

Structural and Vibrational Studies of Solid Ammonia to 120 GPa

Frédéric Datchi, Sandra Ninet, Michel Gauthier, A.Marco Saitta,
Institut de Minéralogie et Physique des Milieux Condensés, CNRS,
Université P&M Curie, 140 rue Lourmel, 75015 Paris, France. E-mail: fd@pmc.jussieu.fr

Like water, ammonia is a major member of the group of simple hydrogen-bonded molecular ices. The study of its high-pressure properties is first of natural interest due to its abundance in the solar system, like in the Jovian planets. Ammonia also presents a fundamental interest in condensed-matter physics as a H-bonded solid. Hydrogen bonds are weaker in ammonia than in water since 3 H atoms share a single lone pair. Whereas the symmetric state of water ice has been observed experimentally, the symmetrization path in ammonia appears more complicated. Actually, the phase diagram is barely known above 10 GPa. The solid transforms to the orthorhombic phase IV above 4 GPa; the presence of new phases has been suggested by Raman [1], Brillouin [2] and IR [3] experiments. But these results are confusing — what are the transition pressures ?, and incomplete — what is the nature of these new phases ?

We have conducted X-ray diffraction experiments up to 120 GPa and polarized Raman scattering on single crystals up to 70 GPa at low temperature. The use of single crystals allowed us to observe for the first time both very weak diffraction peaks and Raman modes and follow their evolution with pressure. Comparison between NH_3 and ND_3 showed significant isotopic effects.

[1] Gauthier, et al, *Phys. Rev. B*, 1988, **37**, 2102-2115. [2] Gauthier, et al., *Sol. State Comm.*, 1988, **68**, 149. [4] Sakashita, et al, *Rev. High Pres. Sc. Tech.*, 1998, **7**, 796-798.

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