

21. STRUCTURAL RESULTS FROM METHODS OTHER THAN DIFFRACTION

21.1-13 STRUCTURAL TRANSFORMATIONS IN TETRA-n-BUTYLAMMONIUM OCTACYANOMETALATES.

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In this work the dynamical and phase situation in octacyanometalates, $M=Mo(V)$ or $W(V)$, is presented. The compounds were investigated by X-ray powder diffraction and wide-line proton magnetic resonance techniques at the temperature range 90-373 K. Diffraction patterns showed three distinct phase regions which have been characterized crystallographically. Moreover, the changes of the second moment and lineshape with temperature are presented. On ground of the dynamical model proposed for the crystal lattice of the compounds a detailed analysis of the experimental data is made. The different kinds of dynamical states of cations and anions are proved to be responsible for the observed effects.

21.1-14 THE REFINEMENT OF THE SPACE GROUP AND PHASE TRANSITION IN CHRYSOTILE-ASBESTOS STRUCTURE. By D.K.Arkhpenko, G.B.Bokiy, N.A.Palchik, V.A.Simonov. Institute of Geology and Geophysics Sib.Branch of the USSR Acad.Sciences 630090-Novosibirsk-90, USSR; Institute of Geol. of Ore Deposits, Petrol.Mineral.Geochem.Acad. Sciences, 109017-Moscow, Staromonetny 35, USSR.

The chrysotile-asbestos structure according to powder diffraction data refers to monoclinic classes (PDF-21-543) and is characterized by three space groups with the same rules of systematic absences: $C_2^3=Cm$; $C_2^3=C2$; $C_{2h}^3=C2/m$.

Phase transition is set up at $T = -40^\circ C$. From the vibrational spectra analyses due to the previously suggested methods (Arkhipenko, Bokiy, Kristallografiya (1977), 22, 6, 1176) it follows: 1. Space group between the groups with the same rules of systematic absences for the initial structure is refined as centrosymmetrical- $C_{2h}^3=C2/m$.

2. Inversion centre loss by phase transition is deduced (space group: $C_2^3=Cm$ or $C_2^3=C2$).

3. The increasing brittling by thermal drop up to $T = -40^\circ C$ with the change of its structure due to phase transition is explained.