

C37	0.1403 (2)	0.1567 (4)	0.7923 (5)	0.076 (3)
C38	0.1137 (2)	0.1615 (3)	0.6912 (5)	0.056 (2)
C39	0.0779 (2)	0.1279 (4)	0.6770 (5)	0.067 (2)
C110	0.0797 (2)	0.4912 (4)	0.5359 (6)	0.068 (2)
C111	0.08782 (14)	0.4093 (3)	0.5108 (5)	0.0559 (19)
C113	0.14287 (13)	0.4324 (3)	0.2980 (5)	0.053 (2)
C114	0.12153 (13)	0.4548 (3)	0.3800 (5)	0.0548 (19)
C210	0.02496 (14)	0.3242 (4)	0.1181 (5)	0.065 (2)
C211	0.05037 (13)	0.3280 (3)	0.2204 (5)	0.0540 (19)
C213	0.10899 (13)	0.1530 (3)	0.1998 (4)	0.0472 (17)
C214	0.07970 (13)	0.2111 (3)	0.1710 (4)	0.0467 (17)
C310	0.05507 (15)	0.1343 (3)	0.5752 (5)	0.0585 (19)
C311	0.06647 (12)	0.1755 (3)	0.4860 (5)	0.0499 (19)
C313	0.15942 (12)	0.2326 (3)	0.6039 (4)	0.0442 (16)
C314	0.12353 (13)	0.2005 (3)	0.5975 (4)	0.0438 (17)
P1	0	0.03919 (11)	1/4	0.0455 (6)
F11	0.04360 (8)	0.0391 (2)	0.2846 (3)	0.0724 (14)
F12	-0.00296 (10)	0.0390 (2)	0.3785 (3)	0.0791 (16)
F13	0	0.1389 (2)	1/4	0.0677 (18)
F14	0	-0.0606 (2)	1/4	0.0668 (18)
P2	0	0.5851 (2)	1/4	0.0786 (10)
F21	0.0309 (2)	0.5179 (3)	0.2664 (5)	0.151 (3)
F22	0.0297 (2)	0.6519 (4)	0.2754 (7)	0.196 (4)
F23	0.0002 (2)	0.5841 (4)	0.3789 (5)	0.165 (3)
P3	0.24086 (5)	0.0400 (2)	0.0536 (2)	0.1000 (9)
F31	0.24495 (13)	0.0426 (4)	0.1833 (4)	0.133 (2)
F32	0.27711 (14)	-0.0087 (4)	0.0608 (5)	0.148 (3)
F33	0.2157 (2)	-0.0320 (6)	0.0502 (7)	0.233 (5)
F34	0.23781 (13)	0.0428 (6)	-0.0761 (4)	0.216 (5)
F35	0.2063 (2)	0.0939 (7)	0.0440 (7)	0.278 (6)
F36	0.2658 (2)	0.1198 (5)	0.0579 (7)	0.209 (4)

Table 2. Selected geometric parameters (\AA , $^\circ$)

Ru—N11	2.061 (5)	Ru—N112	2.067 (4)
Ru—N21	2.063 (5)	Ru—N212	2.064 (4)
Ru—N31	2.056 (4)	Ru—N312	2.068 (4)
N11—Ru—N112	80.38 (17)	N31—Ru—N312	79.62 (15)
N21—Ru—N212	79.47 (17)		

H atoms were placed in calculated ideal positions and refined using a riding model, each with an isotropic displacement parameter set to 1.2 times the equivalent isotropic displacement parameter of the atom to which it is attached.

Program(s) used to solve structure: *SIR92* (Altomare, Cascarano, Giacovazzo & Guagliardi, 1993). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *PLATON* (Spek, 1990), *INSIGHTII* (Biosym Technologies, 1993). Software used to prepare material for publication: *PLATON*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: JZ1107). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structures of Chromium(III) Cyclam Complexes. 6. *trans*-Aqua-hydroxy(1,4,8,11-tetraazacyclotetradecane)chromium(III) Dibromide Hydrate

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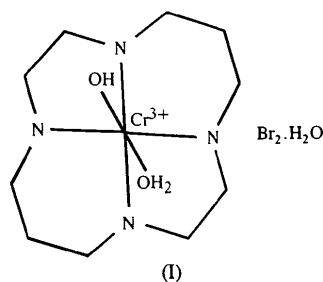
Abstract

The X-ray analysis of the title compound, $[\text{Cr}(\text{OH})(\text{H}_2\text{O})(\text{C}_{10}\text{H}_{24}\text{N}_4)]\text{Br}_2 \cdot \text{H}_2\text{O}$, indicates that the cyclam moiety exists in a chair conformation. The *trans*-axial O atoms bonded to Cr both carry one well defined H atom, with each oxygen also bearing a partially occupied (50%) H atom. The O—Cr—O bond angle is almost linear [$179.6(1)^\circ$] and the O...O vector is tilted by $1.2(2)^\circ$ from the perpendicular to the CrN₄ plane.

Comment

The title compound, (I), is one of a series of salts of the complex ion *trans*-[Cr(cyclam)X₂]⁺, where cy-

clam = 1,4,8,11-tetraazacyclotetradecane. Cyclam is a quadridentate cyclic ligand providing essentially a stable four-donor-atom plane enabling kinetic, photochemical and spectroscopic evaluation of the X₂ ligand to be carried out. When the effective crystal field is assumed to be D_{4h} the spectra can be described by the parameters D_q, D_s and D_t, enabling the crystal field theory to be tested. In principle, tetraaza cyclic ligands present a simpler model for the more complex, naturally occurring porphyrins. Classical examples of porphyrin complexes are those containing manganese prepared and studied by Zaleski (1904) and Taylor (1940). We present the structure of the pink derivative *trans*-[Cr(OH)(H₂O)(cyclam)]Br₂·H₂O as part of our investigation into the roles of exact site symmetry and the field due to neighbouring counterions in determining the form of the electronic spectra of these compounds.



The cyclam moiety provides a tetradentate N-donor ligand, forming with the two axial O atoms an octahedrally coordinated Cr atom (Fig 1). The Cr—N distances have a mean value of 2.064 (3) Å, which is in agreement with those found in other members of this series, including the dicyano complex (Hemmings, Lisgarten, Palmer & Gazi, 1989), the dibromo complex (Lisgarten, Palmer, Hemmings & Gazi, 1990), the dichloro complex (Dealwis, Janes, Palmer, Lisgarten, Maes & Gazi, 1992), the bromo-chloro complex (Chattopadhyay, Palmer, Lisgarten, Wyns & Gazi, 1992) and the dichloro complex (Bouckaert, Maes, Lisgarten, Chattopadhyay, Palmer, Mazid & Gazi, 1993), as well as in related compounds such as *trans*-amminebis(ethylenediamine)-fluorochromium(III) perchlorate (Beveridge, Bushnell & Kirk, 1985). The cyclam ring has geometry similar to that observed in many examples and displays almost perfect non-crystallographic conformational symmetry, $\Delta C_2 = 1.4^\circ$ (Duax & Norton, 1975). The least-squares-planes equation for the Cr³⁺ ion and the four N atoms is $0.9674x' + 0.0246y' + 0.2521z' = 6.0106$, where x' , y' and z' are the coordinates in Å with respect to orthonormal axes (Rollett, 1965). These equatorial ligands and the central Cr ion are coplanar with an r.m.s. deviation of 0.0091 Å. The bond lengths and angles conform within close limits to values quoted for similar compounds. The O(1)··O(2) axial vector is tilted by $1.2(2)^\circ$ from the perpendicular to the CrN₄ plane.

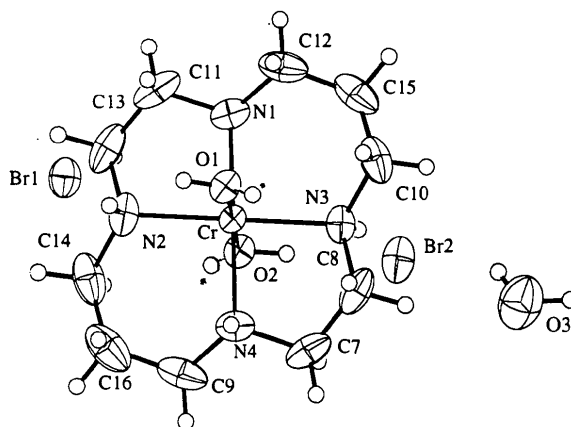


Fig. 1. View of the asymmetric unit perpendicular to the least-squares plane through all atoms. Displacement ellipsoids are plotted at the 50% probability level. The half-occupancy H atoms are indicated by an asterisk.

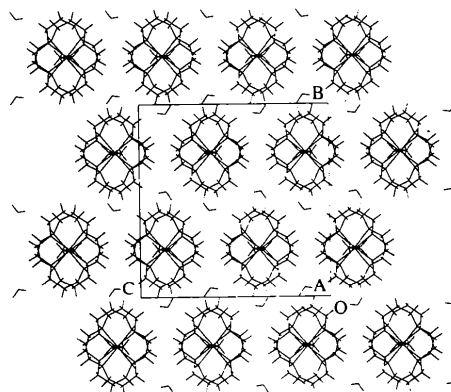


Fig. 2. Packing diagram viewed along *a*o.

Experimental

Crystals were obtained by slow evaporation from aqueous solution.

Crystal data

[Cr(OH)(H₂O)(C₁₀H₂₄N₄)]·
Br₂·H₂O
*M*_r = 465.2
Orthorhombic
Pcab
a = 12.049 (3) Å
b = 17.018 (3) Å
c = 17.071 (3) Å
V = 3500.4 Å³
Z = 8
*D*_x = 1.765 Mg m⁻³

Cu *K*α radiation
 $\lambda = 1.54178$ Å
Cell parameters from 25
reflections
 $\theta = 20\text{--}25^\circ$
 $\mu = 10.838$ mm⁻¹
T = 293 K
Tabular
0.4 × 0.3 × 0.2 mm
Pink

Data collection

Enraf-Nonius CAD-4
diffractometer

*R*_{int} = 0.0325
 $\theta_{\text{max}} = 73^\circ$

ω -2 θ scans $h = -11 \rightarrow 14$
 Absorption correction: $k = -3 \rightarrow 21$
 none $l = -3 \rightarrow 21$
 5558 measured reflections 3 standard reflections
 3493 independent reflections monitored every 100
 2990 observed reflections reflections
 [$I > 2\sigma(I)$] intensity decay: <10%

Refinement

Refinement on F^2 $\Delta\rho_{\max} = 0.199 \text{ e } \text{\AA}^{-3}$
 $R(F) = 0.0629$ $\Delta\rho_{\min} = -0.225 \text{ e } \text{\AA}^{-3}$
 $wR(F^2) = 0.1637$ Extinction correction: *SHELXL92* (Sheldrick, 1992)
 $S = 1.063$ Extinction coefficient: 0.0008 (1)
 3493 reflections Atomic scattering factors from *SHELXL92*
 216 parameters
 $w = 1/[\sigma^2(F^2) + (0.1251P)^2 + 0.018P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = -0.245$
 (U of H15)

N3—Cr1—N4	84.7 (1)	N3—C8—C7	107.9 (3)
O2—Cr1—N2	90.2 (1)	C16—C9—N4	114.0 (4)
O1—Cr1—N2	89.6 (1)	N3—C10—C15	112.1 (4)
N1—Cr1—N2	85.2 (2)	N1—C11—C13	108.7 (3)
N3—Cr1—N2	179.6 (1)	N1—C12—C15	111.9 (4)
N4—Cr1—N2	94.8 (2)	N2—C13—C11	108.5 (3)
C11—N1—C12	114.1 (4)	N2—C14—C16	112.4 (4)
C11—N1—Cr1	106.4 (3)	C12—C15—C10	116.5 (4)
C12—N1—Cr1	115.7 (3)	C9—C16—C14	115.9 (4)
C13—N2—C14	113.5 (4)		
C9—N4—C7—C8	170.0 (4)	N1—C11—C13—N2	56.2 (5)
C10—N3—C8—C7	171.4 (3)	C13—N2—C14—C16	179.0 (4)
N4—C7—C8—N3	-56.9 (4)	N1—C12—C15—C10	-71.6 (6)
C7—N4—C9—C16	-178.7 (4)	N3—C10—C15—C12	71.1 (5)
C8—N3—C10—C15	-178.9 (4)	N4—C9—C16—C14	69.6 (5)
C12—N1—C11—C13	-170.4 (4)	N2—C14—C16—C9	-69.4 (5)
C14—N2—C13—C11	-168.8 (3)		

Preliminary X-ray photographs (Weissenberg and precession) yielded the space group uniquely as *Pcab* and allowed determination of approximate unit-cell dimensions. The structure was solved by the heavy-atom method, all atoms being located in general positions. The H atoms were fixed geometrically except for H atoms attached to N or O: x , y , z and U were refined for H(11) [on N(1)], H(21) [on N(2)], H(31) [on N(3)], H(41) [on N(4)], H(1) and H(15) [on O(1)], H(2) and H(25) [on O(2)], and H(311) and H(312) [on O(3)]. Other H atoms were refined in riding mode with U variable. H(15) and H(25) on the axial O atoms were given fixed occupancy factors of 0.5. The *trans*-axial O atoms bonded to Cr both carry one well defined H atom, the displacement parameter of which refined to an acceptably low value. Each O atom is also associated with a weaker electron density peak at the correct position to define a second H atom. The displacement parameters associated with these minor peaks refine to acceptable values if fixed site occupancy of 0.5 is assumed. This situation can be modelled in terms of disorder across the two O sites of one hydroxy group and one water molecule. One hydroxy group plus two bromide ions thus balance the +3e charge on Cr, as required.

Refinement was performed by full-matrix least squares using the *SHELXL92* (Sheldrick, 1992) program with anisotropic displacement parameters for all non-H atoms, isotropic for H atoms. Geometrical calculations were also carried out using *SHELXL92* and molecular illustrations were prepared using *SNOOPI* (Karaulov, 1993).

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2)

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	U_{eq}
Br1	0.1434 (1)	0.0988 (1)	0.2263 (1)	0.045 (1)
Br2	0.5872 (1)	0.3935 (1)	0.5174 (1)	0.051 (1)
Cr1	0.3687 (1)	0.2464 (1)	0.3725 (1)	0.025 (1)
N1	0.4003 (3)	0.3187 (2)	0.2784 (2)	0.040 (1)
N2	0.4012 (3)	0.1555 (2)	0.2955 (2)	0.042 (1)
N3	0.3359 (3)	0.3366 (2)	0.4500 (2)	0.037 (1)
N4	0.3372 (3)	0.1740 (2)	0.4669 (2)	0.040 (1)
C7	0.3405 (4)	0.2243 (3)	0.5372 (2)	0.055 (1)
C8	0.2811 (4)	0.3007 (3)	0.5188 (2)	0.051 (1)
C9	0.4091 (5)	0.1030 (3)	0.4721 (3)	0.061 (1)
C10	0.2772 (4)	0.4055 (2)	0.4177 (3)	0.053 (1)
C11	0.3964 (4)	0.2686 (4)	0.2081 (2)	0.059 (1)
C12	0.3300 (5)	0.3908 (3)	0.2730 (3)	0.057 (1)
C13	0.4547 (4)	0.1914 (3)	0.2262 (2)	0.059 (1)
C14	0.4638 (4)	0.0882 (3)	0.3281 (3)	0.059 (1)
C15	0.3353 (5)	0.4389 (3)	0.3465 (4)	0.062 (1)
C16	0.4078 (4)	0.0532 (3)	0.4005 (4)	0.068 (2)
O1	0.2101 (2)	0.2441 (2)	0.3404 (1)	0.034 (1)
O2	0.5267 (2)	0.2487 (2)	0.4036 (1)	0.033 (1)
O3	0.3637 (4)	0.4500 (3)	0.6374 (3)	0.084 (1)

Table 2. Selected geometric parameters (\AA , $^\circ$)

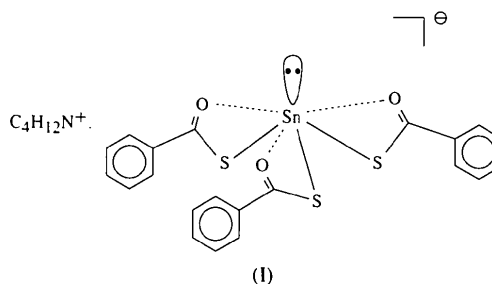
Cr1—O2	1.977 (3)	N3—C10	1.477 (5)
Cr1—O1	1.988 (3)	N3—C8	1.480 (5)
Cr1—N1	2.059 (3)	N4—C7	1.474 (6)
Cr1—N3	2.064 (3)	N4—C9	1.489 (6)
Cr1—N4	2.063 (3)	C7—C8	1.517 (7)
Cr1—N2	2.068 (3)	C9—C16	1.488 (8)
N1—C11	1.473 (6)	C10—C15	1.513 (8)
N1—C12	1.493 (6)	C11—C13	1.521 (8)
N2—C13	1.478 (6)	C12—C15	1.500 (8)
N2—C14	1.480 (6)	C14—C16	1.530 (9)
O2—Cr1—O1	179.6 (1)	C13—N2—Cr1	106.4 (3)
O2—Cr1—N1	91.1 (1)	C14—N2—Cr1	115.9 (3)
O1—Cr1—N1	88.6 (1)	C10—N3—C8	114.2 (3)
O2—Cr1—N3	89.9 (1)	C10—N3—Cr1	116.3 (3)
O1—Cr1—N3	90.4 (1)	C8—N3—Cr1	106.7 (2)
N1—Cr1—N3	95.2 (1)	C7—N4—C9	114.0 (4)
O2—Cr1—N4	88.8 (1)	C7—N4—Cr1	106.6 (3)
O1—Cr1—N4	91.5 (1)	C9—N4—Cr1	115.1 (3)
N1—Cr1—N4	179.9 (2)	N4—C7—C8	108.4 (3)

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: HU1105). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Tetramethylammonium Tris(thiobenzoato-O,S)tin(II)

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Abstract

The synthesis, structure and ¹¹⁹Sn NMR spectrum of the title compound, (C₄H₁₂N)[Sn(C₇H₅OS)₃], are reported. Crystallographic threefold symmetry is present in both the anion and cation. In the [Sn(SOCPh)₃][−] anion, the Sn^{II} coordination geometry is trigonal pyramidal, with the S atoms forming the basal plane and the Sn atom at the apex; the Sn—S distance is 2.592 (2) Å. In addition, weak intramolecular interactions occur between the Sn atom and the carbonyl O atoms [Sn···O 2.967 (2) Å]. The ¹¹⁹Sn NMR chemical shift of the title compound is −227 p.p.m. (MeCN, 295 K).

Comment

The chemistry of metal thiobenzoates has not been extensively investigated (Cras & Willemse, 1987; McCormick, Beremon & Baird, 1984). We have reported the structures of the thiobenzoate complexes of Cd^{II} (Vittal & Dean, 1993), Pb^{II} and Bi^{III} (Burnett, Dean & Vittal, 1993).

Reaction of SnCl₂·2H₂O, Et₃NH⁺·SOCPh[−] and Me₄NCl in the ratio 1:3:1 afforded the title compound, (I), in low yield. The ¹¹⁹Sn chemical shift is −227 p.p.m., the resonance being significantly more shielded than that of [Sn(SPh)₃][−], the chemical shift of which is 140–146 p.p.m. (Arsenault & Dean, 1983; Dean, Vittal & Payne, 1985). Thus, structural information about the [Sn(SOCPh)₃][−] anion is highly desirable.

The structure determination of (I) shows it to consist of discrete anions and cations. Both the Me₄N⁺ and [Sn(SOCPh)₃][−] ions lie on a crystallographic threefold axis; a view of the anion is shown in Fig. 1. The three SOCPh[−] ligands are bonded to Sn^{II} primarily through their S atoms. The coordination sphere around the Sn atom can be described as a trigonal pyramid with the three S atoms occupying the base [S···S distance 3.658 (3) Å] and the Sn atom at the apex. The geometry is consistent with the presence of a stereochemically active lone pair on Sn. The Sn—S distance of 2.592 (2) Å is longer than those of 2.532 (1)–2.552 (1) Å found for trigonal pyramidal [Sn(SPh)₃][−] (Dean, Vittal & Payne, 1985). Weak coordination to the three carbonyl O atoms, however, also occurs in [Sn(SOCPh)₃][−]; the Sn···O distance of 2.967 (2) Å is less than the sum of the relevant van der Waals radii (3.7 Å; Bondi, 1964). The Sn atom is 1.64 (1) Å from the S₃ plane and 0.14 (1) Å from the O₃ plane. The dihedral angle between the SnSCO planes is 101.5 (2)^o. In the PhCOS[−] ligands, the COS planes are twisted from the phenyl ring planes by 18.5 (2)^o.

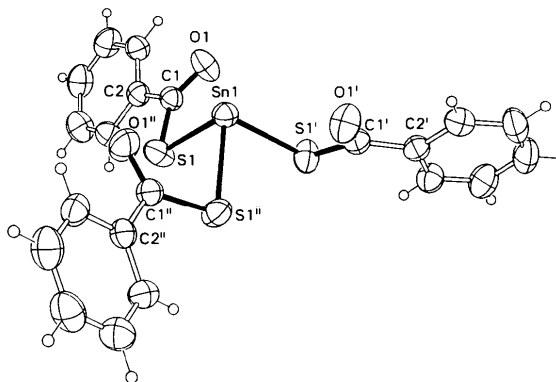


Fig. 1. A view of the [Sn(SOCPh)₃][−] anion showing the labeling of the non-H atoms. Displacement ellipsoids are shown at the 50% probability level and H atoms are drawn as small circles of arbitrary radii.

The methyl groups of the Me₄N⁺ cation are disordered. The two disorder models (occupancies of 0.6 and 0.4) are related by an inversion at N1 along the C8—N1 axis. In the crystal lattice, each Me₄N⁺ cation