to pressures of about 3 GPa, and down to liquid helium temperatures. We present here the results of high pressure powder measurements on the three D2O phases that have interpenetrating sublattices (ices VI, VII and VIII). The node of ordering of tetragonal ice VIII (8G: Td; incomm.) is clearly established, and no evidence is found of partial ordering as the temperature is raised. Ice VII is accurately cubic (8G: Pm3m) with D2O molecules disorderd around their center of mass; there is no evidence of partial ordering at any temperature. The water molecule geometry is normal in both phases, and the hydrogen-bonded first neighbour in ice VIII is confirmed to be more distant than the first non-bonded and the hydrogen-bonded first neighbour in ice VII.

We conclude that the orientational ordering behaviour of these high pressure ices is simpler than thought previously. For our ice VI result to be consistent with those of Kamb, his antiferroelectric ordering must be an artifact of the recovery process, thus throwing doubt on the validity of structural ordering data obtained on samples recovered to ambient pressure.

04.6-7 HYDROGEN-BOND RESEARCH USING THE CAMBRIDGE STRUCTURAL DATABASE. Robin Taylor and Olga Kennard, Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, U.K.

Analysis of data in the Cambridge Structural Database provides detailed information about the basic factors governing hydrogen bond geometry. H...A distances can be correlated with the nature and crystallographic environment of the donor and acceptor groups -for example, R3N+H...O bonds are found to be shorter than H3N+-H...O bonds. D-H...A angles have an energetic preference for linearity or near-linearity, particularly when the H...A distance is short. There is a slight preference for hydrogen bonding in the directions of sp2 lone pairs, but it is arguable whether a similar preference exists for sp3 lone pairs. Donor and acceptor valence bonds appear to be lengthened by hydrogen-bond formation, but this may be an artefact of libration phenomena. Hydrogen bonds involving C-H donors or the 3-centre ("unbraced") arrangement are more common than previously supposed.

04.6-8 CRYSTAL STRUCTURE OF MIIH10(AsO4)4 COMPOUNDS AND HYDROGEN BONDING (MII = Mg, Mn, Ni, Cu and Zn). By M. Chiadini and D. Tran Qui, Laboratoire de Cristallographie, C.N.R.S., Associé à l.U.M.R.C., 166 X, 38042 - Grenoble Cedex, France.

Acidic orthoaesaminic MIIH10(AsO4)4 compounds (MII = Mg, Mn, Ni, Cu and Zn) have been prepared and single crystal grown. X-ray data show that all the series members belong to space group PI and have very close unit cell parameters suggesting normally isomorphism between these salts. Crystal structure of CuIIH10(AsO4)4 (a = 5.391(3), b = 7.631(4), c = 8.298(5), alpha = 105.8(4), beta = 97.62(3) and gamma = 93.84(10)) has been established including hydrogen positions and refined to a final R factor 3.9 % for 2156 reflections. The structure consists of CuO6-AsO4 chains parallel to a-axis. CuO6 and AsO4 tetrahedra are linked together by oxygen corners sharing. Hydrogen localizations confirm the existence of bisacidic and trisacidic groups : AsO2(OH)2 and AsO(OH)3. It was also observed that the triacidic AsO(OH)3 orientation with respect to CuO6-AsO4 chain is significantly different in CuIIH10(AsO4)4 crystal structure and in that of CuIIH10(AsO4)4 (a = 5.5945, b = 7.9249, c = 8.6060, alpha = 105.17, beta = 99.1350, gamma = 91.8500). (Boudjada et al., Acta Cryst. (1980), 836, 133-135). This structural distortion will be discussed in terms of hydrogen bonding.


In acid salts of dicarboxylic acids H2Y we should expect the anion in MW to have one carboxyl group ionized, the other not. In this case the carboxyl groups are linked by H bonds, which are essentially non-symmetric; they are called A-type bonds [Spekman, Structure and Bonding (1972)] and the B-type acid salts PNCH(NH3)2CNHOH. [Blankensteyn, Heerman, Owen & Kroon, Coll. Abstracts E.C.N. B (1983) 161]. We now have solved the crystal structure of the superacid salt of composition NaH(C2H4O7)2, which also appears to be of a mixed A/B type and that of LiH4H406.H2O with unusual cyclic H-bonded carboxylic dimer formation.

NaH2(C2H4O7)2, monoclinic, P21/c, a=6.514 (1), b=9.193 (3), c=3.640 (3) , V=16.00 (3), R=0.08. Two unique reflections [12.2.5c(1)], current R=0.065.

LiH4H406.H2O, monoclinic, P21/c, a=4.886 (1), b=23.361 (5), c=5.310 (1) A, R=0.04. (1), R=0.078.