

Crystal Structure of the Bis(thiourea)iodine(I) Ion

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Summary The crystal structure of the yellow compound of composition $(\text{thiourea})_2\text{I}_2$ has been determined: the compound is bis(thiourea)iodine(I) iodide.

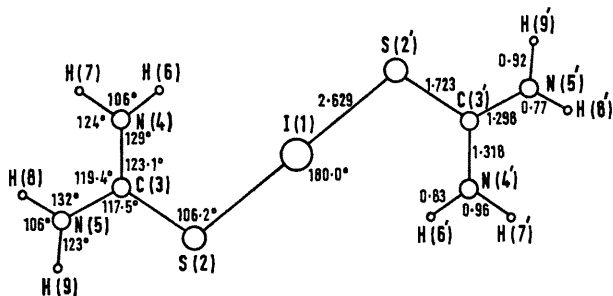
In 1912 Werner¹ described the preparation of a yellow compound formed by interaction of thiourea and iodine in a 2:1 molar ratio. We have determined the crystal structure of this compound, which is bis(thiourea)iodine(I) iodide. The compound was prepared by grinding iodine dissolved in methylene chloride with solid thiourea. Crystals suitable for X-ray studies were grown from methylene chloride solution.

The crystals are monoclinic, space group $C2/c$, with cell dimensions $a = 22.27 \pm 0.02$, $b = 5.290 \pm 0.005$; $c = 9.808 \pm 0.005$ Å; $\beta = 115.31 \pm 0.03^\circ$. There are four units of $\text{C}_2\text{H}_4\text{N}_2\text{S}_2\text{I}_2$ in the cell.

Intensity data were gathered with a Picker automatic diffractometer, using Zr filtered Mo- K_α radiation. Altogether 841 unique reflections were observed. The structure was solved by Patterson and Fourier methods, and refined by full-matrix least-squares techniques. All variable parameters were refined, including anisotropic thermal parameters for non-hydrogen atoms, and isotropic ones for hydrogen. The final R index is 0.025.

The structure consists of separate $[(\text{NH}_2)_2\text{CS}]_2\text{I}^+$ and I^- ions. The anions are located on two-fold axes, whereas the

iodines of the cations are located at centres of symmetry; the cations are not planar, however, presumably owing to a short intramolecular I-N (or I-H) distance. The fold angle defined by I-S-C and S-C-N is 17° . Bond distances and angles are given in the Figure.



FIGURE

So far as we know, this is only the second known example of an I^+ complex, the first being bis(pyridine)iodine(I).²

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¹ E. A. Werner, *J. Chem. Soc.*, 1912, **101**, 2166.

² O. Hassel and H. Hope, *Acta Chem. Scand.*, 1961, **15**, 407.