

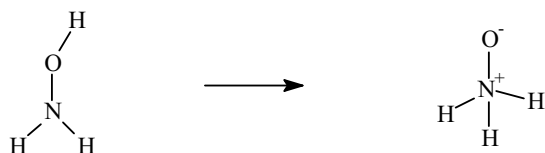
s6.m1.p5 Under Pressure: Hydroxylamine, P.A. McGregor¹, D.R. Allan¹, D.J. Francis², W.G. Marshall², S. Parsons³, C.R. Pulham³, 1. *Department of Physics and Astronomy, The University of Edinburgh, King's Buildings, Mayfield Road, Edinburgh, EH9 3JZ*, 2. *ISIS Neutron Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon, OX110QX*, 3. *Department of Chemistry, The University of Edinburgh, King's Buildings, West Mains Road, Edinburgh, EH9 3JJ*.

Keywords: hydroxylamine, neutron diffraction, pressure.

The hydrogen-bonded systems of water, ammonia and water-ammonia mixtures have been extensively studied under a variety of conditions, and show a rich diversity of structural motifs involving hydrogen bonding. Hydroxylamine (NH₂OH) contains both amine and hydroxy functional groups in the same molecule, and so should also be expected to give rise to a range of interesting structures that are dependent on the relative magnitude of intermolecular interactions. Pressure is a powerful tool for tuning these interactions.

Unlike its fully substituted analogues, eg Me₃N⁺-O⁻, hydroxylamine exists under ambient conditions as the N-OH bonded tautomer rather than the N⁺-O⁻ bonded tautomer.

Preliminary investigations at the University of Edinburgh using Raman spectroscopy showed a substantial increase in the N-O stretching mode that is consistent with the formation of the amine-oxide tautomer.



A fully deuterated sample was prepared for neutron diffraction on PEARL/HiPr at ISIS. With a limited pressure and temperature range, 260-300K and 0-9Gpa, these initial neutron diffraction studies produced convincing evidence of the existence of two high- pressure phases. A third phase was also observed, but we have yet to rule out the possibility that this pattern is due to decomposition of the sample.