The Crystal Structure of Bis(imidazoline-2-thione)cadmium Chloride

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CADMIUM, like zinc, shows a tendency to assume a tetrahedral co-ordination, but only a few crystal structures have been reported.[1] Octahedral co-ordination is more usual and generally achieved in polymeric structures. Tetrahedral co-ordination is now observed in bis(imidazoline-2-thione)cadmium

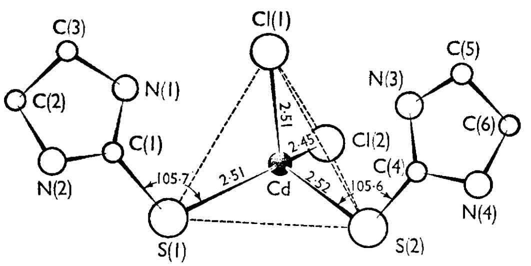

FIGURE 1. $Cd[SC(NHCH_2)_2]_2Cl_2$: *clinographic projection of the molecule.*

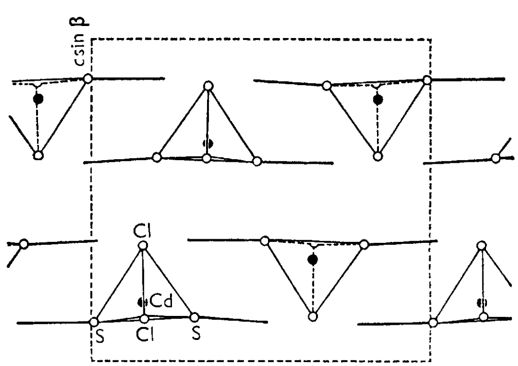

FIGURE 2. *Projection of the structure on* (100). *Bold lines indicate the organic molecules.*

chloride. $Cd[SC(NHCH_2)_2]_2Cl_2$, $M = 387{\cdot}6$, $a = 6{\cdot}26$ (1), $b = 14{\cdot}54$ (2), $c = 14{\cdot}59$ (1) Å, $\beta = 108{\cdot}3°$ ($+01{\cdot}03°$), $Z = 4$, $U = 1265$ Å^3, $D_c = 2{\cdot}02$, $D_m = 2{\cdot}07$ g.cm.$^{-3}$, space group, $P\ 2_1/c$.

Intensities of 1207 non-zero independent reflections were measured photometrically from equi-inclination Weissenberg photographs taken around [100] up to the fifth layer. The structure was solved by standard Patterson and Fourier methods and refined by differential synthesis. At the present stage the R index is 13·8%.

Two chlorine and two sulphur atoms tetrahedrally co-ordinate to cadmium as shown in Figure 1. The distances in the co-ordination polyhedron agree well with those found in bis-(thiourea)cadmium chloride.[2] The two non-equivalent organic molecules are symmetrically tilted with respect to the Cd–S bonds and lie in planes nearly parallel to (001). The structure is built of double layers, parallel to (001), and containing the organic molecules and the chlorine atoms; the coupling of these layers is due to the Cd–Cl and Cd–S bonds, cadmium being situated between each couple of layers as shown in Figure 2.

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[1] K. S. Pitzer, *Z. Krist.*, 1935, **92**, 131.
[2] M. Nardelli, L. Cavalca, and A. Braibanti, *Gazzetta*, 1957, **87**, 138.