08.1–10 CRYSTAL CHEMISTRY OF THE Ba-Nb-S SYSTEM: THE LAYER STRUCTURE OF $Ba_{10+x}Nb_5S_{22}(S_2)$. J.S. Swinnea and H. Steinfink, Materials Science and Eng., University of Texas, Austin, TX and L.E. Rendon-DiazMiron and L. Baños-Lopez, Institute de Materiales, Universidad Nacional Autonoma, Mexico.

Black platy crystals from the product of a reaction mixture of 6BaS:3Nb:7S reacted at 1000°C were hexagonal with a=6.909(4)Å, c=49.25(2)Å, $P6_3/mmc$, Z=2. A pronounced subcell with a=6.91Å, c=5.5Å indicated that this was a layer structure consisting of stacking of close packed BaS_3 layers. Three dimensional x-ray diffraction data were collected from a crystal using MoK_α radiation. From measured 782 structure amplitudes, 608 greater than $2\sigma(F)$ were used to solve the structure. The final R=0.1076,ωR=0.0800; for 91 reflections with $\ell=9n$ R=0.0406 and for the 517 reflections $\ell\neq 9n$ R=0.139. The structure is based on the stacking of close packed BaS_3 layers with the sequence CBDBABDBC BCDCACDCB, where D designates a disordered layer. The disordered layers contain two crystallographically independent Ba with partial site occupancies and disordered S_2 and S ions. Nb occupy octahedral interstices and form two different arrangements; a unit consisting of 3 face sharing octahedra and a unit of 2 face sharing octahedra. These octahedral units are separated by the disordered layers. The Nb-Nb distances in the chain of 3 are 3.29Å and they are 3.57Å in the double unit. The ordered structure probably has the composition $Ba_{21}Nb_{10}S_{44}(S_2)_2$.

08.1–11 STRUCTURES AND GRAPHS OF TETRAHEDRAL FRAMEWORKS. By S. J. Chung*, Th. Hahn**, and W. E. Klee°
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A graph-theoretical method for the generation of tetrahedral framework structures has been reported (Chung & Hahn, Acta Cryst. A31 (1975) S1; Chung, Hahn & Klee, Acta cryst. A40 (1984) 42). These structures can be considered as four-connected three-dimensional periodic nets. They are derived by means of finite, four-regular, connected graphs with labeled multiple edges and loops. The vertices and edges of the finite graphs represent sets of translationally equivalent points and lines, respectively, in the periodic nets. These labeled graphs contain full information on the connectivity of the actual structures and thus can be also used for purposes of classification.
This method has been employed to derive all graphs representing four-connected periodic nets with up to four nodes in a unit cell. From these graphs a number of new, crystal-chemically reasonable tetrahedral framework structures are obtained. They will be characterized, illustrated, and compared with known structures.
Structure determinations of several new compounds will be reported: $CsLiCrO_4$, $CsLiMoO_4$ (cristobalite type, space group $F\bar{4}3m$, positional disorder of oxygens), $N_2H_5LiSeO_4$ (Icmm type, space group $Pc2_1n$), and $(Na_{0.7}Ca_{0.3})(Al_{1.3}Si_{2.7})O_8$ (I4/mmm type, space group $P22_12_1$, complete Si-Al-disorder).
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08.1–12 STRUCTURAL CHEMISTRY OF PHOSPHO-TELLURATES. By N. Boudjada and J.C. Guitel, Laboratoire de Cristallographie, C.N.R.S., associé à l'U.S.M.G., 166 X, 38042 - Grenoble Cedex, France.

A good number of phosphate-tellurate salts have already been described. Up to now, we never observed the existence of a condensed phosphotelluric anion but always the coexistence, as independent units, of the $Te(OH)_6$ group and the phosphoric anion (condensed or not).

$NaH_2PO_4.Na_2HPO_4.Te(OH)_6$ (a monophosphate),

$K_3HP_2O_7.Te(OH)_6.H_2O$ (a diphosphate),

$2(NH_4)_3P_3O_9.Te(OH)_6$ (a trimetaphosphate)

and $(NH_4)_4P_4O_{12}.2Te(OH)_6.2H_2O$ (a tetrametaphosphate)

are examples of such addition compounds recently studied in the laboratory. Main geometrical features of phosphoric and telluric groups in these salts are compared.

Special attention is devoted to an ammonium phosphotellurate, $(NH_4)_2HPO_4.2NH_4H_2PO_4.Te(OH)_6$, where good ferroelectric properties are observed below 48°C.