

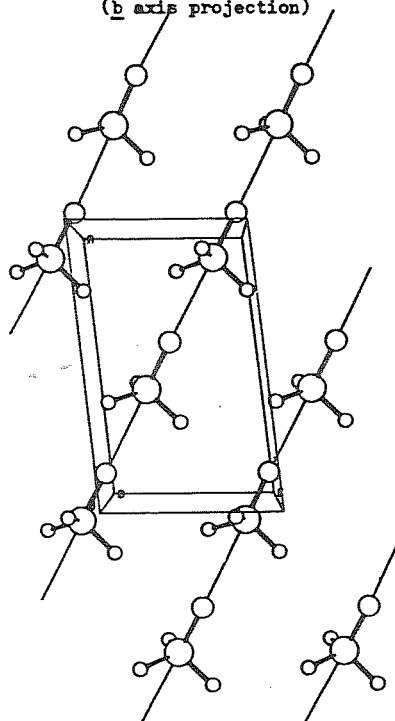
We have, for the first time, established the existence of  $\text{SiO}_2\text{N}_2$  tetrahedra in the pyrosilicate group  $\text{Si}_2\text{O}_7\text{N}_4$  during the structural study of the melilite compound  $\text{Ln}_2\text{Si}_3\text{O}_7\text{N}_4$ . The third silicon atom presents a  $\text{SiN}_4$  nitrided environment.

When calcium is substituted by lanthanide in  $\text{CaSiO}_3$ ,  $\text{LnSiO}_3\text{N}$  compounds are obtained. The cyclic  $\text{Si}_3\text{O}_9$  group of the wollastonite is replaced by the  $\text{Si}_3\text{O}_6\text{N}_3$  entity with existence of  $\text{Si}_2\text{O}_2\text{N}_2$  tetrahedra.

The  $\text{Ca}_4\text{Si}_7\text{O}_{17}\text{F}_2$  cuspidine belongs to the sorosilicate family. The substitution of calcium by lanthanide leads to the  $\text{Ln}_4\text{Si}_7\text{O}_{17}\text{N}_2$  oxynitrides. Nitrogen doesn't take the fluorine position but is linked to silicon. In the  $\text{Si}_2\text{O}_5\text{N}_2$  group the formation of  $\text{SiO}_3\text{N}$  tetrahedra can be observed.

So, as the  $\text{SiO}_4$ ,  $\text{SiN}_4$  and  $\text{SiON}_3$  tetrahedra were already well known, we have pointed out for the first time the evidence of the  $\text{SiO}_2\text{N}_2$  and  $\text{SiO}_3\text{N}$  tetrahedra.

Figure 1. Packing diagram for silyl fluoride (b axis projection)



08.2-37 THE CRYSTAL STRUCTURE OF SILYL FLUORIDE  
AT 96K, by Alexander J. Blake, E.A.V. Ebsworth and Alan J. Welch, Department of Chemistry, University of Edinburgh, Scotland, EH9 3JJ.

A sample of silyl fluoride was sublimed into a Pyrex tube which was then sealed. On cooling the sample on a Weissenberg camera equipped for low-temperature work, a liquid appeared from which a single crystal was grown. Space group ( $P2_1/n$ ) and unitcell parameters were determined before the crystal was transferred - without melting or other phase change - to an Enraf-Nonius CAD4 diffractometer for data collection. Accurate unitcell parameters were obtained by least-squares refinement (G.S. Pawley, J.Appl.Cryst. 1981, 14, 357-361) against an Xray powder profile for the compound obtained by microdensitometry of a film recorded on a Guinier-Simon low-temperature camera.

The structure of silyl fluoride consists of chains of molecules formed by strong F...Si interactions. The F...Si distance of 2.8941(12) Å is well within the sum of the corresponding van der Waals' radii (3.45 Å). The Si - F...Si and F...Si - F angles are 146.03(7) and 178.65(6)° respectively. Perhaps surprisingly, there are no close F...H contacts. The Si has 4 + 1 coordination and a concomitant lengthening of the Si - F bond in the crystal (1.6045(12) Å) as compared with the gas phase value of 1.59465(4) Å (S. Craddock, personal communication) is observed. Full details will be presented for silyl fluoride and for related compounds.

08.2-38 ON THE NON-HOMOGENEITY OF THE PHASE COMPOSITION OF URINARY CALCULI.

Z. Durski and H. Nowaczek, Department of Chemistry, Warsaw Technical University, Warszawa, Poland, and B. Kuzaka, Urological Clinic, Academy of Medicine, Warszawa, Poland.

As the result of the investigations which we have conducted using powder methods on a X-ray diffractometer, we have found that several parts / outer part, central part, nucleus / of the same kidney stone - may have a different phase composition /Tab. I/. This fact is not fully and satisfactorily examined and described in the literature yet. Non-homogeneity of the composition can also effect the quantitative determination of the composition. The stone can be composed from two substances only /e.g. from WEW and WED/ but the quantitative relation of these components in the outer part and in the central part of the stone can be different. There are also such cases, in which one finds in the renal of the same patient a few stones with different phase composition /Tab. II/.

The accurate data will be published in Polski Tygodnik Lekarski / Polish Magazine of Medicine/. The abbreviations applied in this abstract are as follows: WEW - whewellite, WED - weddellite, HAPA - hydroxyl-apatite, STRU - struvite, UA - uric acid.