Isostructural Transformation and Polymorphism of Thiourea Dioxide at High Pressure

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With the notable exceptions of water, ammonia and a very limited number of other examples, there have been relatively few high-pressure structural studies of simple molecular compounds. Such studies can provide fascinating information about intermolecular interactions and pressure-induced phase transition, in particular hydrogen-bonding interactions. Recent results for thiourea and urea obtained from the experiments on neutron beamlines at the UK ISIS facilities have shown a very rich high-pressure behaviour [1].

In the light of these results, we have undertaken neutron and synchrotron studies on thiourea dioxide, which has been selected by virtue of its interesting ambient pressure structure [2].

We report a phase transition between a powder sample of orthorhombic phase I of thiourea dioxide to a new monoclinic phase II at a pressure of 0.54 GPa. This transition has also been observed in a single crystal sample at a pressure of 0.45 GPa. We also report an unusual isostructural transformation in thiourea dioxide at 6.8 GPa that involves the formation of a new hydrogen bond.

[1] Marshall W.G., *ISIS Annual Report*, 2003. [2] Sullivan R.A.L., Hargreaves A., *Acta. Cryst*., 1962, **15**, 675.

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