F7	0.5093 (3)	0.9051 (8)	0.1036 (4)	0.254 (5)
F8	0.4933 (4)	0.9416 (6)	0.1790 (4)	0.234 (5)
F9	0.4674 (3)	0.8140 (5)	0.1468 (4)	0.202 (4)
F10	0.3835 (4)	1.1290 (6)	−0.0311 (3)	0.217 (4)
F11	0.2998 (7)	1.1791 (7)	−0.0226 (6)	0.326 (9)
F12	0.2931 (8)	1.0800 (9)	−0.0742 (3)	0.346 (10)
O1	0.1512 (2)	0.9843 (3)	0.2075 (2)	0.0640 (9)
O2	0.0929 (2)	0.8466 (2)	0.11647 (15)	0.0616 (8)
O3	0.3462 (2)	0.8999 (3)	0.1174 (2)	0.0729 (10)
O4	0.2663 (2)	1.0258 (3)	0.0308 (2)	0.0701 (10)
O5	0.2826 (2)	1.1107 (2)	0.1788 (2)	0.0682 (9)
O6	0.3098 (2)	0.9378 (3)	0.2314 (2)	0.0709 (10)
O7	0.2503 (2)	0.7748 (2)	0.1690 (2)	0.0659 (9)
O8	0.1934 (2)	0.7947 (2)	0.0427 (2)	0.0597 (8)
O9	0.1104 (2)	0.9557 (2)	0.00149 (14)	0.0540 (8)
O10	0.1223 (2)	1.1074 (2)	0.07574 (15)	0.0607 (8)
C1	0.1158 (4)	0.9741 (6)	0.2935 (3)	0.091 (2)
C2	0.1161 (2)	0.9376 (3)	0.2327 (2)	0.0565 (11)
C3	0.0788 (2)	0.8563 (3)	0.2133 (2)	0.0564 (11)
C4	0.0687 (2)	0.8197 (3)	0.1561 (2)	0.0482 (10)
C5	0.0194 (2)	0.7360 (4)	0.1397 (2)	0.0573 (11)
C6	0.4656 (3)	0.8989 (7)	0.1317 (4)	0.102 (2)
C7	0.3929 (2)	0.9350 (4)	0.1002 (2)	0.0615 (12)
C8	0.3873 (3)	1.0002 (4)	0.0555 (3)	0.0721 (15)
C9	0.3243 (3)	1.0379 (4)	0.0232 (2)	0.0615 (12)
C10	0.3251 (4)	1.1040 (7)	−0.0269 (4)	0.106 (3)
C11	0.2963 (4)	1.1863 (4)	0.1438 (3)	0.093 (2)
C12	0.3367 (3)	1.0983 (5)	0.2323 (3)	0.088 (2)
C13	0.3181 (3)	1.0196 (5)	0.2668 (3)	0.083 (2)
C14	0.3034 (4)	0.8538 (4)	0.2611 (3)	0.084 (2)
C15	0.3081 (4)	0.7743 (4)	0.2227 (3)	0.084 (2)
C16	0.2594 (3)	0.7078 (4)	0.1271 (3)	0.077 (2)
C17	0.1989 (3)	0.7078 (3)	0.0733 (3)	0.0699 (14)
C18	0.1348 (3)	0.7975 (4)	−0.0101 (3)	0.0729 (15)
C19	0.1288 (3)	0.8912 (4)	−0.0373 (2)	0.0668 (13)
C20	0.0980 (3)	1.0474 (4)	−0.0225 (2)	0.0658 (14)
C21	0.0714 (3)	1.1048 (4)	0.0194 (2)	0.0638 (13)
C22	0.1005 (4)	1.1628 (4)	0.1172 (3)	0.091 (2)

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

Ba1—O1	2.758 (3)	Ba1—O10	2.832 (3)
Ba1—O4	2.762 (4)	Ba1—O7	2.837 (3)
Ba1—O8	2.806 (3)	Ba1—O6	2.844 (4)
Ba1—O3	2.811 (3)	Ba1—O5	2.846 (3)
Ba1—O2	2.815 (3)	Ba1—O9	2.858 (3)
O4—Ba1—O3	61.16 (11)	O10—Ba1—O5	74.00 (11)
O1—Ba1—O2	62.41 (10)	O6—Ba1—O5	57.82 (11)
O8—Ba1—O7	60.68 (11)	O8—Ba1—O9	60.33 (9)
O7—Ba1—O6	59.71 (11)	O10—Ba1—O9	57.72 (9)

Data collection: *CAD-4/PC* (Enraf–Nonius, 1992). Cell refinement: *CAD-4/PC*. Data reduction: local program (*CAD-4*; Davis, 1975). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEX* (McArdle, 1994). Software used to prepare material for publication: *SHELXL*93.

The authors thank the SERC/EPSRC for support and Dr H. Chudzynska for translating one of the references.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: CF1089). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Bondi, A. (1964). *J. Phys. Chem.* **68**, 441–451.

Dahmen, K.-H. & Gerfin, T. (1993). *Prog. Cryst. Growth Charact.* **27**, 117–161.

Davis, J. (1975). *CAD-4. Program for Data Reduction*. University of London, England.

Enraf–Nonius (1992). *CAD-4/PC Software*. Version 1.5c. Enraf–Nonius, Delft, The Netherlands.

Gardiner, R., Brown, D. W., Kirlin, P. S. & Rheingold, A. L. (1991). *Chem. Mater.* **3**, 1053–1059.

Haymore, B. L., Lamb, J. D., Izatt, R. M. & Christensen, J. J. (1982). *Inorg. Chem.* **21**, 1598–1602.

Inerowicz, H. D., Khan, M. A., Atkinson, G. & White, R. L. (1994). *Acta Cryst.* C**50**, 688–690.

McArdle, P. (1994). *J. Appl. Cryst.* **27**, 438–439.

Motevalli, M., O'Brien, P. & Watson, I. M. (1996). *Polyhedron*, **15**, 1865–1875.

Neumayer, D. A., Studebaker, D. B., Hinds, B. J., Stern, C. S. & Marks, T. J. (1994). *Chem. Mater.* **6**, 878–880.

Norman, J. A. T. & Pez, G. P. (1991). *J. Chem. Soc. Chem. Commun.* pp. 971–972.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**42**, 351–359.

Polyanskaya, T. M., Gatilov, Yu. V., Martynova, T. N. & Nikulina, L. D. (1992). *Zh. Strukt. Khim.* **33**, 190.

Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.

Sheldrick, G. M. (1993). *SHELXL93. Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.

Sluis, P. van der, Spek, A. L., Timmer, K. & Meinema, H. A. (1990). *Acta Cryst.* C**46**, 1741–1743.

Tobaly, P. & Watson, I. M. (1995). *J. Chem. Thermodyn.* **27**, 1211–1219.

Watson, I. M., Atwood, M. P., Cumberbatch, T. J. & Cardwell, D. A. (1994). *J. Mater. Chem.* **4**, 1393–1401.

Acta Cryst. (1996). C**52**, 3030–3033

Tris(*N*,*N*-diethyldithiocarbamato-*S*,*S'*)-nickel(IV) 1,1,2,3,3-Pentacyanopropenide

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(*Received 12 December 1995; accepted 17 July 1996*)

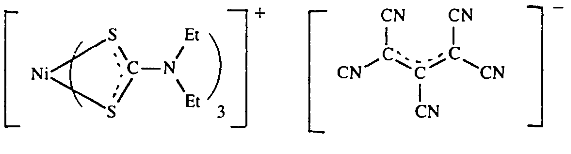
Abstract

The title compound, $[Ni(C_5H_{10}NS_2)_3](C_8N_5)$, forms a structure with sheets consisting of alternate rows of cations and anions. The Ni atom in the cation has distorted octahedral geometry. The planar $[C_3(CN)_5]^-$ anion is significantly distorted from C_{2v} symmetry. The Ni—S distances range from 2.246 (2) to 2.257 (2) Å and the C—C distances in the allyl group of the anion are 1.19 (2) and 1.35 (2) Å.

Acta Crystallographica Section C
ISSN 0108-2701 © 1996

Comment

Since the discovery of the first molecular magnet [Fe(C_5Me_5)$_2$](TCNE) (where C_5Me_5 is pentamethylcyclopentadienyl and TCNE is tetracyanoethylene) (Miller *et al.*, 1987), the reaction of TCNE with metal complexes has attracted a great deal of attention. Recently, another type of molecular magnet, [Mn(TPP)](TCNE) (where TPP is tetraphenylporphinato), which has a chain structure with Mn^{III} atoms bridged by μ_2-TCNE anion radicals, was reported by Miller, Calabrese, McLean & Epstein (1992). It is also known that [Ni(R_2dtc)$_2$] (where R_2dtc is *N*,*N*-dialkyldithiocarbamato) can be oxidized by X_2 (X = Br, I) to [$Ni^{III}X$(R_2dtc)$_2$] (William, Rouwette & Cras, 1972). As the electron capacity of TCNE is between that of Br_2 and I_2, we attempted to synthesize [Ni^{III}(Et_2dtc)$_2$](TCNE), a possible chain complex, by reaction of [Ni(Et_2dtc)$_2$] with TCNE, but obtained the title compound, (I), instead. The $[C_3(CN)_5]^-$ ion can also be prepared directly from TCNE itself (Giraudon, Sala-Pala, Guerchais & Toupet, 1991; Miller *et al.*, 1987).



(I)

The Ni atom has distorted octahedral geometry. The range of Ni—S distances in the cation [2.246 (2)–2.257 (2) Å] is consistent with the description of the metal atom as nickel(IV). Bond lengths and angles of the cation agree well with those found in $[Ni(^nBu_2dtc)_3]^+$ (Avdeef, Fackler & Fischer, 1970; Fackler, Avdeef & Fischer, 1973). The $[C_3(CN)_5]^-$ anion is planar [r.m.s. Δ = 0.031 (11) Å]. The most significant deviations from normal bond distances are C16—C17 [1.19 (2) Å] and C17—C21 [1.66 (2) Å]. A similar distortion was reported in [CuCl($C_{10}H_{10}N_2$)$_2$][$C_3(CN)_5$] (Jensen & Jacobson, 1981). The crystal structure consists of sheets containing alternate rows of cations and anions parallel to (101) (Fig. 2).

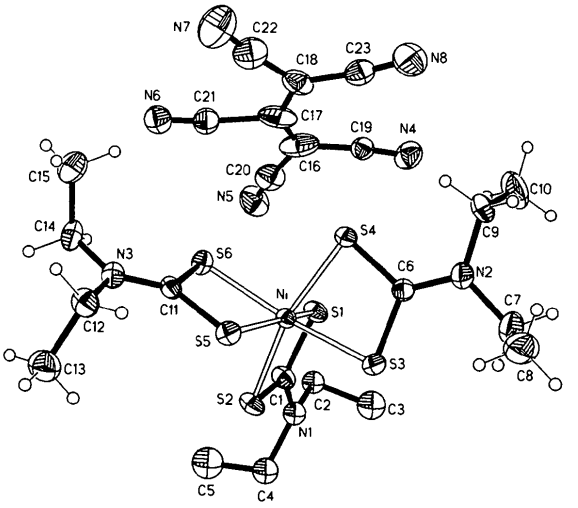


Fig. 1. The molecular structure of (I) showing 20% probability displacement ellipsoids.

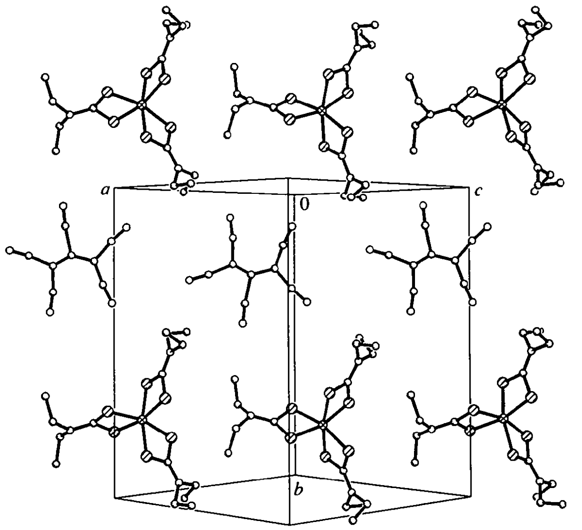


Fig. 2. The packing of cations and anions parallel to (101).

Experimental

TCNE (0.1 g) in toluene (20 ml) was added to an equimolar amount of [Ni(Et_2dtc)$_2$] dissolved in dichloromethane (15 ml). The product was recrystallized from benzene by slow evaporation.

Crystal data

[Ni($C_5H_{10}NS_2$)$_3$](C_8N_5)
M_r = 669.62
Monoclinic
Cc
a = 13.904 (2) Å
b = 17.525 (2) Å
c = 13.406 (2) Å
β = 95.964 (6)°
V = 3248.9 (8) Å^3
Z = 4
D_x = 1.369 Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 25 reflections
θ = 12–13°
μ = 1.010 mm^{-1}
T = 300 (2) K
Plate
0.43 × 0.36 × 0.07 mm
Black

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans

2464 observed reflections [$I > 2\sigma(I)$]
θ_{max} = 24.97°

Absorption correction:
ψ scan (North, Phillips & Mathews, 1968)
$T_{\min} = 0.78$, $T_{\max} = 0.93$
2862 measured reflections
2862 independent reflections

$h = 0 \rightarrow 16$
$k = 0 \rightarrow 20$
$l = -15 \rightarrow 15$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R(F) = 0.0443$
$wR(F^2) = 0.1063$
$S = 1.083$
2862 reflections
338 parameters
H atoms riding with $U(\mathrm{H}) = 1.3U_{\mathrm{eq}}(\mathrm{C})$
$w = 1/[\sigma^2(F_o^2) + (0.052P)^2 + 2.39P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.101$

$\Delta\rho_{\max} = 0.588$ e Å^{-3}
$\Delta\rho_{\min} = -0.267$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
Absolute configuration: Flack (1983)
Flack parameter = −0.02 (3)

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

$$U_{\mathrm{eq}} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Ni	0.97796 (7)	0.74074 (5)	1.14895 (7)	0.0469 (2)
S1	0.9972 (2)	0.7868 (1)	0.9952 (2)	0.0620 (5)
S2	1.1299 (1)	0.7075 (1)	1.1254 (2)	0.0666 (6)
S3	1.0253 (2)	0.8477 (1)	1.2333 (2)	0.0645 (6)
S4	0.8388 (1)	0.8054 (1)	1.1575 (2)	0.0550 (5)
S5	0.9765 (2)	0.6670 (1)	1.2868 (1)	0.0581 (5)
S6	0.9067 (2)	0.6321 (1)	1.0903 (1)	0.0593 (5)
N1†	1.1882 (13)	0.7724 (9)	0.9605 (12)	0.071 (4)
N1′†	1.1652 (10)	0.7452 (8)	0.9340 (10)	0.051 (3)
N2	0.8737 (5)	0.9424 (4)	1.2445 (6)	0.074 (2)
N3	0.9083 (5)	0.5267 (4)	1.2364 (5)	0.062 (2)
N4	0.7331 (9)	0.8998 (6)	0.8942 (9)	0.103 (3)
N5	0.8454 (10)	0.7013 (7)	0.7816 (9)	0.124 (4)
N6	0.6975 (7)	0.5630 (6)	0.9293 (7)	0.095 (3)
N7	0.5311 (13)	0.6307 (9)	1.1177 (12)	0.175 (6)
N8	0.5632 (9)	0.8718 (8)	1.0690 (9)	0.128 (4)
C1	1.1117 (6)	0.7509 (5)	1.0121 (7)	0.067 (2)
C2†	1.1581 (16)	0.8014 (14)	0.8536 (17)	0.071 (6)
C2′†	1.1327 (19)	0.7816 (14)	0.8310 (19)	0.086 (7)
C3†	1.190 (2)	0.8841 (17)	0.872 (2)	0.114 (9)
C3′†	1.1898 (18)	0.8634 (15)	0.8281 (19)	0.090 (7)
C4†	1.289 (2)	0.7379 (16)	0.987 (2)	0.088 (7)
C4′†	1.2628 (18)	0.7105 (15)	0.9531 (19)	0.084 (6)
C5†	1.293 (2)	0.660 (2)	0.945 (3)	0.137 (10)
C5′†	1.331 (2)	0.7642 (16)	1.017 (2)	0.108 (8)
C6	0.9070 (5)	0.8761 (4)	1.2164 (6)	0.054 (2)
C7	0.9407 (9)	1.0001 (6)	1.2979 (10)	0.105 (4)
C8	0.9465 (10)	0.9965 (8)	1.4066 (10)	0.127 (5)
C9	0.7704 (7)	0.9606 (6)	1.2251 (8)	0.090 (3)
C10	0.7514 (11)	1.0112 (7)	1.1335 (11)	0.131 (5)
C11	0.9273 (5)	0.5960 (4)	1.2094 (6)	0.053 (2)
C12	0.9318 (7)	0.5003 (6)	1.3396 (7)	0.076 (3)
C13	1.0276 (8)	0.4587 (7)	1.3552 (10)	0.107 (4)
C14	0.8636 (7)	0.4715 (5)	1.1621 (7)	0.076 (3)
C15	0.7570 (8)	0.4678 (6)	1.1607 (8)	0.094 (3)
C16	0.7268 (12)	0.7521 (10)	0.9035 (12)	0.118 (5)
C17	0.6766 (9)	0.7182 (10)	0.9552 (10)	0.114 (5)
C18	0.6134 (8)	0.7377 (8)	1.0213 (9)	0.096 (4)
C19	0.7253 (7)	0.8365 (6)	0.9025 (8)	0.067 (2)
C20	0.7940 (10)	0.7189 (8)	0.8352 (9)	0.101 (4)
C21	0.6934 (9)	0.6258 (7)	0.9372 (9)	0.096 (4)
C22	0.5698 (10)	0.6739 (10)	1.0727 (10)	0.116 (4)
C23	0.5897 (8)	0.8127 (7)	1.0457 (9)	0.088 (3)

† Site occupancy of 0.5 assumed.

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

Ni—S1	2.255 (2)	N7—C22	1.14 (2)
Ni—S2	2.246 (2)	N8—C23	1.153 (14)
Ni—S3	2.252 (2)	C16—C17	1.19 (2)
Ni—S4	2.256 (2)	C16—C19	1.48 (2)
Ni—S5	2.257 (2)	C16—C20	1.49 (2)
Ni—S6	2.251 (2)	C17—C18	1.35 (2)
N4—C19	1.121 (12)	C17—C21	1.66 (2)
N5—C20	1.11 (2)	C18—C23	1.40 (2)
N6—C21	1.107 (12)	C18—C22	1.48 (2)
S1—Ni—S2	76.25 (8)	C17—C16—C19	119.7 (19)
S1—Ni—S3	96.02 (9)	C17—C16—C20	127.1 (17)
S1—Ni—S4	92.87 (8)	C19—C16—C20	113.2 (13)
S1—Ni—S5	164.89 (9)	C16—C17—C18	136 (2)
S1—Ni—S6	94.20 (8)	C16—C17—C21	107.7 (15)
S2—Ni—S3	93.25 (9)	C18—C17—C21	116.8 (14)
S2—Ni—S4	164.24 (9)	C17—C18—C22	116.2 (13)
S2—Ni—S5	93.13 (8)	C17—C18—C23	125.0 (14)
S2—Ni—S6	96.77 (9)	C22—C18—C23	118.8 (11)
S3—Ni—S4	76.35 (8)	N4—C19—C16	171.4 (14)
S3—Ni—S5	95.28 (9)	N5—C20—C16	173.1 (17)
S3—Ni—S6	167.12 (9)	N6—C21—C17	173.9 (15)
S4—Ni—S5	99.52 (8)	N7—C22—C18	172.5 (18)
S4—Ni—S6	95.36 (8)	N8—C23—C18	174.1 (13)
S5—Ni—S6	76.16 (7)		

The diethylamino portion of one Et_2dtc group is disordered over two positions and was refined isotropically with a site occupancy of 0.5 and without H atoms.

Data collection: *CAD*-4 *VAX/PC* (Enraf–Nonius, 1988). Cell refinement: *CAD*-4 *VAX/PC*. Data reduction: *MolEN* (Fair, 1990). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL-Plus* (Sheldrick, 1987). Software used to prepare material for publication: *SHELXL*93.

The authors thank the University of Malaya (R & D grant 09-02-03-0004), the National Nature Science Foundation and the State Science and Technology Commission of China for supporting this work.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: CF1075). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Avdeef, A., Fackler, J. P. & Fischer, R. G. (1970). *J. Am. Chem. Soc.* **92**, 6972–6974.

Enraf–Nonius (1988). *CAD-4 VAX/PC Operator's Manual.* Enraf–Nonius, Delft, The Netherlands.

Fackler, J. P., Avdeef, A. & Fischer, R. G. (1973). *J. Am. Chem. Soc.* **95**, 774–782.

Fair, C. K. (1990). *MolEN. An Interactive Intelligent System for Crystal Structure Analysis.* Enraf–Nonius, Delft, The Netherlands.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Giraudon, J. M., Sala-Pala, J., Guerchais, J. E. & Toupet, L. (1991). *Inorg. Chem.* **30**, 891–899.

Jensen, W. P. & Jacobson, R. A. (1981). *Inorg. Chim. Acta*, **50**, 189–194.

Miller, J. S., Calabrese, J. C., McLean, R. S. & Epstein, A. J. (1992). *J. Adv. Mater.* **4**, 498–500.

Miller, J. S., Calabrese, J. C., Rommelmann, H., Chittipeddi, S. R., Zhang, J. H., Reiff, W. M. & Epstein, A. J. (1987). *J. Am. Chem. Soc.* **109**, 769–781.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1987). *SHELXTL-Plus*. Release 3.4 for Nicolet *R3m/V* Crystallographic Systems. Nicolet Instrument Corporation, Madison, Wisconsin, USA.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1993). *SHELXL93. Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.
William, J., Rouwette, P. H. & Cras, J. A. (1972). *Inorg. Nucl. Chem. Lett.* **8**, 389–391.

Acta Cryst. (1996). C**52**, 3033-3035

β-meso-(5,7,7,12,12,14-Hexamethyl-1,4,8,11-tetraazacyclotetradecane)nickel(II) Diperchlorate Monohydrate

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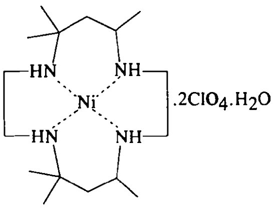
(*Received 24 July 1995; accepted 14 August 1996*)

Abstract

In the title compound, $[Ni(C_{16}H_{36}N_4)](ClO_4)_2.H_2O$, the Ni^{II} ion is four-coordinated by the four N atoms of the macrocyclic ligand. The four N atoms are coplanar to within 0.05 Å and the four H atoms attached to the N atoms are located on the same side of the macrocyclic plane. The configuration of the four chiral nitrogen centres and two chiral carbon centres are (1*RS*,4*SR*,8*RS*,11*SR*) and (5*SR*,14*RS*), respectively. The two five-membered chelate rings are in unstable eclipsed forms and the two six-membered chelate rings are in stable chair forms. The two methyl groups attached to the asymmetric C atoms are equatorial. The perchlorate ions and water O atom are not within the bonding distance of the cation.

Comment

The chemistry of macrocyclic compounds has undergone spectacular growth recently, due to their distinctive coordination and biological significance (Cabbiness & Margerum, 1969). The extreme kinetic inertness and very high thermodynamic stability of tetraamine macrocyclic ligand complexes are of particular stereochemical interest, since they greatly enhance the number of potentially isolable isomers (Liang & Chung, 1980; Lee, Lu, Chung & Lee, 1984). In a previous paper (Lee, Wu & Chung, 1984), we reported the synthesis and characterization of five stereoisomers of Ni^{II} complexes of 5,5,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradecane (1,4-CTH), namely, [Ni(*β-rac*-1,4-CTH)(NCS)$_2$], [Ni(*α-meso*-1,4-CTH)Cl$_2$], [Ni(*β-meso*-1,4-CTH)(NCS)$_2$], [Ni(*γ-meso*-1,4-CTH)(NCS)$_2$] and [Ni(*δ-meso*-1,4-CTH)(NCS)$_2$]. The present paper concerns the crystal structure of one of these isomers, [Ni(*β-meso*-1,4-CTH)](ClO$_4$)$_2$.H$_2$O, (I).



(I)

The Ni^{II} ion is four-coordinated by the amine N atoms, with Ni—N distances in the range 1.915 (5)–1.935 (4) Å, which are normal for planar Ni^{II}–tetraamine complexes. The chelate angles subtended at the Ni atom are normal for the five-membered [87.6 (2) and 89.1 (2)°] and six-membered [89.6 (2) and 93.6 (2)°] chelate rings (Fig. 1). These angles are a compromise between the optimum value of the bond angle at Ni (90°), the Ni—N bond distances and the preferred 'bite' of the chelate. Weak hydrogen bonds are formed among the amino group, water molecules and perchlorate O atoms. This hydrogen-bond network stabilizes the crystal packing and is similar to that found in the red macrocyclic ligand complex of copper(II) perchlorate (Lee, Lee, Juang & Chung, 1985), where hydrogen bond lengths range from 3.10 (5) to 3.39 (6) Å.

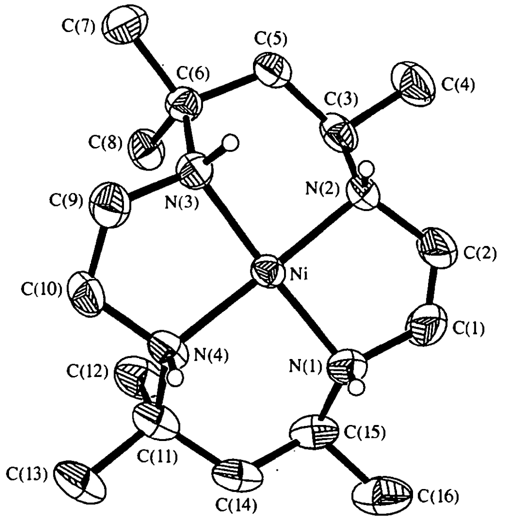


Fig. 1. *ORTEP*II (Johnson, 1976) drawing of a single molecule of (I) with displacement ellipsoids scaled to 30% probability. H atoms attached to N atoms are shown as circles.