

The Crystal Structure of Lead Thiocyanate

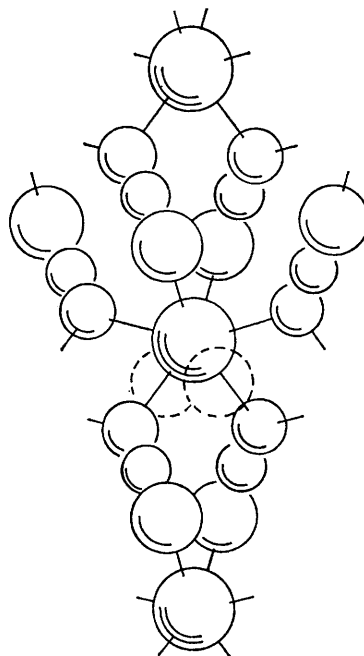
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CRYSTALS provided by Miss Ida Woodward, of Queen's University, Belfast, have been studied by X-ray diffraction (using Cu- $K\alpha$ radiation) with the following results: *Lead thiocyanate*, $\text{Pb}(\text{SCN})_2$, $M = 323.4$. *Monoclinic*, $a = 9.72$, $b = 6.57$, $c = 8.27$ Å, $\beta = 92.0^\circ$, $U = 527.8$ Å³, $D_m(\text{Groth}) = 3.82$, $Z = 4$, $D_c = 4.07$. Space group, Cc or $C2/c$. The latter (No. 15) is consistent with the outcome of a structure analysis based on the intensities of 340 observed reflexions. The structure was solved by the heavy-atom method and refined by three-dimensional least-squares analysis to an R -value of 13.5%. Allowance for absorption, which is heavy, was made only roughly, so that the positions of the carbon and nitrogen atoms are not accurately determined.

The essential features of this neat structure are suggested by the Figure. The lead ion lies on a two-fold axis, its immediate co-ordination being six-fold: a pair of sulphur atoms lie at a distance of $3.05 (\pm 0.01)$ Å and two pairs of nitrogen atoms at 2.70 and 2.72 Å (each ± 0.08). A second pair of sulphur atoms (indicated by the broken circles in the Figure) are at 3.14 Å. Including this last pair, each lead ion makes contact with four sulphur and with four nitrogen atoms from eight different thiocyanate ions, whilst each thiocyanate makes contact with four lead ions—two at each end. The thiocyanate ion does not deviate significantly from linearity, and the S-C and C-N distances are about 1.5_3 and 1.2_6 Å respectively.

A sub-cell defined by $a' = -\frac{1}{2}c$, $b' = b$ and $c' = -a + \frac{1}{2}c$ has $a' = 4.14$, $b' = 6.57$, $c' = 10.69$ Å



FIGURE

The crystal structure of lead thiocyanate viewed in the a -direction, with the b -axis vertical: in order of decreasing radii the circles represent Pb, S, N, and C atoms.

and $\beta = 115^\circ$, parameters which agree well with those given by Groth.

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