Table 2. *Selected geometric parameters (Å, °)*

Ni—O1	1.839 (7)	N1—C6	1.434 (13)
Ni—O2	1.812 (7)	N1—C8	1.314 (13)
Ni—N1	1.852 (8)	C1—C6	1.389 (13)
Ni—N2	1.951 (9)	C8—C9	1.409 (14)
O1—C1	1.342 (15)	C9—C14	1.42 (2)
O2—C14	1.319 (14)		
O1—Ni—O2	176.5 (3)	Ni—N1—C6	111.4 (6)
O1—Ni—N1	87.2 (3)	Ni—N1—C8	125.2 (7)
O1—Ni—N2	89.9 (3)	C6—N1—C8	123.2 (8)
O2—Ni—N1	96.2 (4)	O1—C1—C6	117.7 (8)
O2—Ni—N2	86.7 (4)	N1—C6—C1	111.5 (8)
N1—Ni—N2	176.2 (4)	N1—C8—C9	125.3 (9)
Ni—O1—C1	112.1 (6)	C8—C9—C14	122.3 (9)
Ni—O2—C14	127.3 (7)	O2—C14—C9	123.5 (9)

All H atoms were taken from difference maps and given U_{iso} values 1.3 times the U_{eq} values of their parent atoms and a riding model was adopted.

Data collection: *CAD-4 Express* (Enraf–Nonius, 1993). Data reduction: *MolEN* (Fair, 1990). Program(s) used to solve structure: *SIMPEL* in *MolEN*. Program(s) used to refine structure: *LSFM* in *MolEN*. Molecular graphics: *ORTEP*II (Johnson, 1976) in *MolEN*. Software used to prepare material for publication: *MolEN*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: CF1069). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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***trans*-(5,7,7,12,14,14-Hexamethyl-1,4,8,11-tetraazacyclotetradeca-4,11-diene-*N*,*N'*,*N''*,*N'''*)di(isothiocyanato-*N*)cobalt(III) Thiocyanate**

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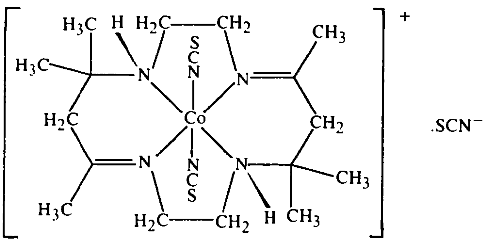
Abstract

The Co^{III} ion in the title compound, $[Co(NCS)_2(C_{16}H_{32}N_4)](SCN)$, is six-coordinate in a distorted octahedral environment, with the four N atoms of the macrocyclic tetradentate ligand equatorial and the N atoms of two isothiocyanato groups axial. The tetradentate macrocyclic ligand is in a planar conformation, with the two five-membered rings in *gauche* conformations and the two six-membered rings in twist conformations. The complex has an *RR* or *SS* configuration for the two chiral amine N centres. Intermolecular hydrogen bonds between the two NH groups and the unbonded thiocyanate anion help stabilize the crystal structure.

Comment

The crystal structures of the copper(II) and nickel(II) complexes of the macrocyclic ligand 5,7,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradeca-4,11-diene have been reported (Curtis, 1964). We report here the crystal structure of the cobalt(III) complex, (I), of this ligand.



(I)

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The Co^{III} ion is six-coordinate in a distorted octahedral environment, with the four N atoms of the macrocyclic tetradentate ligand equatorial and the N atoms of two isothiocyanato groups axial (Fig. 1). The tetradentate ligand is in a planar conformation, with the two five-membered rings in *gauche* conformations and the two six-membered rings in twist conformations. The complex cation is chiral and spontaneous resolution occurs on crystallization. However, no attempt was made to determine the absolute configuration of the crystal used in the structure analysis. The two chiral amine centres have the same optical configuration, either both *R* or both *S*. One of the two isothiocyanato groups coordinated to the Co^{III} ion is almost linear, the other being bent. Intermolecular hydrogen bonds between the two NH groups and the unbonded thiocyanate ion help stabilize the crystal structure (Fig. 2).

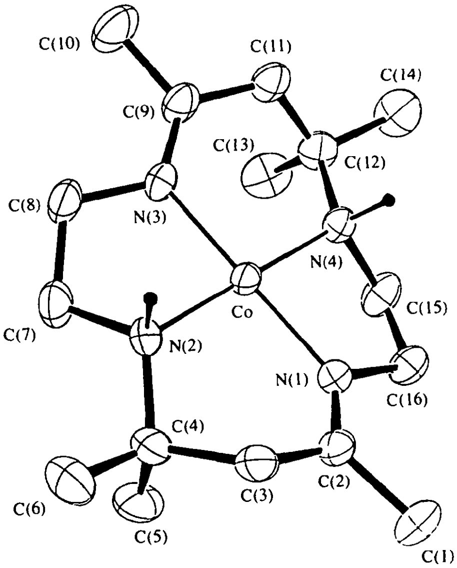

Fig. 1. *ORTEPII* (Johnson, 1976) plot of the title cobalt complex, excluding H atoms except those attached to N(2) and N(4). Displacement ellipsoids are plotted at the 30% probability level.

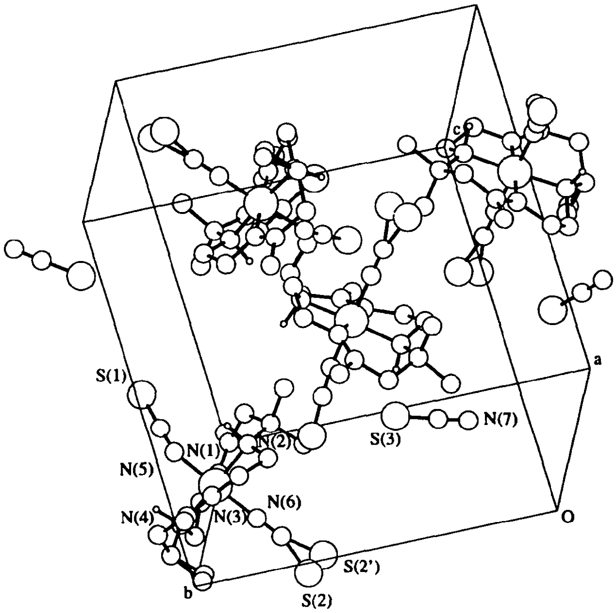

Fig. 2. Packing diagram (*PLUTO*; Motherwell & Clegg, 1976) of the title compound, excluding H atoms except those attached to N(2) and N(4). For clarity, only S and N atoms are labelled. One isothiocyanato group is almost linear, the other is bent. The S atom in the bent isothiocyanato group has split occupancy.

The Co—N distances shown in Table 2 can be classified into three types. These are between metal and isothiocyanato N atoms, metal and amine N atoms or metal and imine N atoms. The three types of bond distance are generally in agreement with the results of previous investigations (Restivo, Horney & Ferguson, 1975; Lu, Chen & Chung, 1992, 1993; Tahirov, Lu, Chen, Lai & Chung, 1993; Lu, Lai & Chung, 1994; Tahirov, Lu, Chen, Chi & Chung, 1994).

Experimental

The ligand as 5,7,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradeca-4,11-diene dihydroperchlorate ($L.2HClO_4$) and *trans*-dichloro(5,7,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradeca-4,11-diene)cobalt(III) chloride were prepared according to the methods described by Hay & Lawrance (1975) and Sadasivan, Kernohan & Endicott (1967). The dichloro complex (1 g) was dissolved in hydrochloric acid solution (10^{-3} *M*, 50 ml). NaSCN (1 g) was added to the resulting solution, which was then stirred for 1 h. Crystals of the title complex were obtained by rotatory evaporation and were recrystallized from aqueous methanol (1/1 *v*/*v*).

Crystal data

$[Co(NCS)_2(C_{16}H_{32}N_4)]$-
(SCN)
$M_r = 513.62$
Orthorhombic
$P2_12_12_1$
$a = 12.169\ (2)$ Å
$b = 13.576\ (1)$ Å
$c = 14.919\ (1)$ Å
$V = 2464.7\ (5)$ Å^3
$Z = 4$
$D_x = 1.384$ Mg m^{-3}

Mo *Kα* radiation
$\lambda = 0.71073$ Å
Cell parameters from 25
reflections
$\theta = 6.41–15.56°$
$\mu = 0.96$ mm^{-1}
$T = 298\ (3)$ K
Parallelepiped
0.44 × 0.31 × 0.25 mm
Deep-red–brown

Data collection

Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction:
ψ scan (North, Phillips & Mathews, 1968)
$T_{min} = 0.75$, $T_{max} = 0.79$
3984 measured reflections
3984 independent reflections

2804 observed reflections
$[I > 1.5\sigma(I)]$
$\theta_{max} = 29.9°$
$h = 0 \rightarrow 17$
$k = 0 \rightarrow 19$
$l = 0 \rightarrow 20$
3 standard reflections
frequency: 60 min
intensity variation: ±1%

Refinement

Refinement on F
$R = 0.051$
$wR = 0.055$
$S = 1.52$
2804 reflections
280 parameters
H-atom parameters not refined
$w = 1/[\sigma(F_o)^2 + 0.0004|F_o|^2]$
$(\Delta/\sigma)_{\max} = 0.020$
$\Delta\rho_{\max} = 0.38$ (7) e Å^{-3}
$\Delta\rho_{\min} = -0.31$ (7) e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$$B_{\rm eq} = (8\pi^2/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$
Co	0.53886 (5)	0.97209 (5)	0.06159 (4)	3.20 (2)
S(1)	0.72757 (12)	1.12890 (12)	0.27029 (13)	6.31 (8)
S(2)†	0.4882 (3)	0.7898 (4)	−0.1970 (3)	10.0 (3)
S(2′)†	0.5276 (3)	0.7446 (3)	−0.1717 (2)	6.03 (14)
S(3)	0.52658 (16)	0.44578 (13)	0.14764 (11)	6.64 (8)
N(1)	0.6932 (3)	0.9854 (3)	0.0358 (3)	3.81 (16)
N(2)	0.5541 (3)	0.8586 (3)	0.1436 (3)	3.94 (16)
N(3)	0.3847 (3)	0.9596 (3)	0.0902 (3)	4.22 (18)
N(4)	0.5241 (3)	1.0889 (3)	−0.0151 (2)	3.91 (17)
N(5)	0.5614 (3)	1.0580 (3)	0.1615 (2)	3.44 (16)
N(6)	0.5210 (4)	0.8871 (3)	−0.0382 (3)	4.9 (2)
N(7)	0.6059 (4)	0.2762 (4)	0.0690 (4)	6.9 (3)
C(1)	0.8903 (4)	0.9763 (6)	0.0682 (5)	7.7 (4)
C(2)	0.7725 (4)	0.9491 (4)	0.0821 (4)	4.8 (2)
C(3)	0.7520 (4)	0.8808 (4)	0.1584 (4)	5.0 (2)
C(4)	0.6605 (4)	0.8031 (4)	0.1495 (4)	5.1 (3)
C(5)	0.6812 (6)	0.7388 (5)	0.0693 (5)	7.3 (4)
C(6)	0.6609 (5)	0.7402 (5)	0.2334 (5)	7.3 (4)
C(7)	0.4550 (5)	0.7978 (4)	0.1318 (4)	5.9 (3)
C(8)	0.3566 (4)	0.8670 (5)	0.1371 (4)	5.5 (3)
C(9)	0.3115 (4)	1.0258 (4)	0.0782 (3)	4.5 (2)
C(10)	0.1944 (4)	1.0143 (6)	0.1078 (5)	7.0 (4)
C(11)	0.3382 (4)	1.1221 (4)	0.0358 (3)	4.7 (2)
C(12)	0.4109 (4)	1.1181 (4)	−0.0485 (3)	5.0 (3)
C(13)	0.3646 (5)	1.0490 (6)	−0.1178 (4)	7.0 (4)
C(14)	0.4144 (6)	1.2239 (6)	−0.0844 (4)	7.3 (3)
C(15)	0.6116 (5)	1.0812 (4)	−0.0839 (3)	5.0 (2)
C(16)	0.7156 (4)	1.0598 (4)	−0.0348 (4)	4.9 (2)
C(17)	0.6300 (4)	1.0886 (3)	0.2075 (3)	3.72 (19)
C(18)	0.5164 (5)	0.8357 (5)	−0.0976 (4)	6.3 (3)
C(19)	0.5722 (4)	0.3469 (4)	0.1015 (4)	4.9 (2)

† Site occupancy = 0.5.

Table 2. *Selected geometric parameters (Å, °)*

Co—N(1)	1.926 (3)	N(4)—C(15)	1.482 (6)
Co—N(2)	1.976 (4)	N(5)—C(17)	1.157 (6)
Co—N(3)	1.932 (4)	N(6)—C(18)	1.130 (7)
Co—N(4)	1.964 (4)	N(7)—C(19)	1.151 (8)
Co—N(5)	1.913 (4)	C(1)—C(2)	1.494 (7)
Co—N(6)	1.896 (4)	C(2)—C(3)	1.490 (8)
S(1)—C(17)	1.609 (5)	C(3)—C(4)	1.539 (8)
S(2)—C(18)	1.644 (7)	C(4)—C(5)	1.502 (9)
S(2′)—C(18)	1.664 (6)	C(4)—C(6)	1.516 (9)
S(3)—C(19)	1.607 (6)	C(7)—C(8)	1.524 (9)
N(1)—C(2)	1.285 (6)	C(9)—C(10)	1.500 (7)
N(1)—C(16)	1.485 (6)	C(9)—C(11)	1.489 (8)
N(2)—C(4)	1.501 (6)	C(11)—C(12)	1.540 (7)
N(2)—C(7)	1.472 (7)	C(12)—C(13)	1.505 (8)
N(3)—C(8)	1.479 (7)	C(12)—C(14)	1.533 (9)
N(3)—C(9)	1.277 (7)	C(15)—C(16)	1.490 (8)
N(4)—C(12)	1.518 (6)		
N(1)—Co—N(2)	96.0 (2)	N(1)—C(2)—C(1)	123.4 (5)
N(1)—Co—N(3)	178.7 (2)	N(1)—C(2)—C(3)	121.5 (4)
N(1)—Co—N(4)	84.1 (2)	C(1)—C(2)—C(3)	114.9 (5)
N(1)—Co—N(5)	87.6 (2)	C(2)—C(3)—C(4)	118.8 (5)
N(1)—Co—N(6)	90.7 (2)	N(2)—C(4)—C(3)	106.5 (4)
N(2)—Co—N(3)	83.5 (2)	N(2)—C(4)—C(5)	112.9 (5)
N(2)—Co—N(4)	177.4 (2)	N(2)—C(4)—C(6)	109.5 (4)
N(2)—Co—N(5)	88.8 (2)	C(3)—C(4)—C(5)	110.2 (5)
N(2)—Co—N(6)	91.3 (2)	C(3)—C(4)—C(6)	108.2 (5)
N(3)—Co—N(4)	96.3 (2)	C(5)—C(4)—C(6)	109.3 (5)
N(3)—Co—N(5)	91.2 (2)	N(2)—C(7)—C(8)	107.0 (4)
N(3)—Co—N(6)	90.5 (2)	N(3)—C(8)—C(7)	108.5 (4)
N(4)—Co—N(5)	88.6 (2)	N(3)—C(9)—C(10)	123.3 (5)
N(4)—Co—N(6)	91.4 (2)	N(3)—C(9)—C(11)	121.7 (4)
N(5)—Co—N(6)	178.3 (2)	C(10)—C(9)—C(11)	115.1 (5)
Co—N(1)—C(2)	126.1 (3)	C(9)—C(11)—C(12)	116.2 (5)
Co—N(1)—C(16)	112.6 (3)	N(4)—C(12)—C(11)	105.2 (4)
C(2)—N(1)—C(16)	120.3 (4)	N(4)—C(12)—C(13)	113.8 (5)
Co—N(2)—C(4)	120.6 (3)	N(4)—C(12)—C(14)	109.6 (5)
Co—N(2)—C(7)	106.6 (3)	C(11)—C(12)—C(13)	111.6 (5)
C(4)—N(2)—C(7)	115.6 (4)	C(11)—C(12)—C(14)	105.5 (5)
Co—N(3)—C(8)	113.8 (3)	C(13)—C(12)—C(14)	110.7 (5)
Co—N(3)—C(9)	125.8 (4)	N(4)—C(15)—C(16)	106.5 (4)
C(8)—N(3)—C(9)	120.2 (4)	N(1)—C(16)—C(15)	109.0 (4)
Co—N(4)—C(12)	119.0 (3)	S(1)—C(17)—N(5)	178.4 (4)
Co—N(4)—C(15)	106.3 (3)	S(2)—C(18)—N(6)	162.2 (7)
C(12)—N(4)—C(15)	116.3 (4)	S(2′)—C(18)—N(6)	167.5 (7)
Co—N(5)—C(17)	141.7 (3)	S(3)—C(19)—N(7)	179.3 (5)
Co—N(6)—C(18)	176.3 (5)		

The title structure was solved by direct and Fourier methods and refined by full-matrix least-squares techniques. H atoms were located by difference Fourier methods and theoretical calculations.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *NRCVAX* (Gabe, Le Page, Charland, Lee & White, 1989). Program(s) used to solve structure: *NRCVAX*. Program(s) used to refine structure: *NRCVAX*. Molecular graphics: *ORTEP*II (Johnson, 1976) and *PLUTO* (Motherwell & Clegg, 1976). Software used to prepare material for publication: *NRCVAX*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: HR1025). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1996). C**52**, 2687-2689

Aqua(1,5,8,12-tetramethyl-1,4,8,11-tetraazacyclotetradecane-*N*,*N*′,*N*″,*N*‴)copper(II) Diperchlorate

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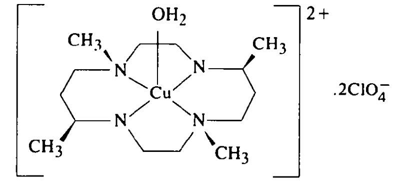
(*Received 14 February 1994; accepted 13 June 1996*)

Abstract

The Cu^{II} ion in the title compound, $[Cu(C_{14}H_{32}N_4)(H_2O)](ClO_4)_2$, is five-coordinate in a distorted square-pyramidal geometry, with the four N atoms of the macrocyclic ligand equatorial and the O atom of the aqua group axial. The tetradentate ligand adopts its most stable conformation with the two six-membered rings in chair conformations and the two five-membered rings in *gauche* conformations. The complex has a 1*SR*,4*SR*,8*SR*,11*SR* configuration for the four chiral N-atom centers and a 5*RS*,12*RS* configuration for the two chiral C-atom centers.

Comment

The macrocyclic ligand 1,5,8,12-tetramethyl-1,4,8,11-tetraazacyclotetradecane exists as two isomers, namely, *C-meso-* and *C-rac*-1,5,8,12-tetramethyl-1,4,8,11-tetraazacyclotetradecane (Miyamura *et al.*, 1987). The crystal structure of the nickel(II) complex of the *C-meso* isomer has been reported previously (Miyamura *et al.*, 1987). This paper reports the crystal structure of the copper(II) complex of *C-rac*-1,5,8,12-tetramethyl-1,4,8,11-tetraazacyclotetradecane, (I).



(I)

The Cu^{II} ion is five-coordinate in a distorted square-pyramidal geometry, with the four N atoms of the macrocyclic ligand equatorial and the O atom of the aqua group axial. The four N atoms are coplanar within ±0.18 Å. The Cu—N distances span a very narrow range [2.030 (3)–2.039 (3) Å] and are similar to the average Cu—N distance of 2.03 (3) Å found for Cu^{II} macrocyclic tetraamine complexes (Lu, Chung & Ashida, 1991). The Cu—O$_{water}$ distance is in good agreement with the usual Cu—O$_{axial}$ distances found in Cu^{II} macrocyclic complexes. The two *N*-methyl groups, the two amine H atoms and the coordinated water molecule are on the same side of the equatorial N_4 plane. The tetradentate ligand adopts its most stable conformation with the two six-membered rings in chair conformations and the two five-membered rings in *gauche* conformations. The two C-methyl groups occupy equatorial positions. The complex has a 1*SR*,4*SR*,8*SR*,11*SR* configuration for the four chiral N-atom centers and a 5*RS*,12*RS* configuration for the two chiral C-atom centers. Hydrogen bonds between perchlorate and the water molecule or NH group stabilize the crystal structure.

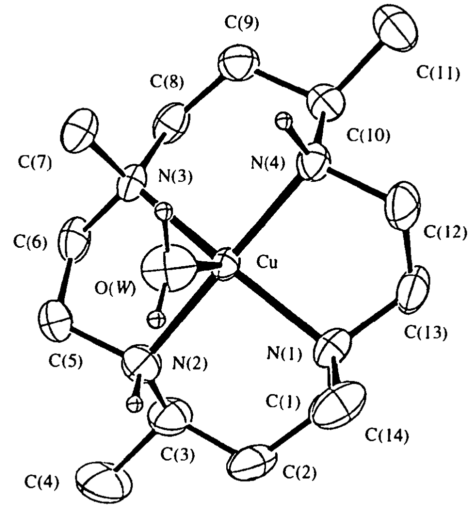


Fig. 1. A perspective view (*SHELXTL-Plus*; Sheldrick, 1986) of the complex cation with the atom-numbering scheme, excluding the perchlorate ions and H atoms attached to C atoms. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

C-rac-1,5,8,12-tetramethyl-1,4,8,11-tetraazacyclotetradecane dihydroperchlorate was prepared according to the method of Miyamura *et al.* (1987). Copper(II) perchlorate hexahydrate