References

Arce, A. J., Deeming, A. J., Donovan-Mtunzi, S. & Kabir, S. E. (1985). *J. Chem. Soc. Dalton Trans.* pp. 2479–2482.

B. A. Frenz & Associates, Inc. (1982). *SDP Structure Determination Package*. College Station, Texas, USA.

Churchill, M. R. & Wasserman, H. J. (1980). *Inorg. Chem.* **19**, 2391–2395.

Demming, A. J., Manning, P. J., Rothwell, I. P., Hursthouse, M. B. & Walker, N. P. C. (1984). *J. Chem. Soc. Dalton Trans.* pp. 2039–2045.

Ditzel, E. J., Gomez-Sal, M., Johnson, B. F. G., Lewis, J. & Raithby, P. R. (1987). *J. Chem. Soc. Dalton Trans.* pp. 1623–1630.

D'Ornelas, L., Choplin, A., Basset, J. M., Hsu, L. & Shore, S. G. (1985). *Nouv. J. Chim.* **9**, 155–157.

Dossi, C., Fusi, A., Pizzotti, M. & Psaro, R. (1990). *Organometallics*, **9**, 1994–1995.

Hodge, S. R., Johnson, B. F. G., Lewis, J. & Raithby, P. R. (1987). *J. Chem. Soc. Dalton Trans.* pp. 931–937.

Johnson, B. F. G., Lewis, J. & Kilty, P. A. (1968). *J. Chem. Soc. A*, pp. 2859–2864.

Johnson, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.

Main, P., Fiske, S. J., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1972). *MULTAN11/82. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

Puga, J., Fehlner, T. P., Gates, B. C., Braga, D. & Grepioni, F. (1990). *Inorg. Chem.* **29**, 2376–2381.

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Low-Temperature Structures of $[py_2H]^+[Co(CO)_4]^-$ (py = Pyridine) and $[(tmen)H]^+[Co(CO)_4]^-$ (tmen = *N*,*N*,*N*′,*N*′)-Tetramethylethylenediamine)

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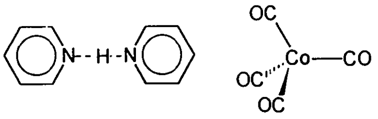
Abstract

The crystal structures of salts arising from the reaction of $HCo(CO)_4$ with pyridine and tetramethylethylenediamine, respectively, have been determined. The former, bis(pyridine) hydrogen tetracarbonylcobaltate(1 −), consists of a $[(C_5H_5N)_2H]^+$ cation, with a symmetrical (within experimental error) N⋯H⋯N hydrogen bond, and a $Co(CO)_4^-$ anion which is distorted towards C_{2v} symmetry. The latter, dimethyl[2-(dimethylamino)ethyl]ammonium tetracarbonylcobaltate(1 −), involves protonated tetramethylethylenediamine, $[(C_6H_{16}N_2)H]^+$, which forms an intramolecular N—H⋯N hydrogen bond, and a $Co(CO)_4^-$ anion of C_s symmetry. No unusual interactions between anions and cations are observed. In each structure the cation exhibits the shortest N⋯N separation observed to date for this hydrogen-bonded cation: 2.634 (4) Å for $[(C_5H_5N)_2H]^+$ and 2.711 (5) Å for the $(tmen)H^+$ cation.

Comment

We have recently synthesized and structurally characterized a number of salts formed from the reaction of $HCo(CO)_4$ with amines or diamines (Brammer, McCann, Bullock, McMullan & Sherwood, 1992; Brammer, Zhao & Ladipo, 1994; Brammer & Zhao, 1994). In some cases the resulting salts exhibit unusual N—H⋯Co hydrogen bonds; in others, particularly when an excess of the (di)amine is used, the resulting salt consists of N—H⋯N hydrogen-bonded cations and non-interacting $Co(CO)_4^-$ anions. The salts reported here, $[(C_6H_5N)_2H]^+[Co(CO)_4]^-$ (1) and $[(tmen)H]^+$ $[Co(CO)_4]^-$ (2), were prepared in the manner previously reported for the preparation of $(Et_3NH)^+[Co(CO)_4]^-$ (Brammer, McCann, Bullock, McMullan & Sherwood, 1992; Calderazzo, Fachinetti, Marchetti & Zanazzi, 1981) and $[(DABCO)H]^+[Co(CO)_4]^-$ (Brammer, Zhao & Ladipo, 1994) using $HCo(CO)_4$ to (di)amine ratios of 1:10 and 1:2.3 for (1) and (2), respectively. Thus, both salts exhibit N—H⋯N rather than N—H⋯Co hydrogen-bonding interactions.



(1)

(2)

The structures of (1) and (2) are shown in Figs. 1 and 2, respectively. Both ions in (2) have exact C_s symmetry; methylene C(12) and C(13) of the anions are disordered about the mirror plane at $y = \frac{1}{4}$. The N⋯N separation in compound (1) is smaller than that previously reported for other salts which include the same or similar N—H⋯N bonded cations (*e.g.* see Table 5). The N⋯N separation in (2) is also markedly shorter than in other examples of monoprotonated tetra-*N*-substituted ethylenediamines (*e.g.* see Doi, Ishida & Inoue, 1990). N···N distances of less than 3.0 Å give rise to the possibility of intramolecular N—H···N hydrogen bonding arising from a *cis* conformation of the diamine, whereas the *trans* conformation leads to N···N separations typically in excess of 3.7 Å and precludes N—H···N hydrogen-bond formation (*e.g.* see Declercq & van Meerssche, 1984). The only related examples in which the N···N separation is less than that of 2.711 Å in (2) are the 'inside-protonated' bicyclo diamines 7-aza-1-azoniabicyclo[5.5.2]tetradecane picrate (N···N 2.554 Å) (White, Alder & Open, 1988*a*) and 7-aza-1-azoniabicyclo[5.4.2]tridecane picrate (N···N 2.474 Å) (White, Alder & Orpen, 1988*b*).

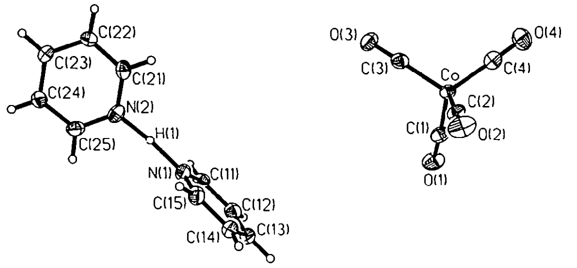


Fig. 1. Structure of $[(C_5H_5N)_2H]^+[Co(CO)_4]^-$ (1) shown with 50% probability ellipsoids for non-H atoms. H atoms are represented as spheres of arbitrary radii.

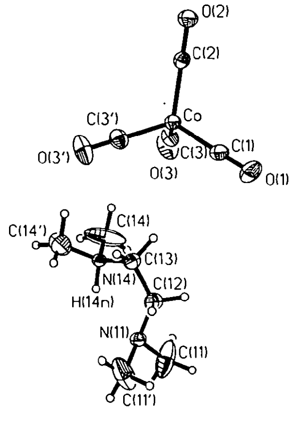


Fig. 2. Structure of $[(tmen)H]^+[Co(CO)_4]^-$ (2) shown with 50% probability ellipsoids for non-H atoms. H atoms are represented as spheres of arbitrary radii. The disorder of C(12) and C(13) is not shown.

Experimental

Compound (1)

Crystal data

$[(C_5H_5N)_2H][Co(CO)_4]$
$M_r = 330.2$
Monoclinic
$P2_1/c$
$a = 7.079$ (3) Å
$b = 14.290$ (4) Å
$c = 14.828$ (5) Å
$\beta = 93.22$ (3)°
$V = 1497.7$ (9) Å^3
$Z = 4$
$D_x = 1.464$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 35 reflections
$\theta = 12.68$–17.26°
$\mu = 1.161$ mm^{-1}
$T = 128$ (5) K
Plate-like
0.50 × 0.45 × 0.15 mm
Yellow
Crystal source: crystallized from pyridine solution

Data collection

Siemens *R*3*m*/*V* diffractometer
ω–2θ scans
Absorption correction: empirical (ψ scans)
$T_{min} = 0.406$, $T_{max} = 0.524$
3247 measured reflections
2890 independent reflections
2236 observed reflections
$[F > 3\sigma(F)]$

$R_{int} = 0.0287$
$\theta_{max} = 30.0$°
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 21$
$l = -21 \rightarrow 21$
3 standard reflections monitored every 50 reflections
intensity variation: ±3%

Refinement

Refinement on *F*
$R = 0.0417$
$wR = 0.0440$
$S = 1.42$
2236 reflections
234 parameters
Only coordinates of H atoms refined
$w = 1/[\sigma^2(F) + 0.0003F^2]$

$(\Delta/\sigma)_{max} = 0.018$
$\Delta\rho_{max} = 0.56$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ 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) *for* (1)

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

	x	*y*	*z*	U_{eq}
Co	0.1248 (1)	0.2440 (1)	0.2034 (1)	0.022 (1)
C(1)	0.0927 (5)	0.1838 (2)	0.3062 (2)	0.030 (1)
C(2)	0.3656 (5)	0.2536 (2)	0.1856 (2)	0.027 (1)
C(3)	0.0228 (5)	0.3561 (2)	0.2176 (2)	0.027 (1)
C(4)	0.0119 (5)	0.1862 (2)	0.1101 (2)	0.029 (1)
O(1)	0.0741 (4)	0.1486 (2)	0.3745 (2)	0.042 (1)
O(3)	−0.0420 (4)	0.4284 (2)	0.2279 (2)	0.036 (1)
O(2)	0.5267 (4)	0.2607 (2)	0.1731 (2)	0.044 (1)
O(4)	−0.0601 (4)	0.1498 (2)	0.0477 (2)	0.044 (1)
N(1)	0.4796 (4)	0.6676 (2)	0.5884 (2)	0.026 (1)
C(11)	0.3595 (5)	0.6072 (2)	0.6228 (2)	0.028 (1)
C(12)	0.4088 (6)	0.5149 (2)	0.6396 (2)	0.031 (1)
C(13)	0.5881 (6)	0.4854 (2)	0.6197 (2)	0.031 (1)
C(14)	0.7126 (5)	0.5482 (2)	0.5843 (2)	0.029 (1)
C(15)	0.6531 (5)	0.6393 (2)	0.5693 (2)	0.028 (1)
N(2)	0.3778 (4)	0.8440 (2)	0.5681 (2)	0.025 (1)
C(21)	0.2878 (4)	0.8744 (2)	0.4922 (2)	0.026 (1)
C(22)	0.2323 (4)	0.9659 (2)	0.4820 (2)	0.024 (1)
C(23)	0.2674 (4)	1.0272 (2)	0.5532 (2)	0.024 (1)
C(24)	0.3604 (5)	0.9951 (2)	0.6318 (2)	0.027 (1)
C(25)	0.4135 (5)	0.9028 (2)	0.6372 (2)	0.028 (1)

Table 2. *Selected geometric parameters* (Å, °) *for* (1)

Co—C(1)	1.776 (3)	N(1)—C(15)	1.338 (5)
Co—C(3)	1.775 (3)	C(11)—C(12)	1.383 (5)

C(1)—O(1)	1.146 (4)	C(12)—C(13)	1.385 (6)
C(3)—O(3)	1.144 (4)	C(13)—C(14)	1.382 (5)
N(1)—C(11)	1.333 (4)	C(14)—C(15)	1.383 (4)
N(2)—C(25)	1.338 (4)	N(2)—C(21)	1.335 (4)
Co—C(2)	1.745 (4)	C(21)—C(22)	1.371 (4)
Co—C(4)	1.764 (3)	C(22)—C(23)	1.384 (4)
C(2)—O(2)	1.170 (5)	C(23)—C(24)	1.383 (4)
C(4)—O(4)	1.155 (4)	C(24)—C(25)	1.373 (4)
C(1)—Co—C(2)	110.0 (1)	C(1)—Co—C(3)	105.2 (1)
C(2)—Co—C(3)	110.8 (1)	C(1)—Co—C(4)	111.8 (1)
C(2)—Co—C(4)	108.7 (2)	C(3)—Co—C(4)	110.3 (1)
Co—C(1)—O(1)	177.0 (3)	Co—C(2)—O(2)	179.3 (3)
Co—C(3)—O(3)	179.1 (3)	Co—C(4)—O(4)	178.4 (3)
C(11)—N(1)—C(15)	119.9 (3)	N(1)—C(11)—C(12)	121.7 (3)
C(11)—C(12)—C(13)	118.5 (3)	C(12)—C(13)—C(14)	119.6 (3)
C(13)—C(14)—C(15)	118.6 (3)	N(1)—C(15)—C(14)	121.6 (3)
N(2)—C(21)—C(22)	121.5 (3)	C(21)—N(2)—C(25)	120.1 (3)
C(22)—C(23)—C(24)	119.3 (3)	C(21)—C(22)—C(23)	118.8 (3)
N(2)—C(25)—C(24)	121.3 (3)	C(23)—C(24)—C(25)	118.9 (3)

Compound (2)

Crystal data

$(C_6H_{17}N_2)[Co(CO)_4]$
$M_r = 288.2$
Orthorhombic
Pnma
$a = 19.528\ (5)$ Å
$b = 9.518\ (2)$ Å
$c = 7.408\ (2)$ Å
$V = 1376.9\ (6)$ Å^3
$Z = 4$
$D_x = 1.390$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 50 reflections
$\theta = 8.35–14.79°$
$\mu = 1.251$ mm^{-1}
$T = 128\ (5)$ K
Needles
0.50 × 0.18 × 0.16 mm
Colorless
Crystal source: crystallized from thf solution

Data collection

Siemens *R*3*m*/*V* diffractometer
ω–2θ scans
Absorption correction: empirical (ψ scans)
$T_{\min} = 0.453$, $T_{\max} = 0.503$
3748 measured reflections
1691 independent reflections
1231 observed reflections $[F > 3\sigma(F)]$

$R_{\text{int}} = 0.0213$
$\theta_{\max} = 27.5°$
$h = -25 \rightarrow 25$
$k = -12 \rightarrow 0$
$l = 0 \rightarrow 9$
3 standard reflections monitored every 50 reflections intensity variation: ±3%

Refinement

Refinement on *F*
$R = 0.0452$
$wR = 0.0455$
$S = 1.48$
1231 reflections
99 parameters
$w = 1/[\sigma^2(F) + 0.0003F^2]$
$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.51$ e Å^{-3}
$\Delta\rho_{\min} = -0.52$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (2)

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

	x	*y*	*z*	U_{eq}
Co	0.3922 (1)	3/4	0.5020 (1)	0.021 (1)
O(1)	0.4495 (2)	3/4	0.8665 (5)	0.045 (1)
O(2)	0.2435 (2)	3/4	0.5364 (4)	0.035 (1)
O(3)	0.4385 (1)	0.9934 (3)	0.2968 (4)	0.049 (1)
C(1)	0.4281 (2)	3/4	0.7228 (6)	0.029 (1)
C(2)	0.3024 (2)	3/4	0.5218 (6)	0.025 (1)
C(3)	0.4204 (2)	0.8985 (4)	0.3794 (4)	0.030 (1)
C(11)	0.7679 (3)	0.8734 (5)	0.4599 (5)	0.074 (2)
N(11)	0.7293 (2)	3/4	0.4152 (5)	0.024 (1)
C(12)†	0.6630 (3)	0.7214 (9)	0.4980 (8)	0.034 (3)
C(13)†	0.6066 (3)	0.7124 (7)	0.3892 (7)	0.028 (2)
N(14)	0.6186 (2)	3/4	0.1941 (5)	0.021 (1)
C(14)	0.5924 (2)	0.8759 (6)	0.1057 (8)	0.086 (2)

† Disordered about the mirror plane at $y = \frac{3}{4}$.

Table 4. *Selected geometric parameters* (Å, °) *for* (2)

Co—C(1)	1.779 (5)	Co—C(2)	1.759 (4)
Co—C(3)	1.768 (3)	O(1)—C(1)	1.144 (6)
O(2)—C(2)	1.155 (5)	O(3)—C(3)	1.147 (4)
C(11)—N(11)	1.435 (5)	N(11)—C(12)	1.458 (6)
C(12)—C(13)	1.367 (8)	C(13)—N(14)	1.507 (6)
N(14)—C(14)	1.458 (6)	N(14)—H(14N)	0.913 (53)
C(1)—Co—C(2)	108.4 (2)	C(1)—Co—C(3)	110.4 (1)
C(2)—Co—C(3)	110.7 (1)	C(3)—Co—C(3$^{\text{i}}$)	106.1 (2)
Co—C(1)—O(1)	178.2 (4)	Co—C(2)—O(2)	179.4 (4)
Co—C(3)—O(3)	178.7 (3)	C(11)—N(11)—C(12)	121.5 (4)
C(11)—N(11)—C(11$^{\text{i}}$)	109.9 (5)	N(11)—C(12)—C(13)	118.6 (5)
C(12)—C(13)—N(14)	115.2 (5)	C(13)—N(14)—C(14)	124.8 (4)
C(14)—N(14)—C(14$^{\text{i}}$)	110.5 (5)	C(13)—N(14)—H(14N)	102.1 (33)
C(14)—N(14)—H(14N)	109.0 (17)		

Symmetry code: (i) $x, \frac{1}{2} - y, z$.

Table 5. *Comparison of geometries* (Å) *of* $[(C_5H_5N)_2H]^+$ *cations*

Anion	N···N separation	Reference
$[Co(CO)_4]^-$	2.634	This work
$[Cr(O)OC(CF_3)_2C(CF_3)_2O_2]^-$	2.644	Nishino & Kochi (1990)
$P_2S_8^-$	2.656	Minshall & Sheldrick (1978)
$[WCl_4(py)_2]^-$	2.733	Brenčič, Čeh & Leban (1986)
$[WBr_4(py)_2]^-$	2.735	Brenčič, Čeh & Leban (1979)
$[ZnBr_2Cl(py)]^-$	2.739	Villarreal-Salinas & Schlemper (1979)
$[Fe_2Cl_6(\mu\text{-}O)]^{2-}$	2.745	Drew, McKee & Nelson (1978)

For compound (2), methylene and methyl H atoms were refined using a riding model with a fixed isotropic displacement parameter $U = 0.08$ Å^2. x and z of the ammonium H atom at $y = \frac{3}{4}$ were allowed to refine freely but a fixed isotropic U of 0.05 Å^2 was assigned to this atom. Disorder of the cation about the mirror plane results in enlarged displacement parameters for the methyl C atoms C(11) and C(14).

All calculations were performed using *SHELXTL-Plus* (Sheldrick, 1991).

Financial support from the Donors of the Petroleum Research Fund, administered by the American Chemical Society, as well as from the University of Missouri Research Board and Weldon Springs Fund is gratefully acknowledged.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: MU1106). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Brammer, L., McCann, M. C., Bullock, R. M., McMullan, R. K. & Sherwood, P. (1992). *Organometallics*, **11**, 2339–2341.

Brammer, L. & Zhao, D. (1994). *Organometallics*, **13**, 1545–1547.

Brammer, L., Zhao, D. & Ladipo, F. T. (1994). *J. Am. Chem. Soc.* Submitted.

Brenčič, J. V., Čeh, B. & Leban, I. (1979). *Acta Cryst.* B**35**, 3028–3030.

Brenčič, J. V., Čeh, B. & Leban, I. (1986). *Z. Anorg. Allg. Chem.* **538**, 212–220.

Calderazzo, F., Fachinetti, F., Marchetti, F. & Zanazzi, P. F. (1981). *J. Chem. Soc. Chem. Commun.* pp. 181–183.

Declercq, J.-P. & van Meerssche, M. (1984). *Bull. Soc. Chim. Belg.* **93**, 235–236.

Doi, M., Ishida, T. & Inoue, M. (1990). *Acta Cryst.* C**46**, 676–678.

Drew, M. G. B., McKee, V. & Nelson, S. M. (1978). *J. Chem. Soc. Dalton Trans.* pp. 80–84.

Minshall, P. C. & Sheldrick, G. M. (1978). *Acta Cryst.* B**34**, 1378–1380.

Nishino, H. & Kochi, J. K. (1990). *Inorg. Chim. Acta*, **174**, 93–102.

Sheldrick, G. M. (1991). *SHELXTL-Plus*. Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Villarreal-Salinas, B. E. & Schlemper, E. O. (1979). *J. Cryst. Mol. Struct.* **8**, 217–237.

White, J. M., Alder, R. W. & Orpen, A. G. (1988*a*). *Acta Cryst.* C**44**, 664–666.

White, J. M., Alder, R. W. & Orpen, A. G. (1988*b*). *Acta Cryst.* C**44**, 1467–1469.

Acta Cryst. (1995). C**51**, 48–50

[*N*,*N*-Bis(2-aminoethyl)-*N*′-(2-aminoethylidene)ethane-1,2-diamine]chlorocobalt(III) Perchlorate

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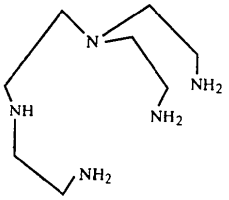
Abstract

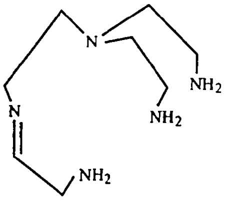
The structure of the title compound, $[CoCl(C_8H_{21}N_5)]2ClO_4$, consists of octahedral $[Co(trenenim)Cl]^{2+}$ cations [where trenenim = *N*,*N*-bis(2-aminoethyl-*N*′-(2-aminoethylidene)ethane-1,2-diamine] with two perchlorate anions acting as counterions. The bond lengths and angles about N(2) and C(3) provide clear evidence for the presence of an imine bond. A short Co—N(2) distance of 1.863 (2) Å reflects the fact that this N atom is an imine N atom. The corresponding Co—N distance in the related saturated system $[Co(trenen)Cl]^{2+}$ [where trenen = *N*,*N*,*N*′-tris(2-aminoethyl)ethane-1,2-diamine] is also substantially shorter than the others. In both cases, the secondary N atom on the appended arm has a stronger affinity for Co^{III} than the primary and tertiary N atoms within the ligand framework.

Comment

The coordination chemistry of pentadentate ligands has attracted our attention because these ligands can be applied in the synthesis of binuclear complexes linked by a single bridging group. We have recently reported the synthesis and X-ray structure of $[Co(trenen)Cl]Cl(ClO_4).H_2O$ (Gatehouse, Martin, McLachlan, Platts & Spiccia, 1992) and the peroxo-bridged complex $[(trenen)CoO_2Co(trenen)](ClO_4)_4$ (Gatehouse, McLachlan, Martin, Martin & Spiccia, 1991), where trenen is the pentadentate ligand, *N*,*N*,*N*′-tris(2-aminoethyl)ethane-1,2-diamine (1). In these complexes, the disposition of the ligand is such that the Cl and O atoms from the peroxide bridge are *trans* to the secondary N atom. A further feature of these complexes is the short Co—N(secondary) distance compared with the other Co—N distances. We report here the X-ray structure of $[Co(trenenim)Cl](ClO_4)_2$, where trenenim is *N*,*N*-bis(2-aminoethyl)-*N*′-(2-aminoethylidene)ethane-1,2-diamine (2). This structure is of interest because the complex is the precursor to $[Co(trenen)Cl]^{2+}$ (Gatehouse *et al.*, 1992) and $[(trenen)CoO_2Co(trenen)]^{4+}$ (Gatehouse *et al.*, 1991).



(1) trenen



(2) trenenim

Fig. 1 shows the structure of the complex cation $[Co(trenenim)Cl]^{2+}$ and the perchlorate counter ions. The primary coordination sphere of the Co^{III} atom comprises five N atoms from the trenenim ligand and one Cl atom. As in the previously reported peroxo and chloro complexes of trenen (Gatehouse *et al.*, 1991; Gatehouse *et al.*, 1992), the chloro ligand is *trans* to the secondary N atom because the ligand

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