1. freezing of one type of AO_4 libration
2. ordering of the two-dimensional hydrogen bridge system
3. AO_4 dimer switching
4. proton ordering within a hydrogen bridge

A complete survey of all known transitions will be presented and examples of the different ordering mechanisms will be analysed in view of experiment and theory.

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Pawlowski, A., Pawlaczyk, Cz., Hilczer, B.: *Solid State Ionics* 44 (1990) 17-19.
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MS11.05b.06 STRUCTURE DETERMINATION AT HIGH PRESSURES FROM MOLECULAR DYNAMICS SIMULA-TIONS. S. K. Sikka, Surinder M. Sharma, R. Chidambaram, High Pressure Physics Division, Bhabha Atomic Research Center Bombay - 400 085

We describe the use of molecular dynamics (MD) simulations to determine the structures of some high pressure phases which give only a few Bragg peaks in their diffraction patterns. In α-quartz, Kingma et al[1] had reported the diffraction pattern of a new phase before amorphization at 21 GPa. Using the coordinates derived from MD simulations, employing the pair potentials of Tsuneyuki et al[2], we got x-ray patterns in excellent agreement with experimental results - indicative of a tripling of the α-quartz unit cell in its basal plane. A monoclinic cell could then be derived.[3]

In $LiCsSO_4$, there has been a controversy about the number and nature of pressure induced phases. We have carried out x-ray diffraction studies on this and have detected two c-c transitions at 4 and 7 GPa and amorphization at ~ 19 GPa[4]. Our data rule out the earlier conjecture that the 4 GPa transition is the orthorhombic to monoclinic (a low temperature phase) one. Instead the x-ray pattern here strongly resembles the one calculated from the coordinates of 9.8 GPa phase of $LiKSO_4$ as computed by an earlier MD simulation[5]. This new structure is related to the ambient one through the softening of the (1/3,1/2,0) mode and has higher oxygen coordination for Li atoms.

Another application to solve the intermediate structure between fcc and hcp structures of Xe in the pressure range 12-75 GPa will also be described.

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Analysis of Atomic Displacement Parameters

MS11.06.01 NORMAL MODE ANALYSIS FROM ELASTIC DIFFRACTION DATA IS POSSIBLE! WHY AND HOW? H. B. Bürgi, Labor für Kristallographie, Freiestr. 3, Universität, CH-3012, Bern, Switzerland

It is generally believed that atomic mean square displacement parameters (ADP) obtained from an elastic diffraction experiment provide information on the motion of individual atoms, but cannot say anything on the cooperative displacements of groups of atoms unless assumptions of questionable validity are made. This opinion is correct with respect to ADP's pertaining to a single temperature; it is untenable, however, when ADP's at several temperatures are available. Why is this so?

ADP's can be considered as a superposition of the contributions from many normal modes. The absolute atomic displacements of a mode depend on its energy (ν), its effective or reduced mass (μ), on temperature (T) and on relative displacement (A) according to $A*h/(8*\pi^2*\mu*\nu)*coth [h*\nu/(2*k*T/]$. At sufficiently low temperatures this expression can be approximated by $A*h/(8*\pi^2*\mu*\nu)$. At sufficiently high temperatures the corresponding approximation is $A*k*T/(4*\pi^2*\mu*\nu^2)$.

Now, suppose that a mean squared displacement U is the result of a superposition of two normal modes only and that it has been measured at a low and at a high temperature; then
$U(lowT) = A1*h/(8*\pi^2*\mu1*\nu1) + A2*h/(8*\pi^2*\mu2*\nu2)$
$U(high T) = A1*k*T/(4*\pi^2*\mu1*\nu1^2)+A2*k*T/(4*\pi^2*\mu2*\nu2^2)$.

From the two independent observations the two normal frequencies can be determined, provided A1 and A2 are known. This simple argument can be generalized to more than two frequencies and to the corresponding relative displacements if the coth-dependence and the three-dimensional information contained in the ADP's are taken into account. In practice, ADP's need to be measured at a sufficient number of appropriate temperatures.

MS11.06.02 MODELLING THE THERMAL MOTION OF FREELY ROTATING MOLECULES. R. T. Downs and L. W. Finger, Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Rd. N.W., Washington D.C. 20015, phone: (202) 686-2410 x 2469, e-mail: downs@gl.ciw.edu

All molecular gas-phases become crystalline when subjected to sufficient pressure. Spectroscopic studies show that the molecules are freely rotating while near the freezing point for many of these phases. As pressure increases the motion is constrained and a lowering of symmetry occurs. In order to model the freely rotating molecule we calculated molecular electron-density wave functions using the *Gaussian92* program for energy-optimized model molecules. The electron-density was then spherically averaged in order to mimic the rotations. The Fourier transform of this spherically averaged electron density provides the scattering factor for the rotating molecule. The displacement parameters obtained from the structure refinement then provide estimates of translational motion.

MS11.06.03 LATTICE-DYNAMICAL CALCULATION OF ATOMIC DISPLACEMENT PARAMETERS (ADPs). Carlo M. Gramaccioli and Francesco Demartin, Università degli Studi, Via Botticelli 23, I-20133, Milano, Italy, Tullio Pilati, CNR-CSRSRC, Via Golgi 19, I-20133 Milano, Italy

ADPs comparable with the corresponding values obtained from crystal structure refinement can be derived from Born-von Karman lattice dynamics. A rigid ion model has been assumed, where atomic charges and VFF parameters have been deduced from best fit to the vibrational frequencies of a series of similar compounds, either molecular crystals or even ionic, non-molecular