The Crystal Structure of Dithiocyanatobis(thiosemicarbazide)nickel(II)

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THE preparation and magnetic properties of the dithiocyanatobis(thiosemicarbazide) of nickel have been reported.[1] In connection with our work on the stereochemistry of thiocyanate complexes we have now determined and refined the crystal structures. The complex compounds of Ni^{II} with thiosemicarbazide, the structures of composition $[NiSO_4(thio)_2(H_2O)_2]$ and $[Ni(thio)_2]$[2,3] are known.

The following data were obtained, using Cu-K_α radiation:

$[Ni(NCS)_2(NH_2{\cdot}CS{\cdot}NH{\cdot}NH_2)_2]$,$C_4H_{10}N_8NiS_4$, M 357·13. Monoclinic, $a = 5{\cdot}27_5$, $b = 7{\cdot}81_3$, $c = 16{\cdot}01$ Å, $\beta = 91°\ 25'$, $U = 659{\cdot}89$ Å^3, $D_m = 1{\cdot}770$, $Z = 2$, $D_c = 1{\cdot}769$. Space group $P2_1/c$ (No. 14); molecular symmetry: I_1 with Ni in a special position.

Structure analysis was based on intensities recorded photographically for some 512 independent reflexions. The structure was solved by the heavy-atom method, and the co-ordinates and the isotropic temperature factors refined by least-square analysis, using three-dimensional data, to a final R value of 0·13. Estimated average deviations are ±0·019 for Ni–N, ±0·022 for S–C, ±0·026 for N–N, and ±0·028 Å for C–N; for angles round Ni, deviations do not exceed ±1°, while for the other atoms maximum deviations are within ±2°.

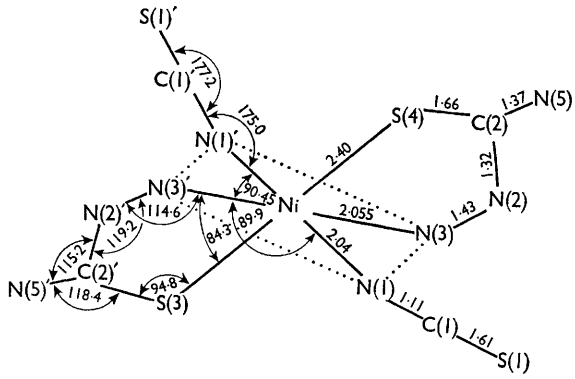

FIGURE. *Schematic view of the co-ordination polyhedron round the nickel atom*

The Figure shows the schematic structure as seen in the projection (100). The thiosemicarbazide molecules and the nickel atom lie in a plane, to which the bond between the nitrogen atoms of the rhodano-groups is normal.

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