

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, Institute of Ore Deposits, Petrology, Mineralogy and Geochemistry of RAN, IKRAN Moscow. LNPO "Burevestnik" St. Petersburg, Russia.

$Or_{62}Ab_{36}An$  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  $Fe^{3+}$  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,  $t=50^\circ C$ , using crystal-monochromator KAP and anti-contamination.

By measuring x-ray intensity  $FeL_{\beta}/L_{\alpha}$  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  $FeL_{\alpha}$  and  $FeL_{\beta}$  and total concentration of iron by EPMA, we designate: