08. 1–16 *FRAMEWORKS AND A CLASSIFICATION SCHEME FOR INORGANIC AND INTERMETALLIC STRUCTURE TYPES.*
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The 2.400 cubic structures of inorganic compounds (ICSD, Bergerhoff, Bonn) and the 1.800 cubic ones of intermetallic compounds (MDF, Calvert, Toronto) can be grouped into about 400 structure types. These types have been described and classified with the aid of nearly 200 frameworks.
The symbolism permits a classification into families, main- and subclasses. 40 % of the cubic structure types belong to the I-, P- and F-family (E. Hellner, Structure and Bonding (1979) 37, 61).Example:
F(Cu-type) with the subclass J(O-framework in ReO_3,$CaTiO_3$), F_2(8th order, O-framework in spinel) with subclasses T(O-framework in cristobalite, Cu-framework in $MgCu_2$) and [F"$_2$-I(4t)] (S-framework in tetrahedrite).
Another 40 % of the cubic structure types belong to the corresponding polyhedra families. In these cases the equipoints of the frameworks of the I-, P- or F-family are replaced by polyhedra (centered or not).Examples:
I *W-type, O-framework in Cu_2O*
I[4t] *F-framework in SiF_4, S-framework in Tl_3VS_4*
I[6o] *F-framework in SiF_6,*
I_2[6o] *in garnet $Ca_3Al_2(SiO_4)_3$ and Hg_3TeO_6; in $RhBi_4$, in $(NH_4)_4Fe(CN)_6\cdot 1,5H_2O$*
I[12i] *Al-framework in WAl_{12}; O-framework in $NaMn_7O_{12}$, $Cu_3Ta_2Ti_2O_{12}$, and in $In(OH)_3$.*
The heterogeneous (O and H_2O)-framework in alumn $KAl(SO_4)_2\cdot 12H_2O$ can be described as F(6o)+F'(6o)+P$^{\frac{1}{2}}_{\equiv}$x(4t).
In addition there exist less comprehensive families and polyhedra families derived e.g. from the
Y** *complex for Si(III)-H.P. and in Th_3P_4 and $CaTlS_2$, the*
±Y *complex for N_2, for FeSi, in FeS_2 and CO_2, the*
S *complex for Ga(II)-H.P., in Cu_3As and in $K_2Mg(SO_4)_3$.*
Other families are derived from heterogeneous frameworks:
[I+W] *for ß-W(A15)type, in α-O_2 and KGe,*
[D+T'] *for $MgCu_2$, in argyrodite Ag_8GeS_6*
[¯Y(3l)+D$^{\frac{x}{\equiv}}$] *for ß-Mn, Au_4Al, in ß-$SnWO_4$ and $RbAg_4J_5$.*
The 3.500 tetragonal inorganic structures with about 900 structure types (including 250 types of intermetallic compounds) add distorted types derived from cubic ones: indium with distorted F;
Pa, ß-Np, ß-Hg with distorted I;
BiIn, TlF, AsCe with distorted F, F' (NaCl) etc.
Different orders complete the families:
order 2 : F_{112} *in stannite, chalcopyrite, α-$ZnCl_2$, ß-Cu_2HgJ_4;* I_{112} *in CuTi*
order $2\frac{1}{2}$: F_M *in $MoNi_4$ with* $M = \frac{3}{2},\frac{1}{2},0/-\frac{1}{2},\frac{3}{2},0/0,01$
order 3 : I_{113} *in BBe_4, $TaSi_2$*
order 4 : I_{114} *in Pd_5Ti_3, Al_5Ni_2Zr*
order 6 : I_{116} *in $PbPdTl_2$*
order 7 : I_{117} *in Cu_4Ti_3*
order 9 : I_{331} *in V_4Zn_5*
Layer descriptions for the cubic structures of Cu, NaCl, ZnS, $CaTiO_3$, Mg_2AlO_4, $MgCu_2$ etc. are extended to the hexagonal stacking variants like Mg, Sm, Am, wurtzite, hexagonal perovskites, hexagonal spinels, Laves phases etc. with the aid of the nets H(3^6), G(6^3) and N(3636) and the Jagodzinski symbols. Edge-centered stackings of H(3^6) nets with the corresponding symbols f, q or d for the 2-, 3- and 4-layer types are realized in Pa, $MoSi_2$, $CrSi_2$, α-Pu, $TiSi_2$.

08. 2–1 INFERENCES ON STRUCTURAL RELATIONSHIPS BASED ON SIMILARITIES BETWEEN POWDER PATTERNS IN THE CASE OF Na-Ca-SILICATES. By R.X. Fischer* and E.Tillmanns, Institut für Geowissenschaften, Universität Mainz, Germany
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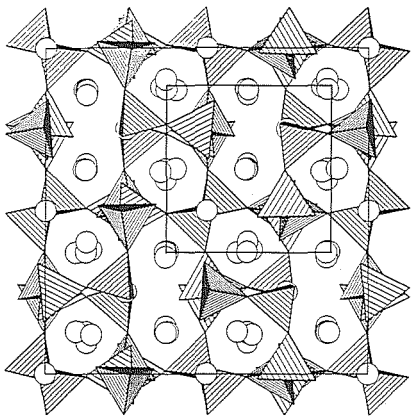
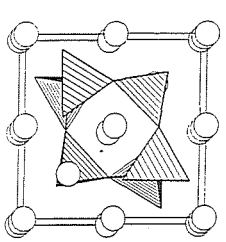
According to similarities in powder diagrams the crystal structures of Na_2CaSiO_4, $Na_2Ca_2Si_3O_9$ and $Na_4CaSi_3O_9$ are known to be closely related. Usually the comparison of powder patterns is used to infer structural relationships. In some cases this leads to wrong conclusions as for $Na_4CaSi_3O_9$ which is supposed to be isostructural to the six-ring aluminate $Ca_3Al_2O_6$ but actually is a 12-ring silicate (Fischer and Tillmanns, Z. Krist. (1984) in press). The structure of $Na_4CaSi_3O_9$ is related to the orthosilicate Na_2CaSiO_4 (Fischer, thesis (1983) Universität Mainz) and to the six-ring silicates of high and low temperature modifications of $Na_2Ca_2Si_3O_9$ (Fischer and Tillmanns, N. Jb. Miner. Mh. (1983), 1983, 49-59) by a similar substructure for the cations. It fits a cubic or pseudocubic cell of 7.5 Å. The subcell parameters are:

compound	subcell param. a [Å]	α [°]	superstructure symmetry
Na_2CaSiO_4	7.443	90	cubic
high-$Na_2Ca_2Si_3O_9$	7.448	88.88	rhombohedral
low -$Na_2Ca_2Si_3O_9$	7.469	88.93	trigonal
$Na_4CaSi_3O_9$	7.544	90	cubic

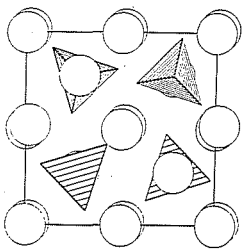
the figure shows projections of the crystal structures of these compounds. a) $Na_4CaSi_3O_9$ with the 7.5 Å-subcell b) h-$Na_2Ca_2Si_3O_9$ in rhombohedral setting (l-$Na_2Ca_2Si_3O_9$ has a slightly distorted structure) c) Na_2CaSiO_4 with one out of 12^4 different arrangements for the SiO_4-tetrahedra in the unit cell. Compared to the scattering power of the cations the influence of oxygen on the intensities is very weak and does not sufficiently affect the powder pattern.



$Na_4CaSi_3O_9$ // [001]



h– $Na_2Ca_2Si_3O_9$ // $[001]_{rh}$



Na_2CaSiO_4 // [001]