(c) hydrogens with H(D)0...S > 3.1 Å C(H(D)...0 > 2.70 Å), far outside the usual hydrogen bond range.

Vibrational spectroscopic investigations on isotopically dilute (H and D) single crystals, measured at 295 K and 75 K, showed uncoupled O-H(D) stretching frequencies in the range $\tilde{\nu}$ = 2345-2665 (3145-3620) cm$^{-1}$. According to the Badger-Bauer rule these frequencies would correspond to hydrogen bond energies of 5-40 kJ mol$^{-1}$. Reasonable assignments of the observed frequencies to the individual hydrogen bonds could be made. For the approximately linear O-H(D)...S type bonds with H(D)...S = 2.35 Å (O...S = 3.3 Å) uncoupled O-H(D) frequencies of $\tilde{\nu}$ = 2400-2520 (3220-3410) cm$^{-1}$ were observed, the specific values depending significantly on the chemical nature of the S acceptor atoms. Despite large H(D)...S distances (2.71-2.85 Å) the bifurcated O-H(D)...S,S bonds show stretching frequencies which are similar to those of linear O-H(D)...S bonds with H(D)...S = 2.35 Å. The type (c) hydrogen atoms observed in Na$_3$As$_4$D$_8$O$_4$ and NaAs$_4$S$_8$S$_2$O$_4$ exhibit O-H(D) frequencies of $\tilde{\nu}$ = 2665 (3620) cm$^{-1}$ which indicate some crystal field interactions with the surrounding atoms.

04.6-04 THE CRYSTAL STRUCTURE OF THE ADDITION COMPOUND OF FLUOROSILICIC ACID WITH UREA. By Se-Yang Zhang, Mei-Cheng Sheo, Xiao-Jie Xu and You-Chi Teng, Institute of Physical Chemistry, Peking University, Beijing, China; Yu-Qin Tu, Institute for Plant Protection Research, Chinese Academy of Agricultural Sciences, Beijing, China.

The addition compound ([NH$_4$)$_2$CO]$_2$H$_2$SiF$_6$ crystallizes in tetragonal space group P 4$_1$/2$_1$ with lattice parameters $a$=9.263(4) Å, $c$=17.898 (6) Å and $Z$=4. The structure was solved by direct method and refined for 1562 independent MoK$_\alpha$ counter data. The R index is 0.082 and Rw=0.032. The result reveals that the crystal structure consists of octahedral fluorosilicate anions and ureated protons ([NH$_4$)$_2$CO]$_2$H$^+$OC(NH$_2$)$_2$. The strength of the hydrogen bonds of intermediate strength, we have undertaken X-ray studies of 2,2',4,4'-tetrahydroxybenzophenone, 2,4-dihydroxybenzophenone and 3,0.6-0.7 Å, $c$=4.702(1)Å (153K) and $a$=5.972(2), $b$=4.822(1) (200K)

Although hydrogen atoms were included with anisotropic temperature factors in both refinements, a difference map showing the electron density of the H atoms shows the inadequacy of the conventional model. At 153K the H atoms are well localized with one on the 3 fold axis and 3 on mirror planes but at room temperature the unique H atom appears to be disordered off the threefold axis. The relation of this disorder to that proposed by Knop et al. will be discussed.

04.6-05 HYDROGEN BONDING IN (NH$_4$)$_2$TiF$_6$. By L. Tun and I.D. Brown, Institute for Materials Research, McMaster University, Hamilton, Ontario, Canada. 155 4ML.

A recent study (Knop, Westerhaus and Falk, 1980 Can. J. Chem., 58, 867) of infrared spectra of the ammonium ion in (NH$_4$)$_2$TiF$_6$ at different temperatures shows that the stretching frequency of all N-H bonds increases with decreasing temperature. The negative values of dv/dT for the N-atoms have been explained by supposing that at low temperatures the hydrogen atoms form trifurcated bonds as required by the space group symmetry but that at higher temperatures the ammonium ion is rotationally disordered to form stronger hydrogen bonds with particular F atoms. In order to examine this hypothesis we have used x-ray diffraction to refine the structure of (NH$_4$)$_2$TiF$_6$ at room temperature and at 153K to R = 0.02. The crystal is triclinic, space group P$ar{3}m1$ with $a$=5.920(2), $b$=4.702(1)Å (153K) and $a$=5.972(2), $b$=4.822(1) (200K)

Financial support of this work by the National Science Foundation (Grant CHE77-08325) is gratefully acknowledged.