08.2–48   CRYSTAL STRUCTURES OF SYNTHETIC IRON AND ALKALI METALS PHOSPHATES. By O.V.Yakubovich,M.A.Simonov,O.K.Mel'nikov,Departement of Geology,Moscow State University,Moscow,USSR.

The crystal structures of four orthophosphates were determined using the X-ray structure analysis methods(4-circle "Syntex" P$\bar{1}$ diffractometer,λMoK_α-radiation,specialized E-XTL computing system).

n°	compound	unit cell parameters(Å)		sp.gr.	z	number of ref.	R$_{hkl}$ (%)
1	KFe$_4^{2+}$[PO$_4$]$_3$	a	6,273(3)	Pmnn	4	1112	4,1
		b	16,513(8)				
		c	9,808(4)				
2	H$_{1,5}$Fe$_{0,5}^{3+}$Na$_5$ [PO$_4$]$_2$F$_2$	a	10,463(7)	P$\bar{3}$	3	1136	6,3
		c	6,596(4)				
3	Na$_3$Fe[PO$_4$]$_2$ (OH)$_2$F	a	9,050(2)	P$\frac{4}{m}$nm	4	500	6,0
4	K$_2$Na$_5$Fe$_7^{2+}$Fe^{3+} [PO$_4$]$_{12}$(OH)$_2$	a	16,53(2)	C$\frac{2}{c}$	4	3056	3,9
		b	10,084(9)				
		c	24,64(3)				
		β	105,75(7)°				

The structures were solved without chemical analysis data. The formulae were obtained by structure determination. The presence of K,Na Fe,P,F in the composition of the compounds is confirmed by qualitative X-ray spectral analysis data. The Fe^{3+} cations are located in octahedra(2,3). The Fe^{2+}polyhedra (1,4) are octahedra and five-vertex figures(orthorhombic pyramids, distorted trigonal bipyramids). The anion tetrahedra(4),octahedra(2),seven-vertex-(3,4),eight-vertex-(4) and nine-vertex figures (3) are singled out around the larger Na$^+$, the distorted trigonal prisms(1),eight-vertex figures and octahedra(4) show up around K$^+$

The cation function of hydrogen atoms was revealed on the basis of the analysis of local valency balance on anions in (2). In the structures some positions are statistically half occupied by Fe(2) and Na(3) For the structure of synthetic arrojadite(4), a number of positions is occupied statistically incompletely by Fe^{2+},Na,K,P. Two P-tetrahedra are linked via a common face, one is filled up statistically by 75%,while the other - by 25%.

08.2–49   POLYTELLURIDES OF THE EARLY 3d-TRANSITION METALS. By Kurt O. KLEPP Institut für Anorganische Chemie, Technische Hochschule Aachen, D-5100 AACHEN (F.R.G.)

Though the ditellurides of Mn, Fe and Co with pyrite or marcasite structure are well known, no polytellurides of the earlier 3d-transition metals have so far been described. Synthesis at moderate temperatures (<700K) has led to the detection of the first polyanionic tellurides of V and Cr. They crystallize with novel and peculiar structures.

VTe$_2$, s.g. C2/m with a = 14.341(5), b = 3.595(2), c = 9.051(3) Å, ß = 109.51(3)°, Z = 6, crystallizes with a layered structure. The layers are built up by edge-sharing VTe$_6$-octahedra and run parallel to (201). The formation of Te-Te-bonds within the layers causes severe distortions of the octahedra. The polyanionic group formed is an infinite zig-zag-chain running parallel to the b-axis. The Te-Te distance within the chain is 2.84 Å, the bond angle is 78.5°.

CrTe$_{1.95}$Cl$_{0.05}$, s.g. P2$_1$/m with a = 14.174(8), b = 3.863(3), c = 14.552(8) Å, ß = 96.44(4)°, Z = 10, was obtained by a transport reaction with HCl/AlCl$_3$. Though a chromium ditelluride does not exist under ordinary conditions, a compound very close to this composition is stabilized by less than one wt% chlorine. The crystal structure is characterized by an infinite framework of CrTe$_6$-octahedra sharing edges and faces. There are four Te$_2$-pairs in the unit cell, the average bond distance is 2.80 Å. Cl in part replaces one of the ten crystallographically independent tellurium atoms.

CrTe$_3$, s.g. P2$_1$/c with a = 7.887(6), b = 12.22(2), c = 11.56(1) Å, ß = 118.41(2)°, Z = 8, is characterized by a layered structure. The layers (Fig.1) run parallel to the bc-plane. They are built up by tetrameric units of edge-sharing CrTe$_6$-octahedra which are in turn linked together by common Te-atoms and Te-Te bonds. The polyanionic species formed are Te$_2$-pairs as well as Te$_3$-chains. The Te-Te-bond distances are close to 2.81 Å, the bond angle within the chain is 86.17°.

Magnetic measurements on these compounds are in progress. Their results and a discussion of the crystal structures will be given at the conference.
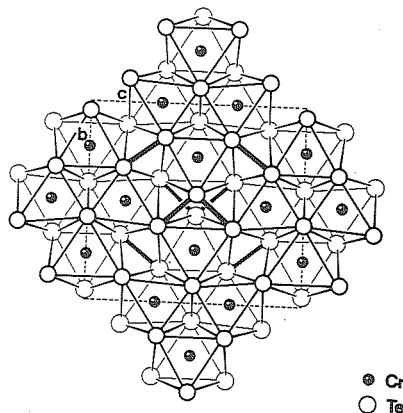

Fig 1) The infinite layers of CrTe$_3$. Te-Te-bonds are indicated by bold lines.