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EFFECT OF PRESSURE ON RAMAN-SPECTRA OF SOLID HCl AND HBr

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Résumé - Des résultats de diffusion Raman sur HCl et HBr, à des températures de 100 à 250 K et des pressions jusqu'à 40 GPa sont présentés. Une nouvelle procédure de chargement avec ces produits réactifs est décrite. L'argon et l'azote sont utilisés comme milieux transmetteurs de pression. Dans HBr, une nouvelle phase a été détectée - probablement avec des liaisons hydrogène symétriques - à 100 K et à des pressions supérieures à 32 GPa.

Abstract - Raman data are presented for HCl and HBr at temperatures between 100 and 250 K and pressures up to 40 GPa. A new procedure is described for loading a DAC with these reactive materials. Argon and nitrogen are used as pressure media. A new phase, probably with symmetric hydrogen bonds, is detected in HBr at 100 K and pressures above 32 GPa.

Three phases are reported for each HCl and HBr at ambient pressure. In the high temperature phase I, the halogen atoms occupy face-centered cubic positions while the H atoms exhibit a 12-fold disorder. Phase III is orthorhombic, space group C\textsubscript{12}, with planar zig-zag hydrogen bonded chains /1/. The orthorhombic "phase II" has been considered as a separate phase with proton disorder, however, the differences between "phase II" and III may be very gradual without any crystallographic phase transition.

A new loading procedure had to be developed for loading the diamond anvil cell (DAC) with the chemically reactive HCl and HBr. The reactive gas is first liquified by controlling the temperature of a small glass tube (fig. 1). A glass capillary is filled up with the liquid and kept in liquid N\textsubscript{2} until it is needed for the next preparation. To load the gasketed DAC, it is cooled to liqu. N\textsubscript{2}-temperature in an insulated box (fig. 2). Turbulences in the N\textsubscript{2}-atmosphere are prevented by covering the box with two transparent plates. A glass capillary with the crys-
talline samples is cracked beside the cell. A crystal is selected and brought into the sample chamber. Either $\text{N}_2$ or $\text{Ar}$ are used as pressure media.

The present experiments were performed with a DAC that has been described previously /2/. The 488 nm and 514 nm lines of an argon-ion laser were used to excite the Raman-spectra and the ruby fluorescence. Back-scattered light was analysed using a double monochromator and photon counting techniques. The resolution was kept at 3 cm$^{-1}$.

Typical Raman-spectra of HBr under pressure at 100 K are shown in fig. 3. At about 32 GPa a drastic change is seen in the spectra. The strong intramolecular peaks as well as two peaks in the lattice region vanish. On the other hand, a new lattice peak appears. From group theoretical arguments it can be concluded, that these changes indicate a transition into a phase with symmetric hydrogen bonds. Under the assumption of a zellengleich transition into a phase with space group $D_{2h}^7$, the three remaining peaks of this phase IV can be assigned as shown in fig. 4.

The temperature variation of the intramolecular modes of HBr at 3.4 GPa is illustrated in fig. 5. The spectra at temperatures below 185 K can be assigned to the orthorhombic phase III. Spectra at temperatures above 200 K are typical for phase I. The phase boundary between the cubic and the orthorhombic phase is represented by the continuous line in the P-T-phase diagram of HBr (fig. 6).

The Raman-spectra of HCl are very similar to the spectra of HBr. The effect of pressure on the Raman-frequencies of HCl at 100 K is given in fig. 7. Fig. 8 shows the P-T-phase diagram of HCl. A phase transition into a symmetric phase was not observed for HCl in the present pressure range up to 42 GPa.
Fig. 5 - Temperature variation of the intramolecular modes in HBr.

Fig. 6 - P-T-phase diagram of HBr.

Fig. 7 - Effect of pressure on Raman-frequencies of HCl.

Fig. 8 - P-T-phase diagram of HCl.

References:
/1/ ANDERSON A., TORRIE B.H. and TSE W.S., J. of Raman Spectroscopy 10, (1981); 149