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The Crystal Structure of Nickel(II) Bis(dithiocarbamate)

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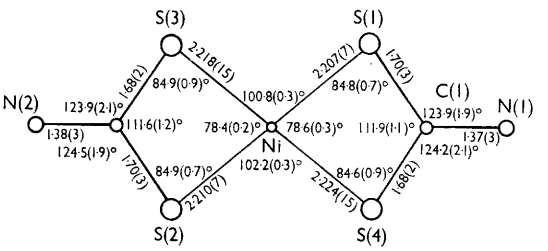
Though the structures of several metal complexes of substituted dithiocarbamic acids have been studied,[1] nothing has yet been done with unsubstituted dithiocarbamates. We have now prepared the following compounds and studied them by *X*-ray methods, using Cu-K_α radiation:

Ammonium dithiocarbamate, $NH_2CS_2NH_4$, $M=$ 110·2. *Orthorhombic*, $a = 5{\cdot}639$ (4), $b = 8{\cdot}272$ (2), $c = 10{\cdot}663$ (3) Å, $U = 497{\cdot}4$ Å^3, $D_m = 1{\cdot}46$, $Z = 4$, $D_c = 1{\cdot}471$; *space group*, *Pbcm* or $Pbc2_1$.

Cobalt(III) *tris*(*dithiocarbamate*), $(NH_2CS_2)_3Co^{III}$, $M = 335{\cdot}4$. *Monoclinic*, $a = 7{\cdot}13$ (3), $b = 10{\cdot}11$ (1), $c = 16{\cdot}32$ (2) Å, $\beta = 100{\cdot}8°(7)$, $U = 1156$ Å^3, $D_m = 1{\cdot}96$, $Z = 4$, $D_c = 1{\cdot}926$; *space group*, $P2_1/c$.

Nickel(II) *bis*(*dithiocarbamate*), $(NH_2CS_2)Ni^{II}{}_2$, $M = 243{\cdot}0$. *Monoclinic*, $a = 8{\cdot}96$ (2), $b = 9{\cdot}825$ (5), $c = 11{\cdot}28$ (2) Å, $\beta = 129{\cdot}3°$ (1), $U = 769{\cdot}0$ Å^3, $D_m = 2{\cdot}09$, $Z = 4$, $D_c = 2{\cdot}098$; space group, $P2_1/c$.

The structure of this last has been determined and refined by differential syntheses based on 1292 independent, photographically-determined intensities, leading to an *R*-value of 11·2%. Bond-distances and -angles are shown in the Figure; they are not significantly different from those found in the α-form of nickel(II) bis-(*NN*-diethyldithiocarbamate).[2] If bond-distances only are considered, the whole molecule is practically centrosymmetrical about the metal atom; but this symmetry is not complete, since the four S-atoms and the Ni-atom deviate slightly but significantly from coplanarity. The four (heavy) atoms of each ligand molecule are coplanar.



Figure

Apart from the four S-atoms two other atoms make contacts with the Ni: these are an H-atom at 2·85 Å and an S-atom at 3·60 Å. Metal–hydrogen contacts of this type have already been noted.[3]

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[1] G. Peyronel, *Z. Krist.*, 1941, **103**, 157.
[2] M. Bonamico, G. Dessy, C. Mariani, A. Vaciago, and L. Zambonelli, *Acta Cryst.*, 1965, **19**, 619.
[3] M. Bonamico, G. Dessy, A. Mugnoli, A. Vaciago, and L. Zambonelli, *Acta Cryst.*, 1965, **19**, 886; N. A. Bailey, J. M. Jenkins, R. Mason, and B. L. Shaw, *Chem. Comm.*, 1965, 237; J. A. Ibers, *Abstr. Amer. Cryst. Assoc.*, 1965, B 10.