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The Preparation and Characterisation of Tris(pyrrole-N-carbodithioato)-cobalt(III) Hemikisdichloromethane. Crystal and Molecular Structure and Solution Properties

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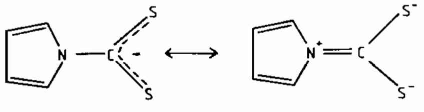
The title compound was obtained as monoclinic crystals belonging to the space group $P2_1/c$ *with* $a = 11.252(3)$, $b = 18.062(2)$, $c = 10.980(2)$ Å, $\beta = 111.30(2)^\circ$ *and* $Z = 4$. *Refinement with diffractometer data measured with CuKα radiation converged to give a conventional R index of 0.070. The* $Co-S_6$ *coordination geometry is distorted octahedral; some of the important bond lengths are Co–S, 2.267(3); S---S, 2.801(5); C–S, 1.675(9); (sulfur bonded) C–N, 1.388(11) Å. The average ligand bite angle is 76.3°, and the compound is isostructural with the Fe analogue.*

The green cobalt(III) complex is diamagnetic in the solid state and in solution in non-coordinating solvents. The solution visible absorption spectrum is typical of other tris(N,N'-disubstituted dithiocarbamato)cobalt(III) complexes having effective D_3 *symmetry.*

Introduction

Structural studies of tris-dithiocarbamato transition metal complexes have been extensive. Single crystal X-ray structure determinations include those of Co(III) [1, 2], Cr(III) [3–5], Fe(III) [4–6], Fe(IV) [7, 8], Ni(IV) [9], Ru(III) [10–12], Rh(III) [3, 5, 13], Ir(III) [4, 5, 12], and Mn(III) [3] compounds. There has been recent interest in the formation of metal complexes of the dithiocarbamate ligand derived from the reaction of carbon disulfide and heterocyclic nitrogen compounds such as pyrrole. The anion of the ligand may be represented [14, 15] by two resonance forms *1(a)* or *1(b)*.



1(a) 1(b)

A variety of metal complexes of this ligand including Cr(III) [15], Fe(III) [6, 14, 15], Co(II) [14], Pt(II) [14], Pd(II) [14], Cu(II) [14], Zn [15], Cd(II) [14] have been prepared and characterised. The recent structural study of tris(pyrrole-N-carbodithioato)-iron(III) [6] indicates that resonance form *1(b)* makes an insignificant contribution to the overall structure and the compound is the most extreme example of a low-spin tris-chelated iron(III) species yet reported. The predominant form of the coordinated ligand is that depicted in *1(a)*.

Although this type of ligand is effective in stabilising lower oxidation states of the coordinated metal [15] the reported isolation of a cobalt(II) species of pyrrole-N-carbodithioate is surprising because rapid oxidation to tris-chelated cobalt(III) species of the dithiocarbamate ligands usually occurs [16]. In our hands, using either cobalt(II) or -(III) salts as starting materials, only dark green *diamagnetic* compounds have been obtained. Accordingly, a single crystal X-ray structure determination of the isolated compound and absorption and C-13 nuclear magnetic resonance spectral measurements were carried out to ascertain the solid and solution structural properties of the compound.

Experimental

Preparation of Compounds

The sodium salt of pyrrole-N-carbodithioic acid was prepared as an approximately 1 *M* solution in dimethylsulfoxide [15]. Tris(pyrrole-N-carbodithioato)cobalt(III) was prepared as follows: The solution containing the sodium salt of the ligand (15 cm^3) was added to a stirred solution of $Co(NH_3)_6Cl_3$ (1 g in 10 cm^3 H_2O). An orange-brown material that formed initially changed to a dark green product which was collected after 6 hr. The product was washed thoroughly with water, dried *in vacuo* and recrystallized from chloroform/petroleum ether to yield 0.3 g of dark green diamagnetic needle shaped crystals (unsuitable for collection of X-ray data). *Anal.* Calc. for $CoC_{15}H_{12}N_3S_6$: C, 37.10; H, 2.49; N, 8.65; S, 39.6. Found: C, 37.14; H, 2.41; N, 8.53; S, 39.6%.

Recrystallisation from dichloromethane/heptane yielded a crystalline material containing 0.75 mol of heptane per mol of compound. *Anal.* Calc. for $CoC_{20.25}H_{16}N_3S_6$: C, 43.37; H, 4.31; N, 7.49; S, 34.31. Found: C, 43.12; H, 4.27; N, 7.50; S, 34.0%. Crystals suitable for X-ray structure analysis were obtained by slow evaporation of a dichloromethane solution of the heptane solvate to give the hemikis-dichloromethane solvate. *Anal.* Calc. for $CoC_{15.5}H_{13}N_3S$ Cl: C, 35.23; H, 2.65; N, 7.95; S, 36.4. Found: C, 35.44; H, 2.70; N, 8.06; S, 36.2%.

Instrumentation

Noise decoupled C-13 n.m.r. spectra were recorded of $CDCl_3$ solutions referenced to tetramethylsilane (0 ppm) as an internal reference on a JEOL PS100P pulsed Fourier Transform spectrometer operating at 25.15 MHz. Visible absorption spectra were measured on a Beckman Model DK2A spectrophotometer. Infrared spectra of the compound as potassium bromide discs were measured on a Perkin Elmer Model 457 spectrometer.

Crystal Data for the Hemikisdichloromethane Solvate

Although several attempts were made to use the heptane solvated species, solvent loss occurred, and this together with a marked tendency towards twinning precluded a structure analysis of the compound in this form. Only the hemikisdichloromethane solvate was obtained in a form suitable for the structure determination. Oscillation and Weissenberg photographs showed that the crystals were monoclinic and systematic extinctions, $h\ 0\ l\ (l = 2n + 1)$ and $0\ k\ 0\ (k = 2n + 1)$, indicated the space group $P2_1/c$. Accurate cell parameters were determined by least squares from 2θ values measured for 20 high-angle reflections on a four-circle diffractometer with CuKα radiation ($\bar{\lambda}$ = 1.5418 Å). The crystal density was determined by flotation in an aqueous solution of K_2HgI_4.

Crystal data: Asymmetric unit, $CoC_{15.5}H_{13}N_3S_6$-Cl. Monoclinic, space group $P2_1/c$, FW 527.9, a = 11.252(3), b = 18.062(2), c = 10.980(2) Å, β = 111.30(2)°; V = 2079 Å^3, D_m = 1.67(2), D_c = 1.686 Mg m^{-3}, Z = 4, F(000) = 1068; μ(CuKα) = 131.1 cm^{-1}.

Data Collection

The crystal used for the diffraction data collection was dark green in colour and had approximate dimensions 0.34 × 0.33 × 0.28 mm. It was mounted by means of Araldite adhesive in a sealed Lindemann glass tube. Three-dimensional intensities were recorded with CuKα radiation (graphite crystal monochromator, $\bar{\lambda}$ = 1.5418 Å) on a Rigaku-AFC four-circle diffractometer at 17 °C. The intensities were recorded by an ω–2θ scan with a 2θ scan rate of 2° min^{-1} and 10 s stationary background counts. The three reference reflections monitored every 50 reflections showed no significant variation in intensity over the data collection period. Of the 3422 unique reflections measured to a 2θ maximum of 130°, the 2390 with values for which $|F_o| > 4\sigma|F_o|$ were used for the structure refinement. The scattering factors for C, N, S, and Cl were from Cromer and Mann [17] for Co from Doyle and Turner [18] and for H were those of Stewart, Davidson and Simpson [19]. Anomalous dispersion corrections, $\Delta f'$ and $\Delta f''$ were made for the non-hydrogen atoms using the values of Cromer and Liberman [20].

Because of the difficulty in assigning indices to the crystal faces which were ill-defined, and because the crystal was approximately cubic in shape, no absorption corrections were made to the intensities which were corrected only for Lorentz and polarisation factors.

Structure Analysis

The structure was solved by the heavy atom method. The coordinates of the Co atom were derived from the vector map and the non-hydrogen atom sites of the complex molecule were located on the Fourier distribution phased on the Co atom contribution to the structure factors. Refinement with individual isotropic temperature factors given to the atoms yielded an R index of 0.20 for $R = \Sigma\|F_o| - |F_c\|/\Sigma|F_o|$. From the subsequent difference map, the sites of the C and Cl atoms of the dichloromethane molecule were located. At this stage of the analysis it was apparent that the methylene group of the dichloromethane molecule was subject to two-fold disorder while the chlorine atoms were ordered. Consequently, the chlorine atom was included in the analysis with an occupancy factor of 1.0 while the bonded carbon atom was assigned an occupancy factor of 0.5. Full-matrix least-squares refinement with anisotropic temperature factors given to the non-hydrogen atoms converged at R = 0.070 and $R_w = (\Sigma w\|F_o| - |F_c\|^2/\Sigma w|F_o|^2)^{1/2}$ = 0.076. In the final refinement cycles, the H atoms of the complex molecule were included at idealised positions and were given a common isotropic temperature factor which refined to B = 3.95 Å^2. The H atoms of the dichloromethane were not included in the analysis.

In the least squares refinement, the function minimised was $\Sigma w(|F_o| - |F_c|)^2$ with terms weighted according to $w = (\sigma^2(F_o) + 0.0004(F_o)^2)^{-1}$. For the final refinement, three low-angle terms with high intensity, 0 4 1, 0 0 2, $\bar{1}$ 0 2, whose $|F_o|$ values when compared with their $|F_c|$ values indicated that they were affected by extinction, were omitted. The mean

TABLE I. Final Atomic Co-ordinates of the Non-hydrogen Atoms ($\times 10^4$) with Their Estimated Standard Deviations in Parentheses, and Equivalent Isotropic Temperature Factors ($Å^2$).

Atom	x	y	z	B_{eq}[a]
Co	620(1)	2007(1)	2211(1)	1.63
S(1)	−1312(2)	2348(1)	725(2)	1.13
S(2)	1876(2)	2697(1)	1430(2)	1.01
S(3)	722(2)	935(1)	1178(2)	0.96
S(11)	−771(2)	1584(1)	3089(2)	1.02
S(22)	931(2)	3061(1)	3386(2)	0.98
S(33)	2296(2)	1390(1)	3684(2)	0.95
C(1)	−1895(8)	1960(5)	1772(9)	0.82
N(1)	−3167(7)	1935(4)	1598(8)	0.89
C(11)	−4165(9)	2148(5)	464(11)	1.66
C(12)	−5280(10)	2069(6)	700(13)	2.59
C(13)	−4956(10)	1791(6)	2022(12)	2.38
C(14)	−3669(10)	1720(6)	2541(11)	1.80
C(2)	1887(9)	3307(5)	2594(9)	0.67
N(2)	2633(7)	3935(4)	2885(7)	0.55
C(21)	3590(10)	4105(6)	2407(10)	1.78
C(22)	4123(12)	4751(6)	2954(12)	3.02
C(23)	3465(12)	4999(6)	3770(12)	2.41
C(24)	2573(10)	4477(5)	3738(11)	1.88
C(3)	1936(8)	720(5)	2572(8)	0.51
N(3)	2528(7)	29(4)	2763(8)	1.07
C(31)	2255(11)	−555(5)	1899(12)	1.52
C(32)	2988(11)	−1133(6)	2502(12)	1.87
C(33)	3762(11)	−904(6)	3790(12)	2.16
C(34)	3444(10)	−197(5)	3937(11)	1.65
C(35)[b]	765(21)	4880(12)	372(22)	1.78
Cl	−471(4)	4558(2)	853(4)	4.70

[a] Calculated from the refined anisotropic thermal parameters, $B_{eq} = 8\pi^2 U_{eq}$. [b] Atom included with an occupancy factor of 0.5.

TABLE II. Interatomic Distances (Å) with Their Estimated Standard Deviations in Parentheses.

Co–S(1)	2.278(3)	N(1)–C(11)	1.394(12)
Co–S(2)	2.273(3)	N(1)–C(14)	1.402(12)
Co–S(3)	2.268(3)	N(2)–C(21)	1.393(12)
Co–S(11)	2.249(3)	N(2)–C(24)	1.373(12)
Co–S(22)	2.255(3)	N(3)–C(31)	1.377(12)
Co–S(33)	2.280(3)	N(3)–C(34)	1.388(12)
S(1)–C(1)	1.671(9)	C(11)–C(12)	1.378(14)
S(2)–C(2)	1.684(9)	C(13)–C(14)	1.356(14)
S(3)–C(3)	1.685(9)	C(21)–C(22)	1.349(15)
S(11)–C(1)	1.680(9)	C(23)–C(24)	1.368(14)
S(22)–C(2)	1.670(9)	C(31)–C(32)	1.346(14)
S(33)–C(3)	1.661(9)	C(33)–C(34)	1.352(14)
C(1)–N(1)	1.374(11)	C(12)–C(13)	1.452(16)
C(2)–N(2)	1.378(11)	C(22)–C(23)	1.426(16)
C(3)–N(3)	1.394(11)	C(32)–C(33)	1.426(16)
		C(35)–Cl	1.76(3)

parameter shift-to-error ratio at convergence was 0.004:1. The largest peak on the final difference map was of height 1.1 e $Å^{-3}$ close to the Co atom. The major calculations were carried out using the SHELX 76 program [21]. The final atomic coordinates for the non-hydrogen atoms together with their estimated standard deviations are given in Table I. Bond lengths and angles are shown in Tables II and III respectively. A perspective drawing of the complex molecule including the numbering system is shown in Fig. 1, while Fig. 2 illustrates the crystal packing. Both diagrams were prepared from the output of ORTEP [22]. Anisotropic thermal parameters, calculated H-coordinates, and listings of

TABLE III. Bond Angles (°) with Their Estimated Standard Deviations in Parentheses.

Angles (°) within CoS_6 Core			
S(1)–Co–S(11)	76.5(1)	S(1)–Co–S(33)	165.5(1)
S(2)–Co–S(22)	76.4(1)	S(2)–Co–S(11)	166.6(1)
S(3)–Co–S(33)	76.0(1)	S(3)–Co–S(22)	169.0(1)
S(1)–Co–S(2)	98.3(1)	S(11)–Co–S(22)	91.7(1)
S(2)–Co–S(3)	97.4(1)	S(22)–Co–S(33)	95.2(1)
S(3)–Co–S(1)	94.7(1)	S(33)–Co–S(11)	93.2(1)
S(1)–Co–S(22)	95.2(1)		
S(2)–Co–S(33)	93.9(1)		
S(3)–Co–S(11)	95.4(1)		
Angle (°) between Co–S–C			
Co–S(1)–C(1)	84.5(3)	Co–S(22)–C(2)	85.3(3)
Co–S(11)–C(1)	85.3(3)	Co–S(3)–C(3)	85.1(3)
Co–S(2)–C(2)	84.6(3)	Co–S(33)–C(3)	85.2(3)

(continued overleaf)

TABLE III. *(continued)*

Angles (°) in Ligand 1

S(1)–C(1)–S(11)	113.6(5)	C(11)–N(1)–C(14)	109.0(8)
S(1)–C(1)–N(1)	124.6(7)	N(1)–C(11)–C(12)	107.3(10)
S(11)–C(1)–N(1)	121.8(7)	N(1)–C(14)–C(13)	108.6(10)
C(1)–N(1)–C(11)	125.1(9)	C(11)–C(12)–C(13)	108.0(10)
C(1)–N(1)–C(14)	125.8(8)	C(14)–C(13)–C(12)	107.2(10)

Angles (°) in Ligand 2

S(2)–C(2)–S(22)	113.1(5)	C(21)–N(2)–C(24)	109.6(8)
S(2)–C(2)–N(2)	123.4(7)	N(2)–C(21)–C(22)	107.6(10)
S(22)–C(2)–N(2)	123.5(7)	N(2)–C(24)–C(23)	106.9(10)
C(2)–N(2)–C(21)	125.7(8)	C(21)–C(22)–C(23)	107.6(11)
C(2)–N(2)–C(24)	124.6(8)	C(24)–C(23)–C(22)	108.1(10)

Angles (°) in Ligand 3

S(3)–C(3)–S(33)	113.6(5)	C(31)–N(3)–C(34)	108.6(8)
S(3)–C(3)–N(3)	121.9(7)	N(3)–C(31)–C(32)	108.2(10)
S(33)–C(3)–N(3)	124.5(7)	N(3)–C(34)–C(33)	107.9(10)
C(3)–N(3)–C(31)	127.4(9)	C(31)–C(32)–C(33)	107.9(10)
C(3)–N(3)–C(34)	123.8(8)	C(34)–C(33)–C(32)	107.4(10)

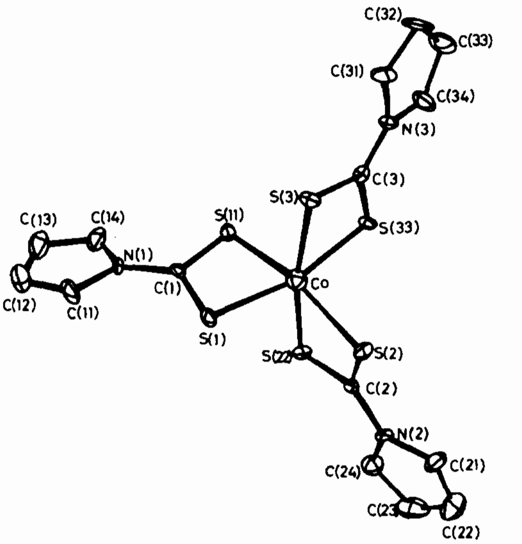


Fig. 1. A perspective view of the complex molecule with thermal ellipsoids scaled to 50% probability.

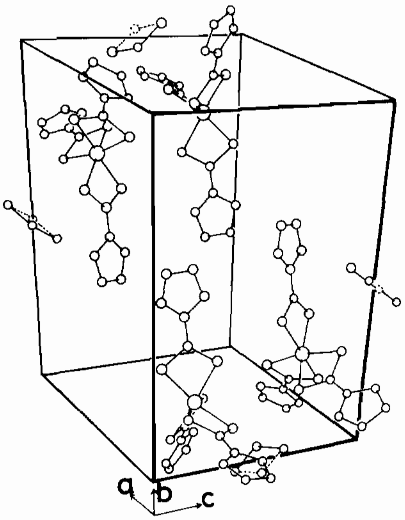


Fig. 2. Crystal packing.

observed and calculated structure amplitudes have been deposited as supplementary data.

Results and Discussion

The dark green diamagnetic tris(pyrrole-N-carbodithioato)cobalt(III) [abbreviated to Co(pcd)$_3$] was isolated in crystalline form as the dichloromethane and heptane solvates. Preliminary attempts to solve the structure of the heptane containing species were not successful because it was not possible to find the exact location of the heptane molecule, although unresolved maxima in electron-density maps indicated its approximate site. However, successful

TABLE IV. Structural Parameters for the CoS_6 Core in Selected Tris(dithiocarbamato)cobalt(III) Complexes.

Compound	$\bar{r}$ (Å)	$\bar{d}$ (Å)	$\bar{s}$ (Å)	$\bar{h}$ (Å)	b	$\bar{\alpha}(\alpha_1, \alpha_2, \alpha_3)$	$\bar{\phi}(\phi_1, \phi_2, \phi_3)$	$\bar{\psi}(\psi_1, \psi_2, \psi_3)$
$Co(H_2dtc)_3$	2.276	2.817	3.36	2.39	1.24	76.5(76.3, 76.7, 76.4)	45.2(45.8, 44.1, 45.6)	31.9(32.5, 30.8, 32.3)
$Co(Me_2dtc)_3$	2.264	2.799	3.33	2.39	1.24	76.4(76.5, 76.4, 76.2)	44.7(44.7, 43.7, 45.8)	31.5(31.4, 30.6, 32.6)
$Co(Et_2dtc)_3$	2.258	2.786	3.32	2.39	1.23	76.2(75.9, 76.8, 75.9)	43.7(43.6, 43.9, 43.6)	30.7(30.8, 30.6, 30.8)
$Co(pcd)_3 \cdot 0.5CH_2Cl_2$	2.267	2.801	3.34	2.38	1.24	76.3(76.5, 76.4, 76.0)	45.1(42.4, 47.2, 45.5)	32.0(29.7, 33.8, 32.5)

structure solution was achieved for the dichloromethane solvate and the results of the structure analysis are given here.

The structural solution represents with the tris(morpholinedithiocarbamato)cobalt(III) benzene solvated compound [5], a rare case of a successful solution of a solvated tris(N,N'-disubstituted-dithiocarbamato)cobalt(III) species. The present structure may also be compared with the isostructural $Fe(pcd)_3 \cdot 0.5CH_2Cl_2$ whose crystal and molecular structure have been recently reported [6].

The cobalt atom is surrounded by a distorted octahedral arrangement of six sulfur atoms, the distortion being toward trigonal prismatic geometry. Structural parameters for compounds of real or approximate D_3 symmetry have been used to characterise $Co-S_6$ polyhedra [23, 24]. These include the average C–S bond length ($\bar{r}$), the average intraligand S---S distance ($\bar{d}$), and the average chelate bite angle ($\bar{\alpha}$). In cases where an exact C_3 symmetry axis is not present a C_3 reference axis (C_3-ref) is defined by the following: The plane containing the midpoints of the lines joining the ligating S atoms is calculated and the normal to this plane containing the cobalt atom is taken as C_3-ref. The parameters $\bar{\phi}$ which is the average projection of $\bar{\alpha}$ onto a plane normal to C_3-ref, and $\bar{\psi}$, the average angle of pitch between the chelate ring and C_3-ref, are then calculated. The parameter h is the height of the polyhedron and $\bar{s}$ is the average distance between sulfur atoms of adjacent ligands [25]. The results of calculations for the structurally characterised tris(N,N'-disubstituted dithiocarbamato)cobalt(III) complexes, $Co(R_2dtc)_3$, R = H [26], R = Me [2], R = Et [1] and the present compound, $Co(pcd)_3$ are shown in Table IV. There is clearly a marked similarity of the coordination geometry of all of these cobalt(III) complexes. For tris-bidentate complexes of regular octahedral geometry, $\alpha = 90°$, $\phi = 60°$, $\psi = 35.3$ and the chelate rings are orthogonal. All the compounds in Table IV are distorted toward the trigonal prismatic limit $\phi = \psi = 0$. Significant distortion from orthogonality of the chelate rings occurs. The parameter b (=d/r), the 'normalised bite' has been used by Kepert [27, 28] to characterise a series of distorted trigonal prismatic structures where *b* is in the range 1.05–1.25. The present compound has a value within this range.

In the coordinated ligand of $Co(pcd)_3 \cdot 0.5CH_2Cl_2$ the mean C–S bond length of 1.675(9) Å is significantly shorter than that found in the other tris(dithiocarbamato)cobalt(III) complexes [1, 2, 26, 29] and indicates that *1a* makes a major contribution to the overall structure. In addition, the average (sulfur bonded) C–N bond length, 1.388(1) Å, is significantly longer than observed in the related tris(dithiocarbamato)cobalt(III) complexes above (1.319–1.321 Å). Such a lengthening of this bond is also in

TABLE V. Equations of Least-squares Planes and Distances (Å) of Atoms from these Planes.[a]

Plane 1	$0.1118X - 0.8697Y - 0.4808Z + 4.2532 = 0$
Plane 2	$-0.5916X + 0.4257Y - 0.6847Z - 0.1269 = 0$
Plane 3	$0.8242X + 0.4180Y - 0.3820Z - 0.5110 = 0$

Plane 1		Plane 2		Plane 3	
Co	−0.008(2)	Co	−0.023(1)	Co	−0.012(1)
S(11)	0.011(2)	S(22)	0.034(2)	S(33)	0.017(2)
C(1)	−0.015(9)	C(2)	−0.045(10)	C(3)	−0.023(9)
S(1)	0.011(2)	S(2)	0.034(2)	S(3)	0.017(2)

[a] *X, Y,* and *Z* are expressed in Å referred to orthogonal axes parallel to *a, b* and *c**. All atoms listed were included in calculation of the planes.

TABLE VI. Intermolecular Approach Distances (Å) less than 3.75 Å. Transformations of the coordinates (*x, y, z*) are denoted by superscripts: I(*x*, ½ − *y*, ½ + *z*); II (−*x*, −½ + *y*, ½ − *z*); III (*x*, ½ − *y*, −½ + *z*); IV (−1 + *x*, *y*, *z*); V (−*x*, ½ + *y*, ½ − *z*).

Cl······N(2)	3.58	S(3)····S(22)$^{\mathrm{III}}$	3.64
Cl······C(2)	3.48	S(2)····S(33)$^{\mathrm{III}}$	3.62
Cl······C(24)	3.73	S(11)···S(1)$^{\mathrm{III}}$	3.71
C(35)···C(21)	3.45	Cl······S(11)$^{\mathrm{III}}$	3.58
C(35)···N(2)	3.28	C(12)···S(2)$^{\mathrm{IV}}$	3.75
C(33)···C(35)$^{\mathrm{I}}$	3.74	C(23)···C(14)$^{\mathrm{V}}$	3.47
S(11)···C(35)$^{\mathrm{I}}$	3.62	Cl······C(3)$^{\mathrm{V}}$	3.49
S(22)···S(2)$^{\mathrm{I}}$	3.41	Cl······C(34)$^{\mathrm{V}}$	3.46
S(11)···C(35)$^{\mathrm{II}}$	3.51	Cl······C(31)$^{\mathrm{V}}$	3.71
N(3)····Cl$^{\mathrm{II}}$	3.31		

accord with structure *1a*. It is of interest to note that the infrared spectrum of the compound in the solid state exhibits a very strong absorption at 1330 cm^{-1}, a value in the region assigned to a C–N (single bond) stretching mode. Similar compounds having structures wherein *1b* predominates normally show an absorption [30] in the range 1450–1600 cm^{-1}. The results shown in Table V indicate that, as expected, the cobalt–ligand donor atom systems are close to planarity. The average bond lengths in the pyrrole moiety are as expected and are similar to those found in the corresponding iron(III) complex [6].

The molecules of the metal complex are well separated from each other within the unit cell (Fig. 2 and Table VI). In particular no unusually short contacts are observed between the complex molecule and the dichloromethane. The reason for the three short sulfur–sulfur intermolecular distances, significantly shorter than the sum of the van der Waal radius for sulfur (3.7 Å) in S(2)———S(3), 3.41 Å, S(3)———S(22), 3.64 Å and S(2)———S(33), 3.62 Å is not apparent. The dichloromethane molecule is not coordinated and occupies a site of C_i symmetry (0 0 ½). The carbon atom is subject to two-fold disorder.

In solution of non-coordinating solvents the compound retains its diamagnetic character as shown by the observation of resonance signals in its C-13 spectrum at δ = 116.1 and 117.7 ppm (pyrrole ring carbon atoms) and 213.8 ppm ($-CS_2$) in $CDCl_3$ relative to tetramethylsilane. The solution ($CHCl_3$) visible absorption spectrum of the compound has maxima at 627 nm (ϵ = 500) and 500 nm (shoulder, ϵ = 2030). Such values are typical of other tris(N,N'-disubstituted dithiocarbamato)cobalt(III) complexes having effective D_3 symmetry [16, 31].

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