

## 08-Inorganic and Mineralogical Crystallography

number of samples are the homogenous solid solutions of ulvospinel and magnetite. The unit cell parameters display the wide variations - from  $8.390 \pm 0.005 \text{ \AA}$  to  $8.485 \pm 0.005 \text{ \AA}$ . The latter value is close to the end member of the isomorphous series, indicating the existence of complete solid solution between ulvospinel and magnetite. Some samples reveal the exsolution intergrowth of ilmenite and titanomagnetite or hematite and titanomagnetite. The structure parameters have been correlated with geodynamic conditions of oceanic basalts formation.

**PS-08.03.04 REFINEMENT OF SUOLUNITE STRUCTURE** By Nicheng Shi\*, Libing Liao, Zhesheng Ma, X-Ray Lab., China University of Geosciences, Beijing 100083, China.

Suolunite is a mineral discovered in China in 1965. It is the only natural silicate in which  $\text{CaO}:\text{SiO}_2:\text{H}_2\text{O}=1:1:1$ . Its structure was first determined by Weissenberg photographic method in 1965. But only x and y coordinates of nonhydrogen atoms were obtained. Our Lab. restudied its structure in 1974 and obtained all z coordinates of the nonhydrogen atoms. The deviation factors for  $F(hk0)$  and  $F(hkl)$  were 17.2% and 18.3% respectively. This study is to refine suolunite structure and to find out as much hydrogen atoms as possible. The intensity data of suolunite was collected on RASA-IIS Rigaku auto-four-circle diffractometer.  $\text{MoK}\alpha$  radiation, graphite monochromator.  $2\theta$  range for data collection:  $3^\circ < 2\theta < 120^\circ$ . Intensity data were corrected for PL factor. 1519 intensities were collected in total and 1281 separate intensities, for which  $|F| > 3\sigma |F|$ , were used in the refinement. The unit cell parameters of suolunite are:  $a=11.119(3) \text{ \AA}$ ,  $b=19.776(3) \text{ \AA}$ ,  $c=5.9900(8) \text{ \AA}$ ,  $V=1317.18(5) \text{ \AA}^3$ . Orthorhombic system. Space group is  $Fdd2$ .  $D_x=2.71 \text{ g/cm}^3$ . The least-squares refinement reduces the R factor to 0.032 for anisotropic temperature factors. Coordinates of all nonhydrogen atoms and some hydrogen atoms were obtained. The refinement result indicates that z coordinates of all atoms in suolunite are away from  $1/4$ ,  $1/2$  and  $3/4$  to some extent. The bond lengths and bond angles showed that the double tetrahedra in suolunite are the most stretched. The Si-O-Si angle of it is very close to  $180^\circ$ , which attracts attention from many crystalchemists.

**PS-08.03.05 CRYSTAL STRUCTURE OF AN OMPHACITE WITH SPACE GROUP Pn** By Z. S. Ma, N. C. Shi and Q. F. Zhang, X-Ray Laboratory, China University of Geosciences, Beijing 100083, China.

Omphacite with space group Pn occurred in eclogite of Zhucheng, Shandong Province, China. Analysis by electron microprobe gave:  $\text{SiO}_2$  54.409,  $\text{TiO}_2$  0.084,  $\text{Al}_2\text{O}_3$  9.207,  $\text{FeO}$  3.285,  $\text{MnO}$  0.012,  $\text{MgO}$  10.317,  $\text{CaO}$  16.264,  $\text{Na}_2\text{O}$  5.123,  $\text{K}_2\text{O}$  0.005,  $\text{Cr}_2\text{O}_3$  0.005, sum 98.712 (wt %) corresponding to  $(\text{Ca}_{0.88}\text{Na}_{0.12})_{0.99}(\text{Mg}_{0.88}\text{Fe}_{0.10}\text{Al}_{0.02})_{1.02}(\text{Si}_{10})$ .

The crystal ( $0.25 \times 0.6 \times 0.32 \text{ mm}$  in size) was selected and mounted on RASA-IIS Rigaku 4-circle automated diffractometer, with  $\text{MoK}\alpha$  radiation, a graphite monochromator, a  $2\theta-\omega$  scan, the scanning constant  $\Delta\omega=1.282+0.5\tan\theta$ , a speed of  $4^\circ/\text{min}$ . 1833 diffractions were collected in the range of  $3^\circ < 2\theta < 65^\circ$ , of which 905 ( $F > 3\sigma |F|$ ) were used for structure refining. The possible space group is  $P2_1/n$  or Pn. The Pn space group was confirmed by the results of structure refinement.  $a=9.607(4)$ ,  $b=8.774(4)$ ,  $c=5.245(1) \text{ \AA}$ ,  $\beta=106.63(3)^\circ$ ,  $V=423.62 \text{ \AA}^3$ ,  $Z=4$ ,  $D_x=2.483 \text{ g/cm}^3$ . The structure was solved by direct methods (SHELX-76). Atomic coordinates, occupancies, isotropic and anisotropic temperature factors were carried out which finally led to reduction of R to 0.051. The polyhedra of Ca-O, Na-O and Mg-O underwent stronger distortions (the ranges of bond length Ca-O  $2.35 \sim 2.72 \text{ \AA}$ ; Na-O  $2.34 \sim 2.73 \text{ \AA}$ ; Mg-O  $1.97 \sim 2.14 \text{ \AA}$ ; Al-O  $1.91 \sim 2.08 \text{ \AA}$ ) than polyhedra of omphacite with  $P2_1/n$ , which caused the symmetry to be reduced. Probably, the occurrence of omphacite with Pn indicated it being of lower formation temperature than omphacite with  $P2_1/n$ .

**PS-08.03.06 FICHELITE. A NATURALLY OCCURRING HYDROCARBON MINERAL.** Mace H.A., and Peterson R.C., Department of Geological Sciences, Queen's University, Kingston, Ontario K7L 3N6 (Canada).

The mineral fichtelite ( $\text{C}_{19}\text{H}_{34}$ ) is a naturally occurring saturated hydrocarbon that is generally found in the remnants of pine-tree trunks in peat and lignite beds in the Fichtel Gebirge region of Germany. It is a fossil resin of abietic acid, which is a component of rosin found in pine trees.

Single crystals up to 4 mm were obtained from a mass of crystals (4 cm across), which existed on a piece of pine wood. The clear, colourless crystals exhibited a platy habit with well-defined crystal faces. The monoclinic space group,  $P2_1$ , was obtained using precession techniques. Unit cell dimensions were determined to be  $a = 10.7060 \text{ \AA}$ ,  $b = 7.4585 \text{ \AA}$ ,  $c = 10.8236 \text{ \AA}$  and  $\beta = 105.840^\circ$ .

The structure was determined by direct methods using 1229 unique reflections obtained with  $\text{Mo-K}\alpha$  X-radiation. Full-matrix least-squares refinement of atomic positions and temperature factors produced an  $R_w = 0.039$ . The molecule, a perhydrophenanthrene, consists of three non-linear fused six-membered rings in chair conformation, as well as an attached methyl group on the first ring, an isopropyl group on the third ring, and an angular methyl group. The position and isotropic temperature factors of all but one hydrogen were determined. All obtained bond lengths and angles were consistent with expected values.

The conversion of abietic acid to fichtelite is a result of chemical processes that result in the loss of the carboxylic acid group, as well as the saturation of the carbons contained in the rings along with the gain of hydrogen atoms.

Small red crystals up to 1.5 mm were observed to be intergrown with the fichtelite. Work is currently being carried out to determine the identity and crystal structure of this material.