions of the individual crystals in the twin. A graphical representation of the results is given illustrating this twinning phenomenon.

24.1-22 ON THE RELATION OF BINARY SYSTEM DIAGRAMS. By N.L. Smirnova, E.M. Berzon, Yu.S. Konyaev and N.V. Belov, MGU, 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 f-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 586 basic phases from a total of 882. In the sequence of basic phases $A_3B-A_2B-AB-AB_2-AB_3$ found in the diagrams, for each phase were shown all neighbouring phases into which it transforms (reconstructs) when its composition changes. In this way all basic phase groupings (BF6) were illustrated. It was shown to which ST these phases correspond, so that the basic phases enter into the BF6 with their corresponding ST. Complete groupings of all five basic phases (CBF6) are found only in some diagrams. In most cases there are incomplete basic phase groupings (IBF6). BF6 from individual diagrams and BF6 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 (C6). The existence of C6 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 C6 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.