The Rh—Rh distance is significantly affected by the carboxylato groups. In the title complex, it is intermediate between the Rh—Rh distance in complexes with four carboxylato bridges, 2·38 Å in $Rh_2(HCOO)_4.2H_2O$ (Shustorovich *et al.*, 1975) or 2·386 (3) Å in $Rh_2(CH_3COO)_4(H_2O)_2$ (Cotton, De Boer, La Prade, Pipal & Ucko, 1970) and the analogous distance in complexes which contain no carboxylato bridging groups, *e.g.* 2·936 (2) Å in $Rh_2(dmg)_4(PPh_3)_2C_3H_7OH.H_2O$ (Caulton & Cotton, 1971).

The Rh—O distance in $Rh_2Cl_2(HCOO)_2(phen)_2$ is about 0·04 Å longer than the Rh—O distance in the tetraformato complex (2·03 Å) (Shustorovich *et al.*, 1975) and in $Rh_2Cl_2(HCOO)_2(dipy)_2.4H_2O$ [2·033 (4) Å (Głowiak, Pasternak & Pruchnik, 1984); 2·039 (9), 2·049 (8) Å (Sokol, Porai-Koshits, Kochetkova & Svieshnikova, 1984)]. It is most probable that elongation of the Rh—O bond in the phenanthroline complex results from steric interactions of the dinitrogen ligands, since the *trans* effect of dipyridyl and phenanthroline is practically the same.

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The Structure of $Ni(cyclam)(ClO_4)_2$

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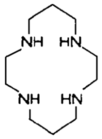
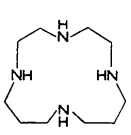
Abstract. Perchlorato(1,4,8,11-tetraazacyclotetradecane)nickel(II) perchlorate, $[Ni(ClO_4)(C_{10}H_{24}N_4)]ClO_4$, $M_r = 457·9$, monoclinic, $P2_1/n$, $a = 9·596$ (2), $b = 13·887$ (6), $c = 13·137$ (3) Å, $\beta = 90·78$ (2)°, $V = 1750·5$ Å^3, $Z = 4$, D_m not determined, $D_x = 1·74$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·7093 Å, μ(Mo $K\alpha$) = 1·47 mm^{-1}, $F(000) = 952$, $R(F) = 0·075$ for 1367 reflections at $T = 158$ K. Known unsubstituted cyclam/isocyclam complexes of Ni^{II} fall into two groups. In the former, the coordination is that of isolated octahedra; these complexes are mauve and paramagnetic. In the latter group (including the present complex) the axially disposed anions are shared between octahedra. These complexes are orange and diamagnetic.

Introduction. Several N_4 macrocycles are known which will act as ligands for transition-metal ions. Crystal structures are known for a number of complexes of one such, 1,4,8,11-tetraazacyclotetradecane (cyclam), (I). Similar complexes are known for isocyclam, 1,4,7,11-tetraazacyclotetradecane, (II). (The structures of many transition-metal complexes with substituted and partially reduced cyclams are also known.)



(I)



(II)

The present structure analysis brings to five the number of unsubstituted cyclam/isocyclam complexes

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of known structure. As detailed in the *Discussion* below, these can be grouped into two classes according to whether the complex consists of isolated octahedra or of octahedra sharing common axial anions.

Experimental. The crystal structure was initially solved at room temperature. It was found that the cyclam ligand and one of the ClO_4^- ions were disordered. Therefore the intensity data were recollected at 158 K, but this did not result in any significant improvement.

An orange crystal, 0·25 × 0·3 × 0·3 mm, of the title compound was used to collect X-ray diffraction data on an automated Picker four-circle diffractometer with graphite-monochromated Mo *Kα* radiation in θ–2θ scan mode with profile analysis (Grant & Gabe, 1978) up to $2\theta_{\max} = 45°$. Intensities were corrected for Lp and measured direct-beam polarization (Le Page, Gabe & Calvert, 1979) but not for absorption.

A total of 2842 reflections (max $h, k, l = 10,14,14$) was measured giving 2296 unique reflections ($R_{\rm int} = 0{\cdot}02$) of which 1367 were significant [$I > 2{\cdot}5\sigma(I)$]. Cell parameters were obtained from least-squares refinement of 36 reflections ($35 < 2\theta < 45°$).

The nickel and two chlorine positions* were located, using the room-temperature intensity data, from the Patterson map, the remaining atoms from F and ΔF syntheses. The cyclam macrocycle exhibits rotational disorder similar to that found in the Ni$^{\rm II}$(isocyclam)-$(ClO_4)_2$ structure (Boeyens, 1983). Also one of the ClO_4^- anions was extensively disordered. Two positions for each of the four N atoms were found. Six of the carbon atoms in one orientation of the cyclam macrocycle lay extremely close to those in the other orientation {[C(1),C(10′)], [C(3),C(2′)], [C(5),C(3′)], [C(6),C(5′)], [C(8),C(7′)] and [C(10),C(8′)]; see Fig. 1}. These atoms were resolved by the best-molecular-fitting program *BMFIT* (Yuen & Nyburg, 1979) using the geometry of the cyclam macrocycle found in the structure of Ni$^{\rm II}$(cyclam)$I_2.H_2O$ (Prasad & McAuley, 1983). The positions of the twelve above C atoms were kept fixed during refinement. Two positions were found for each of three perchlorate oxygen atoms [O(1), O(3), O(4)] of the four atoms attached to Cl(1) and given occupancy 0·5. The remaining oxygen atom, O(2), was given unit occupancy. (The derived geometry of this anion suggests the disorder may be more extensive than this.) The other perchlorate ion, centred on Cl(2), is not disordered. During isotropic refinement, the occupancy of the atoms in the rotationally disordered cyclam macrocycle was found to be 0·5. Attempts at full anisotropic refinement were not successful for many of the atoms in the cyclam rings; their refinement was thus restricted to be isotropic. All other non-hydrogen atoms were successfully refined with anisotropic temperature factors.

Table 1. *Fractional atomic coordinates, their e.s.d.'s and isotropic equivalent temperature factors,* $B_{\rm eq}$

Atoms without e.s.d.'s were fixed in position using *BMFIT* (Yuen & Nyburg, 1979). $B_{\rm eq}$ is the arithmetic mean of the principal axes of the thermal ellipsoid.

	x	*y*	*z*	$B_{\rm eq}$(Å^2)
Ni	0·25139 (14)	0·37831 (15)	0·71358 (11)	2·98 (7)
Cl(1)	0·2435 (3)	0·1357 (3)	0·86104 (25)	4·95 (18)
Cl(2)	0·3003 (3)	0·3705 (3)	0·20589 (24)	5·73 (20)
O(1)	0·2366 (14)	0·2052 (11)	0·9499 (10)	3·0 (8)
O(2)	0·3735 (10)	0·1273 (12)	0·8437 (10)	16·0 (11)
O(3)	0·1409 (16)	0·1485 (15)	0·7984 (13)	7·0 (12)
O(4)	0·2529 (21)	0·0482 (11)	0·9188 (12)	6·1 (11)
O(5)	0·4178 (8)	0·3765 (10)	0·1419 (5)	9·4 (7)
O(6)	0·1758 (7)	0·3778 (8)	0·1457 (6)	6·6 (6)
O(7)	0·3023 (9)	0·2816 (7)	0·2575 (7)	7·4 (6)
O(8)	0·3084 (10)	0·4464 (8)	0·2764 (8)	9·0 (7)
O(1′)	0·2135 (19)	0·2322 (12)	0·8790 (12)	6·1 (11)
O(3′)	0·2608 (23)	0·1373 (24)	0·7466 (12)	10·0 (15)
O(4′)	0·1507 (23)	0·0653 (15)	0·8765 (14)	10·5 (15)
N(1)	0·3932 (17)	0·3152 (12)	0·6351 (12)	2·7 (4)
N(2)	0·4090 (16)	0·4366 (12)	0·7913 (11)	2·0 (4)
N(3)	0·1109 (18)	0·4476 (13)	0·7905 (13)	3·0 (4)
N(4)	0·0964 (18)	0·3206 (13)	0·6379 (13)	3·2 (5)
C(1)	0·5263	0·3559	0·6568	1·6 (4)
C(2)	0·5311 (19)	0·3758 (19)	0·7705 (14)	2·8 (5)
C(3)	0·3946	0·4431	0·9054	2·8 (5)
C(4)	0·2667 (23)	0·5074 (16)	0·9292 (17)	2·9 (6)
C(5)	0·1347	0·4558	0·9068	2·1 (5)
C(6)	−0·0261	0·4045	0·7742	1·8 (5)
C(7)	−0·0320 (20)	0·3809 (21)	0·6592 (15)	3·4 (5)
C(8)	0·1056	0·3172	0·5256	5·0 (7)
C(9)	0·2353 (24)	0·2507 (17)	0·4989 (16)	3·2 (6)
C(10)	0·3655	0·3046	0·5242	3·2 (5)
N(1′)	0·4478 (16)	0·3987 (13)	0·7545 (12)	3·3 (4)
N(2′)	0·2088 (18)	0·4008 (14)	0·8603 (13)	4·1 (5)
N(3′)	0·0512 (16)	0·3566 (15)	0·6805 (12)	3·8 (5)
N(4′)	0·2955 (19)	0·3522 (15)	0·5722 (14)	5·1 (5)
C(1′)	0·4532 (21)	0·3927 (19)	0·8626 (16)	4·0 (6)
C(2′)	0·3347	0·4469	0·9070	2·6 (5)
C(3′)	0·0839	0·4672	0·8799	2·8 (5)
C(4′)	−0·0403 (24)	0·4102 (19)	0·8426 (18)	5·2 (7)
C(5′)	−0·0486	0·4268	0·7203	2·6 (5)
C(6′)	0·0442 (22)	0·3590 (20)	0·5734 (16)	4·3 (6)
C(7′)	0·1661	0·3072	0·5260	4·0 (6)
C(8′)	0·4169	0·2870	0·5532	5·7 (7)
C(9′)	0·5487 (24)	0·3392 (18)	0·5953 (17)	4·5 (7)
C(10′)	0·5494	0·3274	0·7127	4·4 (7)

Calculated H-atom positions with isotropic temperature factors were included in F calculations but were not refined. Refinement was by block-diagonal least squares with weights equal to $1/\sigma^2(F)$ based on counting statistics. $R(F) = 0{\cdot}075$, $wR(F) = 0{\cdot}047$. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Structural disorder was undoubtedly the reason why $R(F)$ did not fall below 0·075. The goodness of fit, S, was 5·3, the maximum ratio of least-squares shift to e.s.d. was 0·35, and the largest peak on the ΔF map was 0·8 e Å^{-3}. All calculations were made with the *NRC* system of programs (Larson & Gabe, 1978) on a Gould 32/9705 computer.

Atomic positional and equivalent isotropic temperature factors are listed in Table 1.*

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* Equivalent positions for $P2_1/n$: x,y,z; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}-x$, $\frac{1}{2}+y$, $\frac{1}{2}-z$; $\frac{1}{2}+x$, $\frac{1}{2}-y$, $\frac{1}{2}+z$.

* Lists of H-atom parameters, anisotropic thermal parameters and structure factors and stereoviews of the crystal packing have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43735 (20 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Discussion. The numbering of atoms in the Ni^{II}-(cyclam) moiety is given in Fig. 1. Bond lengths and bond angles are given in Table 2.

As stated in the *Introduction*, the five known Ni^{II}(unsubstituted-cyclam/isocyclam)X_2 complexes fall into two classes according to whether the structure contains isolated octahedra (cyclam with $X = Cl^-$, NO_3^-)* or whether one of the pair of X anions is interleaved in stacks of successive planar Ni^{II}(cyclam/isocyclam) moieties ($X = I^-$, ClO_4^-). Both the colours and the magnetic moments correlate with these two different modes of coordination (Table 3).

When the cyclam or isocyclam ring is substituted, Ni^{II} complexes of known structure are again either orange (low spin) or mauve (high spin). However, the orange complexes are commonly square-planar with no axial anions present, instead of having axial anions shared with adjacent octahedra. The mauve complexes, on the other hand, consist of isolated octahedra just as for the unsubstituted macrocycles.

The cyclam macrocycle can, in principle, have a number of configurations. In all four known complexes of Ni^{II} it has the centrosymmetric *trans* III form as classified by Bosnich, Poon & Tobe (1965). In the complexes where $X = Cl^-$, NO_3^-, I^-, the centrosymmetry is required crystallographically and Ni^{II} lies on the centre. It is thus exactly coplanar with the four coordinating N atoms. In the present complex ($X = ClO_4^-$), crystallographic centrosymmetry is not required, but when *BMFIT* (Yuen & Nyburg, 1979) is used to compare the ligand of the I^- complex with that of the present complex, the fit is extremely good. Thus the calculated displacement of Ni^{II} from the mean plane of the adjacent N atoms, 0·02 Å, is probably not significant.

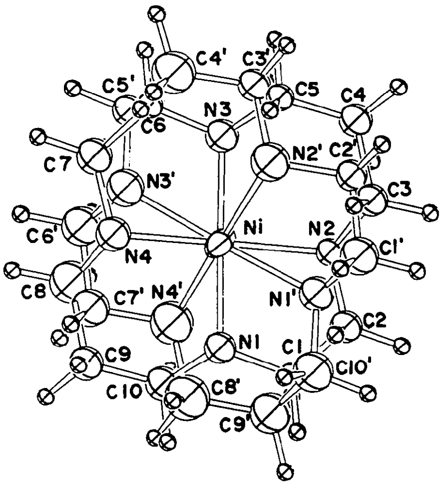

Fig. 1. *ORTEP* plot (Johnson, 1965) of Ni^{II} cyclam (unprimed) and its disordered image (primed). 50% probability spheres based on B_{eq} (B for H atoms set to 1·8 Å^2).

Table 2. *Bond lengths* (Å) *and angles* (°)

E.s.d.'s are not given where the position of either atom was kept fixed during refinement.

Ni–N(1)	1·93 (2)	Ni–N(1′)	1·97 (2)
Ni–N(2)	1·99 (2)	Ni–N(2′)	2·00 (2)
Ni–N(3)	1·95 (2)	Ni–N(3′)	1·99 (2)
Ni–N(4)	1·95 (2)	Ni–N(4′)	1·94 (2)
N(1)–C(1)	1·42	N(1′)–C(1′)	1·42 (3)
N(1)–C(10)	1·48	N(1′)–C(10′)	1·50
N(2)–C(2)	1·47	N(2′)–C(2′)	1·49
N(2)–C(3)	1·51	N(2′)–C(3′)	1·54
N(3)–C(5)	1·55	N(3′)–C(5′)	1·47
N(3)–C(6)	1·46	N(3′)–C(6′)	1·41 (3)
N(4)–C(7)	1·52 (3)	N(4′)–C(7′)	1·51
N(4)–C(8)	1·48	N(4′)–C(8′)	1·50
C(1)–C(2)	1·52	C(1′)–C(2′)	1·49
C(3)–C(4)	1·55	C(3′)–C(4′)	1·51
C(4)–C(5)	1·48	C(4′)–C(5′)	1·62
C(6)–C(7)	1·55	C(6′)–C(7′)	1·51
C(8)–C(9)	1·59	C(8′)–C(9′)	1·55
C(9)–C(10)	1·49	C(9′)–C(10′)	1·55
N(1)–Ni–N(2)	85·5 (7)	N(1′)–Ni–N(2′)	85·6 (7)
N(2)–Ni–N(3)	93·4 (7)	N(2′)–Ni–N(3′)	91·4 (7)
N(3)–Ni–N(4)	86·5 (7)	N(3′)–Ni–N(4′)	89·2 (7)
N(4)–Ni–N(1)	94·6 (7)	N(4′)–Ni–N(1′)	93·9 (7)
Ni–N(1)–C(1)	110·6	Ni–N(1′)–C(1′)	106·6 (1·2)
Ni–N(1)–C(10)	116·8	Ni–N(1′)–C(10′)	115·4 (1·0)
C(1)–N(1)–C(10)	112·6	C(1′)–N(1′)–C(10′)	108·1
Ni–N(2)–C(2)	105·9 (1·2)	Ni–N(2′)–C(2′)	106·7
Ni–N(2)–C(3)	117·1	Ni–N(2′)–C(3′)	115·2
C(2)–N(2)–C(3)	107·6	C(2′)–N(2′)–C(3′)	107·6
Ni–N(3)–C(5)	117·0	Ni–N(3′)–C(5′)	117·1
Ni–N(3)–C(6)	110·4	Ni–N(3′)–C(6′)	104·3
C(5)–N(3)–C(6)	107·3	C(5′)–N(3′)–C(6′)	108·5
Ni–N(4)–C(7)	107·1 (1·2)	Ni–N(4′)–C(7′)	105·8
Ni–N(4)–C(8)	117·8	Ni–N(4′)–C(8′)	116·9
C(7)–N(4)–C(8)	105·1	C(7′)–N(4′)–C(8′)	108·6
N(1)–C(1)–C(2)	106·5	N(1′)–C(1′)–C(2′)	110·1
C(1)–C(2)–N(2)	105·8	C(1′)–C(2′)–N(2′)	103·9
N(2)–C(3)–C(4)	108·5	N(2′)–C(3′)–C(4′)	104·2
C(3)–C(4)–C(5)	111·0	C(3′)–C(4′)–C(5′)	106·0
C(4)–C(5)–N(3)	110·3	C(4′)–C(5′)–N(3′)	103·6
N(3)–C(6)–C(7)	104·6	N(3′)–C(6′)–C(7′)	111·9
C(6)–C(7)–N(4)	106·2	C(6′)–C(7′)–N(4′)	105·9
N(4)–C(8)–C(9)	107·2	N(4′)–C(8′)–C(9′)	106·8
C(8)–C(9)–C(10)	108·4	C(8′)–C(9′)–C(10′)	107·2
C(9)–C(10)–N(1)	114·0	C(9′)–C(10′)–N(1′)	107·5

Table 3. *The two types of* Ni^{II} *cyclam/isocyclam complex*

	Isolated octahedra		Octahedra with shared X anions		
	(cyclam)-Cl_2	(cyclam)-$(NO_3)_2$	(cyclam)-I_2	(cyclam)-$(ClO_4)_2$	(isocyclam)-$(ClO_4)_2$
Colour	mauve[a]	mauve[a]	brown[a]	orange[a]	orange[b]
Magnetic moment, BM at 293 K[a]	3·09	3·06	diam.	diam.	?
Ni–N (Å)	2·066 (3),[c] 2·050 (3)	2·060 (6),[d] 2·050 (5)	1·94 (1),[e] 1·96 (1)	1·93 (2), 1·99 (2), 1·95 (2), 1·95 (2), 1·97 (2), 2·00 (2), 1·99 (2), 1·94 (2)	2·00, 1·99, 1·97[f]

References: (*a*) Bosnich, Tobe & Webb (1965); (*b*) Sabatini & Fabbrizzi (1979); (*c*) Bosnich, Mason, Pauling, Robertson & Tobe (1965); (*d*) Thöm, Fox, Boeyens & Hancock (1984); (*e*) Prasad & McAuley (1983); (*f*) Boeyens (1983).

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* Atomic coordinates for the Cl^- complex have not been published but, from the space group and number of molecules per unit cell, the coordination can only be that of isolated octahedra.

Isocyclam (II) cannot have a centrosymmetric configuration. In the Ni^{II} perchlorate complex it has a mirror plane of symmetry through the appropriate N atoms. In this case, Ni^{II} is significantly (0·30 Å) out of the plane of the coordinating N atoms.

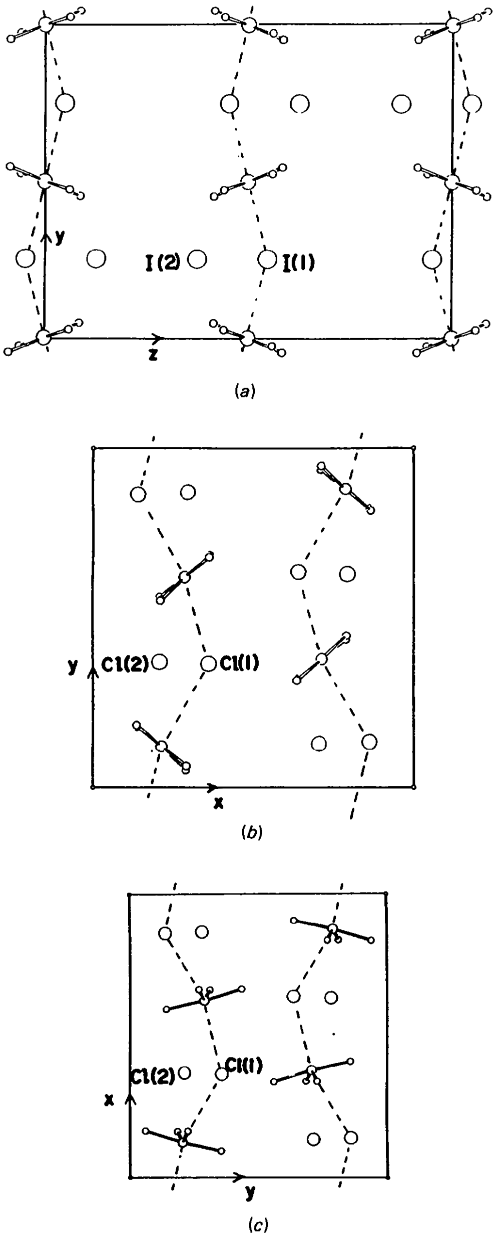

Fig. 2. Crystallographic axial projections of complexes showing only Ni^{II} ions, the four coordinated nitrogen atoms and X^- (either I$^-$, or Cl of ClO$_4^-$): (*a*) cyclam I (Prasad & McAuley, 1983); (*b*) cyclam ClO$_4$ (title compound); (*c*) isocyclam ClO$_4$ (Boeyens, 1983). The Ni$\cdots X \cdots$Ni angles are: (*a*) 151·1, (*b*) 131·4, (*c*) 136·7°.

The nature of the shared axial octahedral coordination is shown by suitable projections of the three diamagnetic complexes, Fig. 2.* It is seen from Fig. 2 that the packing is remarkably similar in all three diamagnetic complexes. In no case is the Ni$\cdots X \cdots$Ni chain linear. (The angles subtended at X are given in Fig. 2. Presumably this angle is not stereochemically significant, merely a consequence of packing requirements.)

The Ni^{II}—N distances found in these complexes are given in Table 3. Those with ioslated octahedra seem to have slightly, but possibly significantly, longer distances than those where X^- is shared between adjacent octahedra. The 'best-fit' distance is calculated as 2·07 Å by Martin, De Hayes, Zompa & Busch (1974) and a value of 2·05 Å is obtained from molecular-mechanics calculations (Thöm, Fox, Boeyens & Hancock, 1984).

Several of the structurally known cyclam/isocyclam complexes exhibit disorder. In the present complex, the ligand itself shows orientational disorder about the nickel ion as it does in the isocyclam perchlorate complex. In both complexes the interleaving perchlorate ions also show orientational disorder. In the isocyclam complex the atomic positions were obtained from rigid-body refinement; in the present case by partially constrained refinement.

In all these Ni^{II} complexes, whether they contain isolated octahedra or not, the proximity of the X^- counterion *cis* to the N donor atoms is governed by the H atoms of the macrocycle which protrude either side of the mean plane. Thus these Ni$^{II}\cdots X^-$ distances are without stereochemical significance. In the present cyclam perchlorate complex, the Cl atom of the disordered, shared ClO$_4^-$ ions does not sit at the centroid of the protruding H atoms of the two adjacent ligands. On one side the shortest Cl$\cdots$H distances are bunched around 3·65 Å, but on the other there are two significantly shorter distances involving Cl(1) at $(\frac{1}{2}-x, \frac{1}{2}+y, 1\frac{1}{2}-z)$: Cl(1)$\cdots$H(N3), 2·86 Å, Cl(1)$\cdots$H(N2), 3·09 Å.

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* Stereoviews of the packing have been deposited.

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Coordination Chemistry of Alkali and Alkaline Earth Cations: the Structure of Bis(3,5-dinitrobenzoato)(tetraethyleneglycol)strontium(II) Monohydrate

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Abstract. μ-(3,5-Dinitrobenzoato-*O*,μ-*O'*)-{2,2'-[oxybis(ethyleneoxy)]diethanol}strontium(II) 3,5-dinitrobenzoate monohydrate, $[Sr(C_7H_3N_2O_6)(C_8H_{18}O_5)]$-$(C_7H_3N_2O_6).H_2O$, $M_r = 722{\cdot}08$, triclinic, $P\bar{1}$, $a = 9{\cdot}070\,(1)$, $b = 13{\cdot}067\,(1)$, $c = 13{\cdot}716\,(1)$ Å, $\alpha = 110{\cdot}74\,(1)$, $\beta = 103{\cdot}91\,(1)$, $\gamma = 95{\cdot}83\,(1)°$, $V = 1441{\cdot}0\,(2)$ Å^3, $Z = 2$, $D_x = 1{\cdot}664$ g cm^{-3}, $\lambda(\mathrm{Cu}\ K\alpha) = 1{\cdot}54184$ Å, $\mu = 36{\cdot}60$ cm^{-1}, $F(000) = 736$, $T = 295$ K, $R = 0{\cdot}052$ for 4605 observed reflections. Sr is coordinated to all five O atoms of tetraethyleneglycol (TEG), to water and both O atoms of the carboxyl group of one dinitrobenzoate (DNB1) and one O atom of the carboxyl group of a centrosymmetrically related DNB1. The centrosymmetrically related Sr atoms are separated by a short distance of 4·401 (1) Å, which results in a closely packed cluster. The terminal OH groups of TEG form hydrogen bonds with the O atoms of the carboxyl group of the second dinitrobenzoate residue (DNB2), which is charge separated from Sr. The water molecule is hydrogen bonded to a terminal O atom of TEG and an O atom of the carboxyl group of DNB2 and thus serves as a link between the Sr clusters. Two neighbouring C—C bonds at one terminal end of TEG are disordered over two positions with site occupation factors of 0·64, 0·36 for one bond and 0·55, 0·45 for the other.

Introduction. With the aim of understanding the intriguing chemical preferences of Na, K, Mg and Ca atoms in natural systems (Williams, 1970), we have undertaken broad-based chemical and crystallographic investigations on alkali and alkaline earth cations in general (Poonia, 1981). With a view to studying interactive differences between seemingly alike cations such as Na and K, and Mg and Ca, we investigated a series of cations in common or comparable environments with regard to charge neutralizer and ligand (Venkatasubramanian, Poonia, Clinger, Ernst & Hackert, 1984). The ligands included cyclic multidentates such as benzo-15-crown-5 (Poonia, Bagdi & Sidhu, 1986) and the double-action acyclic multidentates such as triethanolamine (TEA) and tetraethyleneglycol (TEG) (Poonia & Bajaj, 1979). The charge neutralizers found to be most suitable are 2,4,6-trinitrophenolate (PIC) and 3,5-dinitrobenzoate (DNB). The double-action ligands offer the advantage of stabilizing (bridging) the anion in addition to coordinating with the counter cation so that similar cations can be investigated under a diminished (or lifted) anion effect, especially the trio Ca, Sr and Ba for which within-the-group discrimination is most ticklish. For TEG the systems $M(\mathrm{PIC})_2(\mathrm{TEG})(\mathrm{TEC})$ and $M(\mathrm{DNB})_2(\mathrm{TEG})$ have been selected and the present paper reports the structural aspects of $\mathrm{Sr(DNB)_2(TEG).H_2O}$.

Experimental. Crystals obtained from the Chemistry Department, University of Indore, India. Rod-shaped yellowish crystal, 0·2 × 0·3 × 0·4 mm. Enraf–Nonius

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