ESRF	**Experiment title:** Isomerisation in Phosphorus(V) and Sulphur Compounds	**Experiment number:** CH-25
Beamline: BMl-SNBL	**Date of Experiment:** from: 9 March 1995 to: 13 March 1995	**Date of Report:** 26 August 1996
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Report:

At a wavelength of 0.94734 A, high resolution powder diffraction patterns were measured from capillary samples of stable and metastable $(CH_3)_2SBr_2$, "ionic" and "molecular" Ph_3PCl_2, and $PhPBr_4$.

For the stable form of $(CH_3)_2SBr_2$ the structure has been solved [l], using direct methods, in the space group $P2_1/a$, with lattice parameters a = 11.421 A, *b = 7.386* Å, *c = 7.450* Å, and β = 92.82°. There are four molecules per unit cell. The key structural feature is the charge-transfer interaction between the donor sulphur atom and the bromine acceptor molecule which is coordinated in a near-linear end-on manner to the sulphur atom, figure 1.

Despite its excellent quality, it has proved impossible to index the diffraction from the sample of metastable $(CH_3)_2SBr_2$, figure 2. The cell is perhaps too large for current indexing algorithms, or, more likely, the sample is not single phase. Although metastable $(CH_3)_2SBr_2$ transforms into stable $(CH_3)_2SBr_2$, no peaks from the latter are visible in the diffraction pattern.

The diffraction pattern of $PhPBr_4$ has been indexed with an orthorhombic cell, a = 11.183 Å, *b* = 15.788 Å, and c = 8.050 Å. Attempts to solve the structure by direct methods or Patterson maps are continuing.

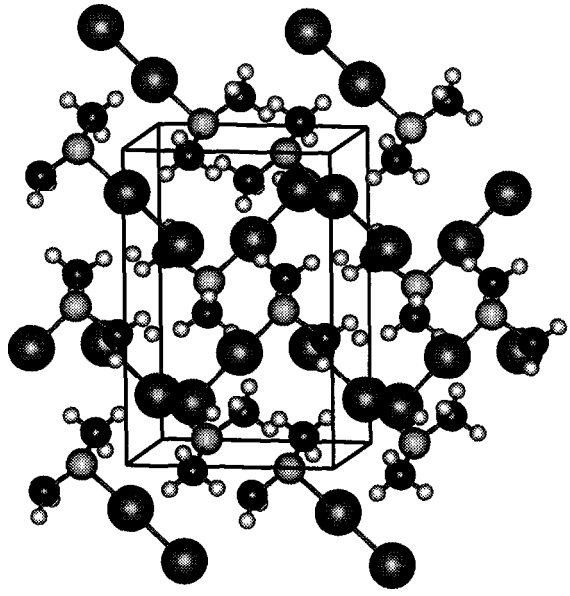

Figure 1. View of the structure of stable $(CH_3)_2SBr_2$

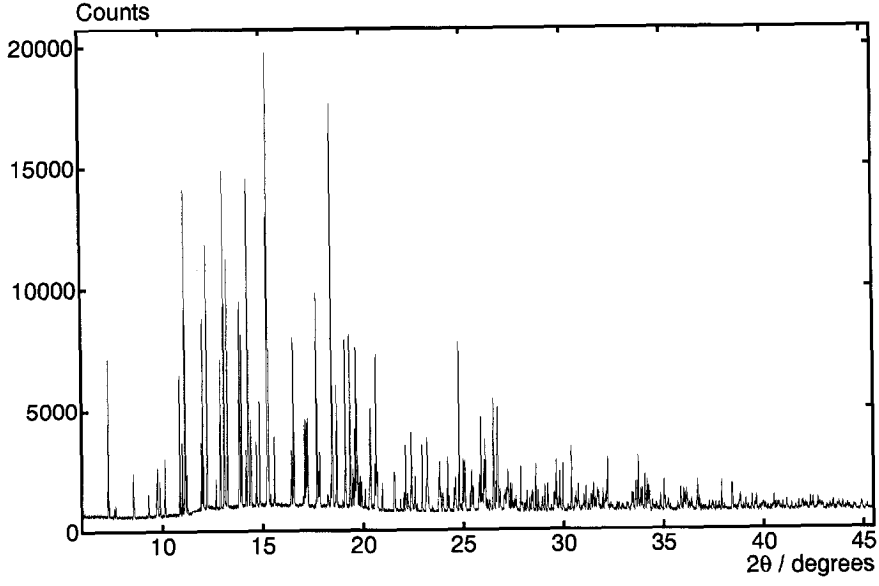

Figure 2. Powder diffraction pattern of metastable $(CH_3)_2SBr_2$

[l] Structural Determination of $(CH_3)_2SBr_2$ Using the Swiss-Norwegian Beam Line at ESRF, A. J. Mora, A. N. Fitch, P. N. Gates and A. Finch, Proceedings of EPDIC 4, Chester 1995, Materials Science Forum, In press.