

an ordered cation vacancy in 3b sites of the structures. Nevertheless, a remaining electron-density of about $3e^-/A^3$ and diffuse strikes observed on precession films indicate, that the assumed rhomboedric space group $R\bar{3}m$ failed.

Table 1 Hexagonal cell parameters

$Ba_2K Ni_2F_9$	a=b= 577.5(2)	c= 2075.6(13)pm
$Ba_2RbNi_2F_9$	a=b= 580.1(1)	c= 2099.4(2)pm
$Ba_2RbFe_2F_9$	a=b= 594.9(1)	c= 2083.7(1)pm
$Ba_2CsNi_2F_9$	a=b= 585.5(1)	c= 2120.9(9)pm
$Rb_4FeFe_2F_{12}$	a=b= 589.1(1)	c= 2903.6(2)pm

08.2-64 INVESTIGATION OF A STOICHIOMETRY OF A METASTABLE CRYSTAL PHASE OF BISMUTH CADMIUM OXIDE WITH SYLLEN'S STRUCTURE BY REITWELD'S METHOD. By S.D.Kyrik, V.A.Kutvitsky, S.V.Misjul, T.I.Karyagina; L.V.Kirensky Institute of Physics, USSR Academy of Sciences, Siberian Branch, 660036 Krasnoyarsk, USSR
The refinement of structure for bismuth cadmium oxide with composition of $5Bi_2O_3 \cdot CdO$ has been carried out by Reitweld's method. Lattice constants are $a=10,220 \text{ \AA}$, $SG - I23$, $R_{prof} = \frac{\sum |y(obs) - y(calc)|}{\sum |y(obs)|} = 0,082$; $R_i = \frac{\sum |I(obs) - I(calc)|}{\sum I(obs)}$ ($I(obs)$, $I(calc)$ are the observed and calculated integral intensities of each reflection; $y(obs)$, $y(calc)$ are the observed and calculated profile point data). The density of charge for tetrahedral sites (2a) of 74e was obtained, that agrees with scheme of Craig and Stephenson (D.C.Craig, N.C.Stephenson, J.Solid State Chem,(1975), 15, 1). For 24f site the density of charge is 70% less than it is for Bi atom. It is explained by the substitution for the Bi part in 24f by Cd. The stoichiometry of compound corresponding by the obtained population coefficient is Bi:Cd = 19:7. Ions Cd (0,67 in the unit cell) located in (2a) lead to the shift of 2,68(0,67·4) oxide atoms being the top of octahedra. The filling of decreased octahedra is realized by Bi ions (Cd ones are too large for this purpose). The charge compensation is provided by the arrangement of 5,36 Cd ions in structure. Finally, cell contains 6Cd and 20Bi. This corresponds to the chemical analysis and to refinement of the structure.

08.3-1 $Y_{13}Pd_{40}Sn_{31}$, A NEW STRUCTURE TYPE INTERPRETED AS AN INTERGROWTH OF SIMPLE STRUCTURE BLOCKS. By K. Cenxual and E. Parthé. Laboratoire de Cristallographie aux Rayons X, Université de Genève, 24 quai Ernest Ansermet, CH-1211 Genève 4, Switzerland.

$Y_{13}Pd_{40}Sn_{31}$, hexagonal, $a = 19.891(7)$, $c = 9.246(6) \text{ \AA}$, $P6/mmm$, crystallizes with a new structure type containing 168 atoms in the unit cell. In a recent crystal-chemical study of the structures of rare-earth-transition metal-borides, silicides and their homologues (Parthé & Chabot (1984) in "Handbook on Physics and Chemistry of Rare Earths" Vol. 6, ch. 48) it was shown that a successful approach to the understanding and memorizing of complicated ternary alloy crystal structures is their interpretation as an intergrowth of segments of different simple, binary or ternary structures. The $Y_{13}Pd_{40}Sn_{31}$ structure can be described as an intergrowth of three kinds of segments: one is a ternary ordering variant of the $CaCu_5$ -type, the second has an atom arrangement similar to that found in the neighbouring phase YPd_2Sn with $MnCu_2Al$ -(Heusler) type structure (Ishikawa et al. (1982) in "Superconductivity in d- and f-Band Metals", Proc. IVth Conf., Kernforschungs-zentrum Karlsruhe), a derivative of the BCC W-type, and the third one consists of a column of trigonal prisms where Pd centred Sn prisms alternate with Sn centred Pd prisms.

It will further be shown that in another ternary stannide structure type, $CeNi_5Sn$ (Skolozdra et al. (1981) Sov. Phys. Crystallogr. 26, 272) binary $CaCu_5$ -type slabs are intergrown with ternary Heusler type slabs.

A detailed account of the present work will be published in Acta Crystallogr. C.

08.3-2 AN ENERGETICAL INTERPRETATION OF THE α Mn STRUCTURE. By K.Schubert, Max Planck Institut für Metallforschung, Inst. f. Werkstoffwiss., Stuttgart, F.R.Germany
The structure of α Mn has been found for instance in the alloy system Mo-Re which may be interpreted by the two-electron-correlations model (Chem.Script.(1982)19,224). The interpretation becomes possible by the electron count $Mo_{1,5,8}Re_{0,7}$ yielding for $Mo_3Re(Cr_3Si)$ type cells $b'b$, c of the spatial correlations which obey the equations $\bar{a} = b'F(1) = bF(2) = cB(4)$ where a =crystal cell matrix, $b'F=5s$ -electron correlation cell of the cubic face centered type, $bF=4d$ -electron correlation cell, cB =peripheral core electron correlation cell of the cubic body centered type, (1)=unity commensurability matrix, (2)=2(1). The assumption of several spatial correlations corresponds to the existence of several energy bands in Mo-Re. At higher Re content the phase $Mo_2Re_3(\beta U)$ type is stable. It is a contractive homeotype of Mo_3Re as the so called secondary layers (Frank, Kasper, Acta Cryst.(1958)11,184,12,483) go over from the Schläfli type 4f4 to 4343f2. The contraction is in agreement with the rule that a decrease of the b -concentration causes closer packed structures. The electron correlations satisfy $a=(9.5;4.9)\bar{A}=bHT(5;3/2)=cU(\sqrt{50};4.5)$ where HT=hexagonal isometric Bravais lattice cell in pseudo tetragonal aspect, U=tetragonal body centered isometric lattice cell. The cell bF in Mo_3Re has changed to bHT in Mo_2Re_3 and cB to cU ; for the brief notation of the commensurabilities see (Chem.Scripta (1982)19,224). The phase $Mo_2Re_3(\alpha Mn)$ type is a stacking homeotype of βU and allows the correlations $a=bC(5)=cU(\sqrt{50};9)$ where C=cubic primitive lattice; the cell bHT in Mo_2Re_3 has changed to bC in $MoRe_3$ and cU has been conserved. The correlations explain the stacking homeotypism of $MoRe_3$ by the rule for stacking in $Cu(3-N)AuZnN$ (Schubert, Kristallstrukturen zweikomponentiger Phasen, Berlin 1964 p.99) The electron concentration $N_e^C=2.16$ is compatible with the valence of Mn found by Humé-Rothery (Phil.Mag.(1948)39,89) in the mixtures Cu-Zn and Cu-Al.