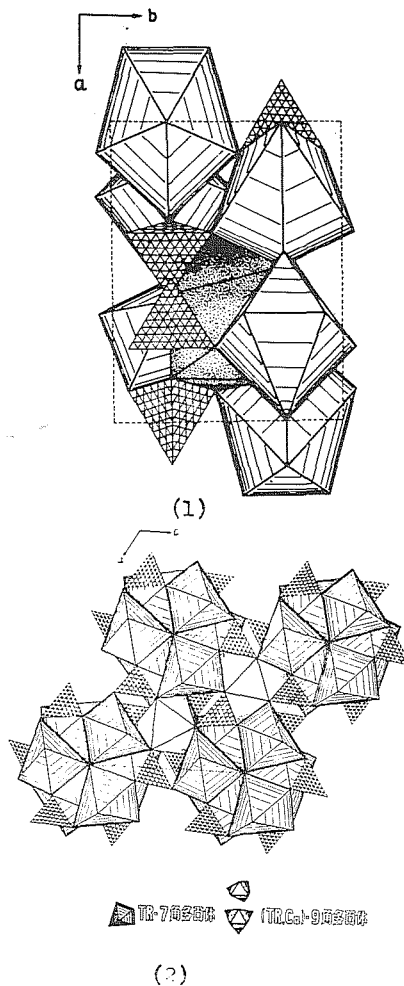


concluded that the  $[5^{12}]$  cages contain  $\text{CH}_4$  molecules while the  $[5^{12}6^2]$  cages contain  $\text{CO}_2$  and  $\text{N}_2$ .

Bond lengths ( $\text{\AA}$ ) and valence angles ( $^\circ$ ) are given in the following table.

	range	mean value of $[5^{12}]$	mean value of $[5^{12}6^2]$	grand mean value
Si-O	1.569-1.596	1.579	1.572	1.576
O-Si-O	107.9-110.4	109.3	109.5	109.5
Si-O-Si	148.2-180	162.9	170.3	168.8

Si-O distances show only little variation, the grand mean value of  $1.576\text{\AA}$  being considerably lower than the value  $1.608\text{\AA}$  deduced by Brown & Gibbs (Amer. Miner. (1969) 54, 1528) for silica frameworks. Si-O-Si angles in M have values up to  $180^\circ$  with a very high grand mean value of  $168.8^\circ$ . The structure of M is a good example of the negative correlation between Si-O distances and Si-O-Si angles reported by Hill & Gibbs (Acta Cryst. (1979) B 35, 25). - Melanophlogite is the first silicate known to contain pentagondodecahedra formed from  $[\text{SiO}_4]$  tetrahedra.



**08.4-09** THE CRYSTAL STRUCTURE OF LESSINGITE, RICH IN LIGHT RARE EARTH, CERIUM. By Li De-yu, Wang Pei-ling & Liu Jian-chen, Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai, China.

The change of symmetry group of apatite from  $P6_3/m$  to that of lessingite,  $P2_1$ , results from the shift of the Si and O atoms from the equivalent positions (6h) and (12i) as produced by distortion of polyhedra with 7- and 9-corners. The substitution of Ca in apatite for TR (to some extent) and the disorder distribution of atoms TR and Ca on the equivalent positions (6h) and (4f) may have contributed to the distortion of the 7- and 9-cornered polyhedra. This is significant for understanding both the characteristics of constituent and structure, and the relationship between the distribution of rare earth elements and the crystal chemistry of compounds with the apatite structure type which are important for laser application.

Unit cell determination was furnished on PW 1100 diffractometer by least-squares refinement:  $a = 9.6283$ ,  $b = 9.6305$ ,  $c = 7.0495 \text{\AA}$ ;  $\gamma = 120.02^\circ$ ;  $Z = 2(\text{TR}_{3.42}\text{Ca}_{1.415}\text{M}_{0.165}\text{Si}_3\text{O}_{12}\text{F})$ ;  $d_{\text{obs}} = 4.877 \text{ g/cm}^3$ ;  $d_{\text{calc}} = 4.918 \text{ g/cm}^3$ .

The atomic coordinates, isotropic and anisotropic thermal parameters were refined to  $R = 0.093$  and  $R_w = 0.083$  for 808 independent reflections by means of least-squares calculations.

The projections of structure of lessingite (XZ) (Fig.1) and (XY) (Fig. 2).