24.1-01 ORDERING OF THE $Pd_{60}Cu_{40}$ ALLOY METALLIC LATTICE AT HYDROGENATION. V.F.Degtyareva, V.E.Antonov, I.T.Belash, E.G.Ponyatovsky. Institute of Solid State Physics, USSR Academy of Sciences, 142432, Chernogolovka, USSR

The electrical resistance of the $Pd_{60}Cu_{40}$ alloy hydrogenized at $P \leqslant 20$ kbar and $T=200^{o}C$ increases during ~50 min, then it remains almost unchanged. Exposure of the sample at $T > 200^{o}C$ decreases the electrical resistance irreversibly, that is the evidence of the non-reversible phase transition. An X-ray study of the hydrogenated samples was made after cooling and subsequent releasing the pressure to atmospheric. For the samples hydrogenized at $T=200^{o}C$ the metallic lattice had a f.c.c. structure with $a=3,897 \pm 0,005$ A (at $-190^{o}C$). This phase should be considered as a hydrogen solid solution on the base of initial f.c.c. lattice of alloy. Samples hydrogenized at $T \geqslant 200^{o}C$ had the metal sublattice, which may by described on the base of a face centered tetragonal pseudo-cell with parameters $a=3,958 \pm 0,08$; $c=3,828 \pm 0,012$A; $c/a=0,967$ (at $-190^{o}C$). The hydrogen content in both cases was $n \lessapprox 0,5$. At the hydrogen release from the samples after annealing at $300^{o}C$, their metal sublattice retained its tetragonal distortion, the degree of tetragonality even increased . These seem to be favourable for the assumption that the observed tetragonal distortions are due to the atomic ordering of the metal sublattice itself occuring in the $Pd_{60}Cu_{40}$-H solution. This assumption is supported by appearance of superstructural diffraction lines in addition to the basis ones.

24.1-02 THE CRYSTAL CHEMISTRY OF DOUBLE SYSTEMS OF VANADATE PYROXENES $M^{+}VO_3$ (M=Li,Na, K,Rb,Cs). R.S.Bubnova, S.K.Filatov, V.S.Grunin, Z.N.Zonn, I.V.Roshdestvenskaya, Institute of silicate chemistry, USSR Academy of Sciences, Leningrad, USSR.

In the $Na_XLi_{2-X}V_2O_6$ system of clinopyroxenes rare continuous isomorphism for Li-Na has been found in the range room-melting point temperatures. The crystal structures of members with X=0.15, 0.66, 1.00 (Бубнова et al, Кристаллография , (1980) 25, 1287), 1,40 and 2.00 have been determined. The space group is C2/c, diopside structural type. In particular:

	X=0.15, R=0.039			X=0.66, R=0.036		
	$x \cdot 10^5$	$y \cdot 10^5$	$z \cdot 10^5$	$x \cdot 10^5$	$y \cdot 10^5$	$z \cdot 10^5$
V	28854	09452	26441	28914	09277	25211
M1	50000	41957	25000	50000	41683	25000
M2	50000	21426	75000	50000	20812	75000
01	11522	10951	16420	11637	09790	15259
02	35469	27029	28328	35218	26342	29165
03	35505	-02561	07009	35617	-00602	04607

In the structure of $NaVO_3$ the Li atoms substitute at first the Na atoms in M1-octahedra up to $LiNaV_2O_6$, and then in M2-octahedra up to $LiVO_3$. The temperature deformations of monoclinic crystals of that series are highly anisotropic. The largest α_2 axis of the deformation tensor is oriented along b-axis, the smallest (negative) α_1 axis is placed near the acute bisectrix of β angle of monoclinity. The degree of $(\alpha_3 - \alpha_1)$ anisotropy of monoclinic ac plane correlates with the speed of β angle change, and decreases with increasing temperature and during the transition from the end members of series to the middle ones.

In the $NaVO_3$(clinopyroxen) - KVO_3(orthopyroxen) system, when $Na/K \geqslant 1$, the isomorphism appears near the end members of series at room temperature and becomes unlimited at 400-450°C. The isomorphism is limited when $Na/K < 1$.

In the orthopyroxen KVO_3-$RbVO_3$ system continuous isomorphism is accompanied by almost linear changes of cell dimensions. In the KVO_3-$CsVO_3$ system isomorphism is limited by intervals 0≈10 and ~90-100 mol.% in system KVO_3-$CsVO_3$.

24.1-03 INFLUENCE OF OPTICAL PUMPING ON FERROELECTRIC PHASE TRANSITION IN PROUSTITE Ag_3AsS_3. I.M.Shmytko, V.Sh.Shekhtman, V.I. Ivanov, Institute of Solid State Physics, the USSR Academy of Sciences, Chernogolovka, Moscow district, 142432, USSR.

Influence of optical pumping on a ferroelectric phase transition of the first order has been investigated in Ag_3AsS_3 at 28K by the method of low-temperature diffractometry. Optical pumping was realized from a highpressure xenon lamp. Temperature hysteresis reduced markedly at 10^5lx and practically vanished at 10^6 lx. If the optical pumping is kept constant at $1-1,5 \cdot 10^6$ lx there appears an interval $\Delta T \sim 1K$ where the self-oscillating regime of the phase transition, i.e. para-ferro-para state ($R3m \leftrightarrow PI$) takes place. Period of oscillation recorded diffractometrically by the reflection intensity of one such phase is 1,5 sec. The effect was observed when the integral power of illumination was high and it vanished when the spectral composition of the incident light lay within the energy gap ($\lambda \simeq 0,6$ mkm). Within the framework of the phenomenological theory of the local field equations, the observed instability of the phase state is related to the appearance in the crystal of a constant electric field due to the optical detection. The employment of an intermittent light involved a drop in the intensity from which the self-oscillations began. At low frequences of the light pulsations the self-oscillations were periodically recurrent in the nature, i.e. the crystal passed over one of the stable (para

or ferro) states. Time between the passages depended on the light intermittence frequency; the self-oscillating regime was reestablished at 10^3 Hertz. Thus, the characteristic time of the physical process that checks the effect is not more than 10^{-3} sec. This also agrees with the assumption of the role of nonlinear effects.

In this manner such processes as the diffusion of excited electrons should be excluded from consideration. The unsuitability of the model of the photovoltaic effect is supported by the results of an independent determination of the change of the lattice parameter. It is shown that the temperature of phase transition increases at high levels of optical pumping, whereas for the proustite (ΔE_g/para < ΔE_g/ferro) the photovoltaic effect has to result in the temperature drop.

24.1-04 THE CALCULATION OF THE STRUCTURAL PARAMETERS FOR THE PYROCHLORE FAMILY OF STRUCTURES. THE STABILITY REGIONS OF THE PYROCHLORE TYPE STRUCTURE. By Ja.E. Cherner, G.A. Gegusina, E.G. Fesenko, Institute of Physics, Rostov State University, Rostov on Don, USSR

The method of real and hypothetical pyrochlores bond lengths and lattice parameters calculation from the chemical composition is presented. The calculated interatomic distances and lattice parameters differ from the experimental ones by 1.5 % and 0.3 % respectively. The established connection between chemical composition and lattice parameters allows 1) to establish the reliability of the experimental structure data; 2) to predict the chemical composition on the basis of precise lattice parameter measurements. By means of the method presented the pyrochlore type structure stability regions are established and the method of the prediction of the formation pyrochlore type compounds having the pre-assigned composition is developed. The efficiency of the above methods is empirically confirmed.

24.1-05 COMPOSITION AND CRYSTAL STRUCTURES OF DOUBLE MOLYBDATES OF UNI- AND BIVALENT METALS. By R.F.Klevtsova, V.G.Kim, L.A.Glinskaya, P.V. Klevtsov, Institute of Inorganic Chemistry, Sib.Dept.Acad.Sci.USSR, Novosibirsk, USSR.

When studying a phase formation in $M_2^{+}MoO_4$ - $R^{2+}MoO_4$(M=Li,Na,K,Rb,Cs; R=Mg,Ni,Co,Fe,Cu,Zn) systems, compounds with the initial component ratios 2:1,1:1,1:2,1:3,1:5 have been found, i.e. 1)$M_4R(MoO_4)_3$; 2)$M_2R(MoO_4)_2$; 3)$M_2R_2(MoO_4)_3$; 4)$M_2R_3(MoO_4)_4$; 5)$M_2R_5(MoO_4)_6$. The synthesized double molybdates have been studied by differential thermal analysis and X-ray methods. The single crystals of these compounds have been grown by the flux method using the melts of the alkaline metal polymolybdates as a solvent. The X-ray study has revealed 12 structure types at the present stage. The tetrahedral coordination of Mo atoms is common to the structures determined. A variety of structure types results from the difference in the coordination of R- and M-polyhedra and ways of their joint. The following kinds of R-polyhedra have been found: tetrahedra and polyhedra with five vertices for some compounds of Zn, slightly distorted octahedra in compounds with Mg,Ni,Co,Fe and largely deformed octahedra with a characteristic distance differentiation (4+2) in compounds of Cu. The coordination numbers for univalent cations vary from 6 to 12. The following extents of the R-polyhedra polymerization have been observed: isolated polyhedra, a pair of edge-sharing octahedra, links of a wolframite-like band of four or six octahedra and an infinite chain of octahedra.

24.1-06 CRYSTAL STRUCTURE FEATURES OF A SERIES OF DERIVATIVES OF 1,2,4-TRIAZOLE. By G.L. Starova, O.V. Frank-Kamenetskaya, V.A. Frank-Kamenetsky, Department of Crystallography, Leningrad State University, Leningrad, U.S.S.R.

On the basis of X-ray crystal structure data of six compounds [1,2,4-triazole, $C_2H_3N_3$, Goldstein et al., Acta Cryst. (1969) B25, 135, (I), 5-amino-1H-1,2,4-triazole, $C_2H_4N_4$, (II), 3,5-diamino-1H-1,2,4-triazole, $C_2H_5N_5$, (III), 3-nitro-1H-1,2,4-triazole, $C_2H_2N_4O_2$, (IV), Closset et al., Bull. Soc. Chim. Belg. (1975) 84, 1023; bis-(3-nitro-1H-1,2,4-triazolyl-5) dihydrate, $C_4H_2N_8O_4.2H_2O$, (V), 3-nitro-(3'-chloro-1H-1,2,4-triazolyl-5,1'), $C_4H_2N_7O_2Cl$, (VI)] (Table) we established the following: 1) Tautomerism. In the crystals of all compounds, the molecules exist in the asymmetric tautomeric form. The ring proton is located near the donor (II) and far from the acceptor (IV) substituent. 2) Conformation. The substituents are insignificantly inclined to the ring plane. Only (III) is not flat. The bis-nitrotriazolyl molecules are centrosymmetric (V) or pseudocentrosymmetric (VI). 3) Molecular interaction. The ring proton participates in strong hydrogen bonds in the crystals of all compounds. All triazole molecules, except (V), interact by N-H...N hydrogen bonding. The triazole ring in (V) is connected with water molecules by N-H...O bonds. Van der Waals forces represent the main bond type in this crystal.