

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 ($\Delta E_0/\text{para} < \Delta E_0/\text{ferro}$) the photovoltaic effect has to result in the temperature drop.

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)

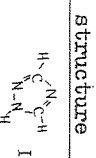
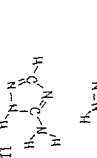
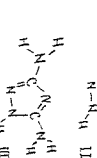
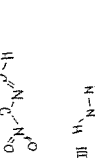
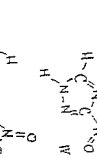
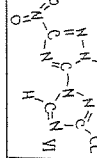
systems, compounds with the initial component ratios 2:1, 1:1, 1:2, 1:3, 1:5 have been found, i.e. 1) $M_4R(MoO_4)_3$; 2) $M_2R(MoO_4)_2$; 3) $M_2R_2(MoO_4)_3$; 4) $M_2R_3(MoO_4)_4$; 5) $M_2R_5(MoO_4)_6$. The synthesized double molybdates have been studied by differential thermal analysis and X-ray methods. 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.

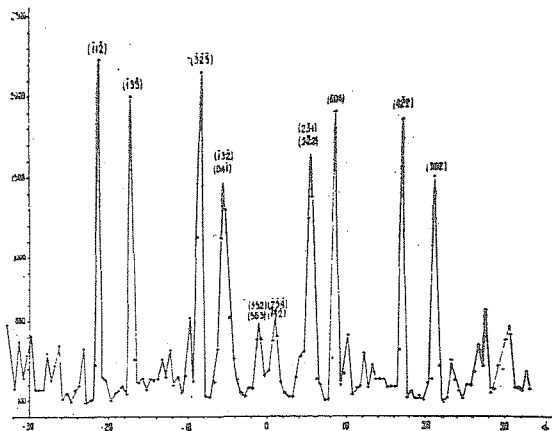
24.1-04 THE CALCULATION OF THE STRUCTURAL PARAMETERS FOR THE PYROCHLORE FAMILY OF STRUCTURES. THE STABILITY REGIONS OF THE PYROCHLORE TYPE STRUCTURE. By Ja.E. Cherner, G.A. Gegusina, E.G. Fesenko, Institute of Physics, Rostov State University, Rostov on Don, USSR

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.

24.1-06 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, $C_2H_4N_4O_2$, (IV), Closset et al., Bull. Soc. Chim. Belg. (1975) 84, 1023; bis-(3-nitro-1H-1,2,4-triazolyl-5) dihydrate, $C_4H_2N_8O_4 \cdot 2H_2O$, (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.

Molecular structure	Hydrogen bonds		Structure model
	A...A	H...A	
	N...N=2.821, C...N=2.500,	H...N=1.83Å, H...N=2.48Å,	<NHN=160° <CHN=147°
	N...N=2.896, N...N=3.080, N...N=3.135,	H...N=2.04Å, H...N=2.27Å, H...N=2.25Å,	<NHN=171° <NHN=154° <NHN=161°
	N...N=2.947, N...N=2.992, N...N=3.101, N...N=3.145,	H...N=2.12Å, H...N=2.11Å, H...N=2.29Å, H...N=2.36Å,	<NHN=161° <NHN=168° <NHN=146° <NHN=151°
	No data		
	N...O=2.650, O...O=3.060,	H...O=1.74Å, H...O=2.23Å,	<NHO=174° <OHO=155°
	N...N=2.922,	H...N=1.96Å,	<NHN=179°
			Chain around 2 ₁
			Corrugated sheets
			Chain around 2 ₁
			Chain along [101]
			Chain along a



Multiple X-ray scattering in FeBO₃.
MoK α . Refl.(111).

24.1-07 MULTIPLE X-RAY SCATTERING BY RHOMBOHEDRAL CRYSTALS. N.N.Faleyev, V.G.Labushkin. Gosstandart, Moscow, USSR.

The multiple X-ray scattering (Renninger's effect (Renninger M., Zeit. Kryst. 113, 99, 1960) was observed in ferrous hematite and borate crystals. X-ray scattering was studied in the direction of forbidden reflections (111), (333), and (555). The evidence for multiple scattering was provided by periodic occurrence of peaks in the process of crystal rotation about the diffraction vector $\vec{\tau}$. In accordance with the symmetry of the reciprocal lattice of the crystals studied the peaks recur every 60°; besides, they are symmetrical relative to the zero mark.

The ratios of the peak intensities to the permitted reflection intensity amount to 1×10^{-4} - 2×10^{-3} . Thus, the effect observed in crystals of rhombohedral symmetry should be taken into account when the nuclear levels are studied in the crystals of this kind by means of synchrotron radiation, as well as in solving other related physical problems.

24.1-08 X-RAY STUDIES OF MAGNETIC STRUCTURE OF ANTIFERROMAGNETIC NiO AND MnO CRYSTALS. N.N.Faleyev, A.A.Lomov, V.G.Labushkin

The angular distribution of CuK α & MoK α X-rays scattering by NiO & MnO crystals in the direction of superstructural magnetic reflections (1/2 1/2 1/2) & (3/2 3/2 3/2) was studied at $T < T_N$ & $T > T_N$ (where T_N is the phase transition temperature). When the CuK α radiation was scattered by NiO crystals, the reflections caused by the magnetic structure of the crystal were observed. The intensity of the reflection (3/2 3/2 3/2) exceeded substantially (about 10 times) both the theoretical predictions (Plazman & Tzoar, Phys.Rev. (1970), B2, 3556) & experimental data (Bergevin & Brunel, (1972), 39A, 141, Phys. Lett). With MnO crystals & MoK α radiation the magnetic structure did not manifest itself in X-ray scattering measurements although the incoherent background level was several times lower than the expected intensity of "magnetic" reflections. The results obtained allow the X-ray technique to be used in magnetic structure studies of crystals. Still greater possibilities lie in the employment of synchrotron radiation.