

$\sin\theta/\lambda < 1.0 \text{ \AA}^{-1}$ , 6692 reflections with  $F/\langle F \rangle > 3\sigma/F$ ,  $R=2.53\%$ ) evidences that KGP and KTP are isostructural. The structures of these two crystals differ mainly in the following features:  $[\text{GeO}_6]$ -octahedra are essentially less distorted than  $[\text{TiO}_6]$  ones, besides, there was hardly any alteration of long and short chemical bonds in the chains of metal-oxygen octahedra. For instance, the corresponding bond lengths are as follows:  $\text{Ge}(1)-\text{O}(\text{Ge}2)$  1.801,  $\text{Ge}(1)-\text{O}(\text{Ge}1)$  1.791,  $\text{Ge}(2)-\text{O}(\text{Ge}2)$  1.813,  $\text{Ge}(2)-\text{O}(\text{Ge}1)$  1.823 Å. The results obtained for KGP are compared to the data available for similar  $\text{KMeOPO}_4$  compounds, where  $\text{Me} = \text{Sn}$  and  $\text{V}$ , as well as for KTP crystals irradiated by fast neutrons.

PS-08.04.10 TEMPERATURE DEPENDENCE OF THERMAL VIBRATION AND POSITIONAL PARAMETERS OF ATOMS IN MAGNETITE. By H. Okudera\*, K. Kihara and T. Matsumoto, Department of Earth Sciences, Faculty of Science, Kanazawa University, Japan.

Crystallographic parameters and their thermal changes in natural magnetite ( $\text{Fe}_3\text{O}_4$ ) have been studied with single crystal X-ray diffraction method in the range from room temperature to 1069K. The cell dimension ( $a$ ), oxygen coordinate ( $u$ -parameter), and atomic mean-square displacements (MSD's) are reversible as a function of temperature below 773K. The cell dimensions of four specimens are determined within the range from 8.3925(7) to 8.3962(3) (Å) at room temperature before heating and agree with the previous reports (e.g., Hamilton, W. C., Pys. Rev., 1958 110, 1050-1057; Fleet, M. E., Acta Cryst., 1981, B37, 917-920). The cell dimension  $a$  with increasing temperature is fitted with the quadratic form:

$a$  (Å) =  $8.3845 + 2.3947 \times 10^{-6} T + 9.338 \times 10^{-8} T^2$  in the range from 299K to 773K. Discontinuity of the first derivative of expansion at 865K, reported by Gorton *et al.* (Trans. Metal. Soc. AIME, 1965, 233, 1519-1525), is not observed in the present magnetite.

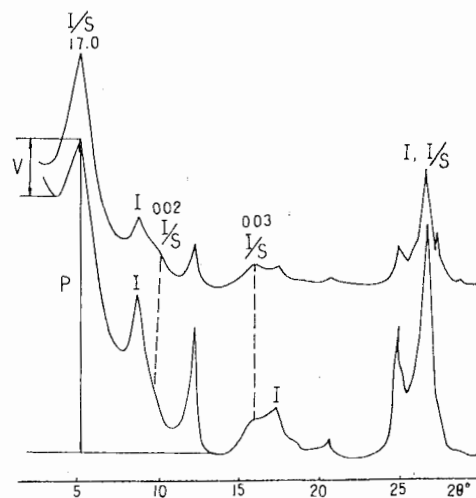
The  $u$ -parameter remains nearly constant at  $u = 0.25487(3)$ , but begins to increase at 623K, suggesting random distribution of  $\text{Fe}^{3+}$  and  $\text{Fe}^{2+}$  over the tetrahedral and octahedral cation sites. This suggests that the structure would be ideally inverse type below 623K and  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  cations would be slightly disordered above the temperature. At the octahedral cation site, the MSD's of atom normal to  $[111]$  has smaller values than that along  $[111]$  at a low temperature. The former, however, has a larger rate of increase with increasing temperature, and becomes larger than the latter above 623K.

PS-08.04.11A PRACTICAL V/P METHOD FOR ESTIMATING SMECTITE LAYERS PERCENTAGE IN MIXED-LAYER ILLITE/SMECTITE AND A STUDY OF FACTORS OF INFLUENCING THE V/P VALUES. By Xi-sheng Lin and Nai-Xuan Zheng, Scientific Research Institute of Petroleum Exploration and Development, Beijing, China.

Smectite layers percentage (%S) has been used to quantitatively describe mixed-layer illite/smectite (I/S). According to the method (R. C. Reynolds, 1970, 1980), the %S should be identified based upon the positions of 002 and 003

reflections of illite/smectite. However, these two peaks are often overlapped with 001 and 002 reflections of illite respectively. An equation  $(\%)S = 66 \cdot \frac{V}{P} + 39$  (shown in Figure) has been derived here, according to the least squares principle, and by using information from E. Perry and J. Hower (1970) and our analyzed data. Obviously, it is easier to use the equation to determine the %S, and the error is 10%. The results suggest that both slit size of diffractometer and contents of I/S in samples affect the V/P values. Size of divergence slit should be fixed at  $1^\circ$  or  $\frac{1}{2}^\circ$

and the equation be changed to  $(66 \cdot \frac{V}{P} + 39) \cdot \sigma_i$  ( $i=1, 2, 3$ ) because of the influence of the contents.  $\sigma_i$  are:  $\sigma_1 = 1.888 - 0.1952 \ln x$ , for  $(\%)S \geq 75$ ;  $\sigma_2 = 1.633 - 0.14 \ln x$ , for  $50 \leq (\%)S < 75$ ;  $\sigma_3 = 1.129 - 0.0013x$ , for  $37 \leq (\%)S < 50$ . Here,  $x$  are referred to the contents. The other factors such as crystallite thickness and lattice distortion, which influence the V/P values, are also discussed in brief.



V/P of 17A peak of ethylene glycol treated mixed-layer illite/smectite  
I, illite I/S, illite/smectite

PS-08.04.12 RECONSTRUCTIVE CRYSTAL-TO-CRYSTAL CONVERSION IN THE SOLID STATE. By U. Eigendorf, G.E. Herberich, T. Wagner, and U. Englert\*, Institut für Anorganische Chemie, RWTH Aachen, Prof.-Pirlet-Straße 1, D-5100 Aachen, Germany. Crystals of the etherate

