are possible. There are 4 single (s,f,d,p), 6 binary (sf,sd,fd,sp,fp,dp), 4 ternary (sfd,sfp,sdp,fdp) and 1 quadruple (spdf) formulas of CC. There are 69 formulas at all. The sfdp–formulas have been distinguished in minerals and these formulas have been compared with 69 formulas. While correlating the formulas of ionic compounds they were divided into the cationic and anionic parts. The formulas of different ranges have been distinguished.

PS–08.04.27 CRYSTAL STRUCTURES OF BORON NITRIDES DETERMINED FROM X-RAY POWDER DATA. By H. Hiraguchi, N. Sudo*, H. Hashizume, S. Nakano (1) and O. Fukunaga (1), Res. Lab. of Engineering Materials, Tokyo Institute of Technology, Nagatsuta, Midori, Yokohama 227, Japan. (1) Dept. of Inorganic Materials, TIT.

The crystal structures of magnesium boron nitride Mg_3BN_3 in the low- and high-pressure forms have been determined *ab initio* from X-ray powder data. The powder patterns were decomposed to estimate individual reflection intensities, which were used to calculate Patterson functions and build try-and-error structure models. The obtained structure parameters were refined by the Rietveld method. 54 and 21 reflections were used to solve the structures of $Mg_3BN_3(L)$ and $Mg_3BN_3(H)$ respectively. Low-pressure $Mg_3BN_3(L)$ has a hexagonal cell (space group $P6_3/mmc$, $Z = 2$) with $a = 3.54453(4)$ and $c = 16.0353(3)$ Å while the high-pressure $Mg_3BN_3(H)$ cell is orthorhombic ($Pmmm$, $Z = 1$) with $a = 3.0933(2)$, $b = 3.1336(2)$ and $c = 7.7005(5)$ Å. The two structures commonly include linear N-B-N molecular anions, considered to play a role in the catalytic property of the material in the reaction converting hexagonal boron nitride into a cubic form at high pressure-temperatures. A 2 % shorter B-N interatomic distance was observed for $Mg_3BN_3(H)$.
Applications of standard direct methods to the $Mg_3BN_3(L)$ intensity data resulted in a very similar structure. High-quality electron density maps have been calculated for this form using the maximum-entropy method with phased structure factors. A separate application of maximum-entropy multisolution program (C. Gilmore *et al.*: *Acta Cryst.* A47, 830 (1991)) to the unphased structure factors yielded quite a similar map in support of the determined structure of $Mg_3BN_3(L)$.

A structure solution from $Sr_3B_2N_4$ X-ray powder data will also be reported.

PS–08.04.28 S_8 : A NEW LOOK AT AN OLD STRUCTURE. By Robin B. English, Department of Chemistry, Rhodes University, South Africa.

The crystalline structures of monoclinic and orthorhombic S_8 are explored using the Dirichlet domain construction.

PS–08.04.29 **TWO-PHASE K-NA FELDSPAR STRUCTURE FROM SICHOTE-ALIN.** By N.
I. Organova*, I. M. Marcille, I. V. Roshdestvenskaja, N. D. Zacharov, Y. A. Nistratov,
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$Or_{62}Ab_{36}An$ is a result of exsolution and consists from K and Na components. For monoclinic K-phase there are $a = 8.542(1)$, $b = 13.0123(19)$ $c = 7.182(10)$, $\beta = 116.054(8)$.
Refinement with massiv from 1091 reflections has been carried out to $R = 2.7\%$. The values of some interatomic distances are: $Si-O_1$ 1.648(1), Si_1-O_3 1.642(1), Si_1-O_4 1.649(1), Si_1-O_5; Si_2-O_2 1.638(1), Si_2-O_3 1.626(2), Si_2-O_4 1.637(1), Si_2-O_5 1.633(1).
Refinement of alkaline occupancy lead to $0.81K + 0.19Na$ for 159 reflections with $\sin\theta/\lambda < 0.5$. Triclinic Na-phase is a periodic polysynthetic periclinic twin with $A = 14a_{Ab}$, what corresponds the TEM observations.

PS–08.04.30
DETERMINATION OF IRON VALENCE IN NATURAL MAGNETITES AND GARNETS BY EPMA. A. By I. P. Laputina*, O. V. Polozova, Institute of Geology of Ore Deposits, Petrography, Mineralogy and Geochemistry {IGEM} Russian Academy of Sciences, Moscow, Russia.

The influence of various valence states of transition elements in chemical compounds on the L-emission spectra is well known. We have shown in earlier papers that the structural-chemical state of iron atoms in natural oxides, silicates and sulphides is exhibited in x-ray emission spectra of $FeK\alpha_{1,2}$ by distinct shifts of the wavelengths and of the band profiles as well as in changes of peak/integral intensity ratio [1].
In this study we attempted to determine the Fe valencies in natural Fe-spinels and garnets by EPMA. Crystal-chemical feature of Fe-O system, possibility of wide exchange between octahedral and tetrahedral sites for Fe^{2+} and Fe^{3+} and Fe^{3+} in different physico-chemical environments make this system very important in the investigations of natural processes, because magnetite and Fe-spinels are often throughgoing minerals formed during several stages of mineralization.
Optimum conditions of investigations have been defined. The measurements were performed at high voltage $E = 10$ kV, $i = 100$ nA, $t = 50$℃, using crystal-monochromator KAP and anti-contamination.
By measuring x-ray intensity FeL_β/L_α in standard natural ferrous oxides with known Fe^{2+}/Fe^{3+} ratios, three characteristic trends with corresponding crystal-chemistry feature were established: 1. for haematite-magnetite-wustite, 2. for haematite-ilmenite, 3. for magnetite-Ti-magnetite-ulvospinel-ilmenite and 4. for natural garnets of the series almandine-andradite. Based on these results, the equations for a quantitative determination of Fe^{2+} and Fe^{3+} were found. Having determined the intensities of FeL_α and FeL_β and total concentration of iron by EPMA, we designate:

$y = FeL_\beta/L_\alpha$, $C = (Fe^{2+} + Fe^{3+})$ and $x = Fe^{2+}/C$.
Then for magnetite (for trend 3) $x = 2$. 13y-0. 51,
for garnets $x = 4$. 17y-2. 08.
The concentrations of Fe^{2+} and Fe^{3+} are calculated using the equations: $Fe^{2+} = x \cdot C$; $Fe^{3+} = (1-x) \cdot C$. We have studied the intensities FeL_β/L_α and the compositions of magnetites in local volume from various differentiates of the Talnakh intrusion of gabbro-dolerite with different oxidation states (Noril'sk, North Siberia). It was found that Fe^{2+}/Fe^{3+} ratio of magnetites is dependent on rock oxidation potential and therefore it can serve as the criterion of physicochemical environment of magma crystallization.

[1] Laputina I. P. Proc. Y11 Europ. Congr. Electron Microscopy and IX Intern. Conf. on X-Ray Opt. and Microanal. , Haaga, 1980, V. 3, p. 154-155.

PS-08.04.31
THE CRYSTAL STRUCTURE OF JAFFEITE AND RELATED COMPOUNDS.

By D. Yu. Pushcharovsk', N. A. Yamnova and Yu. K. Egorov-Tismenko, Moscow State University, 119899 Moscow, Russia.

The crystal structure of jaffeite, $Ca_6[Si_2O_7] \cdot (OH)_6$, from Kombat mine, Namibia (Sarp. H. , Peacor D. R. Amer. Mineral. , 1989, 74, 1203-1206) has been determined by X-ray methods (hexagonal, P3, lattice constants: a 10. 035, c 7. 499 Å, $Z = 2$. 871 reflections, $Ranizo$ 0. 030). Jaffeite and its synthetic analogue are isotypic with fluoborite $B_3[Mg_9(F, OH)_9O_9]$, jeremejevite $B_5[B_3Al_6](OH)_3O_{15}$ and painite $CaZrB \cdot [Al_9O_{18}]$. All these structures contain octahedral frameworks, formed by double bands, in which octahedra share edges. At the contacts of these bands there are trigonal and hexagonal channels. The trigonal channels are filled by pyrogroups $[Si_2O_7]$ (jaffeite), by trigonal Zr-prisms and B-triangles (painite) or by $[BO_3]$ -triangles (fluoborite, jeremejevite). The type of the fillers (Si-O-Si, Zr with B or two B-atoms) determine the similarity of a (b) -cell parameters and the difference of c-parameter in the considered structures.

PS-08.04.32 CRYSTAL STRUCTURE OF $AlCa_2$ $(SO_4)_2F_2Cl \cdot 4H_2O$.
By G. L. Starova', V. S. Fundamenskiy, S. K. Filatov, G. L. Matusevich, L. P. Vergasova. Department of Crystallography, Sankt Petersberg State University, Russia.

The crystal structure of aluminum dicalcium disulphate fluoride dichloride tetrahydrate, $AlCa_2(SO_4)_2FCl \cdot 4H_2O$ has been determined. Space group I 4/m, a = 6. 870 (1), c = 13. 342 (2) Å , $Z = 2$, $D_x = 2$. 353g/cm^3, The 447 unique reflections were obtained with Syntex P2$_1$ diffractometer with Mo radiation for 0. 1x0. 1x0. 05mm colorless plate square crystal. The structure has been solved by direct methods and refined by full-matrix leastsquares to R-factor 0. 046 ($R_w = 0$. 048). Hydrogen atoms have been lo-

cated in difference synthesis.
In the crystal structure of $AlCa_2(SO_4)_2F_2Cl \cdot 4H_2O$ the chains of polyhedra are arranged along [001]. These chains consist of pairs of CaO_4ClF polyhedra alternat with single AlO_4F_2 polyhedra which are rolated along [001] with a difference of 24°. The chains are combined by SO_4-tetrahedra so that all four sulphate oxygen atoms take part in coordinating Ca atoms to form with Cl and F atoms distorted octahedra, which are two nonequal perfect tetragonal pyramids with common base. The stredched one has Cl atom on top, the flattened one an F atom. The Al coordination sphere consists of two F atoms and four oxygen atoms of water moleculecules as flattened perfect tetragonal dipyramide. The Al coordination polyhedron has not direct contacts with SO_4-tetrahedra but interatomic distances analysis performs that in spite of the long distance between oxygen atoms (2. 815Å), a distance from water hydrogen atom to tetrahedron oxygen atom is shortened ($H \cdots O = 2$. 03 (5) Å) and so these atoms have the specific interaction by hydrogen bond to penetrate crystal structure (Fig.).
Bond distances (Å and angles (deg.) in structure: Ca polyhedron: Ca-Cl = 2. 689 (3), Ca-F = 2. 233 (6), Ca-O$_1$ = 2. 366 (3), ClCaF = 180. 0 (1), ClCaO$_1$ = 84. 9 (1), FCaO$_1$ = 95. 0 (1), O$_1$CaO$_1$' = 89. 6 (1), O$_1$CaO$_1$'' = 169. 9 (1).
Al polyhedron: Al-F = 1. 750 (5), Al-O$_2$ = 1. 918 (6), FAlF = 180. 0 (2), FAlO$_2$ = 90. 0 (2), O$_2$AlO$_2$' = 180. 0 (2), O$_2$AlO$_2$'' = 90. 0 (2).
S tetrahedron: S-O$_1$ = 1. 474 (4), O$_1$SO$_1$' = 109. 1 (2), O$_1$SO$_1$'' = 109. 7 (2).

PS-08.04.33 PRINCIPLES OF CRYSTAL CHEMISTRY OF COMPOUNDS CONTAINING TETRAHEDRA $[OT_4]$.
By S. K. Filatov, T. F. Semenova', St. -Petersburg University, Russia.

Revealed are laws of compounds (oxi-salts, oxides) in which the strongest structure fragments are tetrahedra $[OT_4]$, $[OCu_4]$ in particular. Here O is "monatomic" oxygen not present in acid residuals SO_4, SeO_3, CI etc. , hydroxyl groups OH, water molecules H_2O. Such oxygen ions are the most highly charged negative particles, O^{-2} and that is why in gaseous phase, liquids and crystal structures they collect cations around them.
It is known that classic tetrahedra $[TO_4]$ (valency of central atom 7, 6, 5, 4, 3) are polymerized under atmospheric conditions only through their vertices. At the same time tetrahedra $[OT_4]$ (valency of the central atom 2) may be polarized both through the vertices (up to 4 tetrahedra in a vertex) and through the common edge. This sharply increases the diversity of formed polyions $[OCu_x]$ (S. K. Filatov, T. F. Semenova, Doklady Ac. Sc. USSR, 1992, Vol. 322, No3, pp. 536-539).
By now there are the following known types of polyions from tetrahedra $[OCu_4]$: isolated tetrahedra $[OCu_4]^{6+}$ (e. g. , ponomarevite $K_4Cu_4OCl_{10}$); couples of tetrahedra interconnected through the common edge, $[OCu_3]_2^{2+}$ (fedotovite K_2Cu_3O $(SO_4)_3$; chains of tetrahedra interconnected through the vertices, $[OCu_3]_\infty^{4+}$ (kamchatkite KCu_3OCl $(SO_4)_2$); chains of tetrahedra interconnected through the edges, $[OCu_2]_\infty^{2+}$ (piypit $K_4Cu_4O_2$ (SO_4) MeCl); chains of tetrahedra interconnected by turns through the