Grant, D. F. & Gabe, E. J. (1978). *J. Appl. Cryst.* **11**, 114–120.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht).

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

Larson, A. C. & Gabe, E. J. (1978). *Computing in Crystallography*, edited by H. Schenk, R. Olthof-Hazekamp, H. van Koningsveld & G. C. Bassi, p. 81. Delft Univ. Press.

Le Page, Y., Gabe, E. J. & Calvert, L. D. (1979). *J. Appl. Cryst.* **12**, 25–26.

Martin, L. Y., De Hayes, L. J., Zompa, L. J. & Busch, D. H. (1974). *J. Am. Chem. Soc.* **96**, 4046–4048.

Prasad, L. & McAuley, A. (1983). *Acta Cryst.* C**39**, 1175–1177.

Sabatini, L. & Fabbrizzi, L. (1979). *Inorg. Chem.* **18**, 438–444.

Thöm, V. J., Fox, C. C., Boeyens, J. C. A. & Hancock, R. D. (1984). *J. Am. Chem. Soc.* **106**, 5947–5955.

Yuen, P. & Nyburg, S. C. (1979). *J. Appl. Cryst.* **12**, 258.

Acta Cryst. (1987). C**43**, 1042–1045

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

By J. A. Kanters and S. Harder

Laboratorium voor Kristal- en Structuurchemie, University of Utrecht, Padualaan 8, 3508 *TB, Utrecht, The Netherlands*

and N. S. Poonia

Department of Chemistry, Guru Nanak Dev University, Amritsar, 143005 *India*

(*Received* 9 *September* 1986; *accepted* 9 *December* 1986)

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}, λ(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 $M(PIC)_2(TEG)(TEC)$ and $M(DNB)_2(TEG)$ have been selected and the present paper reports the structural aspects of $Sr(DNB)_2(TEG).H_2O$.

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

0108-2701/87/061042-04$01.50

CAD-4 diffractometer. Cell constants from least-squares fit of the setting angles of 24 reflections with θ range 10·0–16·0°. ω–2θ scan, 2θ(max.) = 140°, $\omega = (0{\cdot}60 + 0{\cdot}35\tan\theta)°$, Ni-filtered Cu $K\alpha$ radiation. One half of the reflection sphere, index range $-10 \le h \le 11$, $0 \le k \le 15$, $-16 \le l \le 15$; 5434 reflections measured, all unique, 4605 considered observed $[I > 2{\cdot}5\sigma(I)]$. Two standard reflections ($\bar{1}24$: r.m.s.d 1·07% and $\bar{1}23$: r.m.s.d. 1·08%), measured every 60 reflections. Corrections for Lorentz–polarization effects and linear decay (1·9%). The structure was solved by standard Patterson and Fourier methods. An absorption correction following the *DIFABS* procedure (Walker & Stuart, 1983) was applied on isotropically refined data, min. and max. correction factors being 0·80 (1) and 1·40 (4) on F, respectively. Anisotropic refinement revealed two very short C—C distances (1·34 and 1·30 Å) with nearly eclipsed O—C—C—O torsion angles in the tetraethyleneglycol (TEG) chain and very large U components of the temperature tensor indicating disorder of the two C—C bonds. During subsequent refinement the bond lengths and non-bonded C···O distances involving these C atoms, which were assigned isotropic U values, were restrained to realistic values [C—C 1·520 (5), C—O 1·440 (5) and C···O 2·41 (1) Å] and the site occupation factors (s.o.f.'s) of the C atoms were fixed at 0·70. After refinement difference maps yielded one satellite peak near each of the four disordered C atoms. Because of the satisfactory geometry (C—C and C—O distances and O—C—C—O torsion angles) these peaks were considered as disordered C-atom positions which were refined with the same restraints as above. The occupation factors of the C atoms of the disordered C—C bonds converged to 0·64 for C(311)–C(321) and 0·55 for C(331)–C(341). H atoms of the 3,5-dinitrobenzoate (DNB) molecules and those of the terminal OH groups of TEG were found in the difference maps and included in the refinement. H atoms of TEG were placed at calculated C(sp^3) positions (C—H 1·08 Å) taking into account the occupation factors of the disordered C atoms and refined riding on their carrier atoms. The thermal parameters of all H atoms were fixed at 0·06 Å^2. The refinement on F with 83 atoms and 439 parameters converged to $R(F) = 0{\cdot}052$, $R(wF) = 0{\cdot}054$ with $w = 1/\sigma^2(F)$ and $S = 1{\cdot}19$. The average shift to e.s.d. ratio (Δ/σ) is 0·121 with a max. of 0·893; max. and min. electron densities are 0·65 and −0·87 e Å^{-3}, respectively. Scattering factors from Cromer & Mann (1968). Anomalous-dispersion correction from Cromer & Liberman (1970). Calculations were performed with *SHELX76* (structure determination and refinement) (Sheldrick, 1976), *DIFABS* (absorption correction) (Walker & Stuart, 1983) and *EUCLID* (illustrations and molecular geometry) (Spek, 1982) on the Cyber 180—855 of the University of Utrecht.

Discussion. Fractional atomic coordinates and (equivalent) isotropic thermal parameters are listed in Table 1, selected bond distances, bond angles and torsion angles in Table 2, the strontium coordination in Table 3 and the hydrogen bonds in Table 4. The systematic numbering of the dinitrobenzoates (DNB) and the disordered tetraethyleneglycol (TEG) molecule is shown in Fig. 1.*

Table 1. *Fractional coordinates for the non-*H *atoms with their equivalent isotropic thermal parameters* (Å^2)

	x	y	z	U_{eq}*
Sr	0·04622 (4)	−0·09813 (3)	0·10136 (3)	0·0411 (1)
C(11)	−0·2921 (5)	−0·2682 (3)	−0·2279 (3)	0·042 (1)
C(12)	−0·3238 (5)	−0·3831 (4)	−0·2573 (3)	0·046 (2)
C(13)	−0·4587 (5)	−0·4465 (3)	−0·3382 (3)	0·045 (2)
C(14)	−0·5653 (5)	−0·4005 (4)	−0·3904 (3)	0·047 (1)
C(15)	−0·5286 (5)	−0·2869 (4)	−0·3594 (3)	0·047 (1)
C(16)	−0·3959 (5)	−0·2189 (3)	−0·2789 (3)	0·045 (1)
C(17)	−0·1443 (5)	−0·1994 (4)	−0·1380 (3)	0·049 (2)
N(11)	−0·4883 (5)	−0·5686 (3)	−0·3721 (3)	0·057 (1)
N(12)	−0·6360 (4)	−0·2333 (3)	−0·4172 (3)	0·067 (1)
O(11)	−0·1132 (3)	−0·0961 (2)	−0·1151 (2)	0·098 (2)
O(12)	−0·0642 (4)	−0·2496 (3)	−0·0916 (2)	0·072 (1)
O(13)	−0·3899 (5)	−0·6082 (3)	−0·3302 (4)	0·122 (2)
O(14)	−0·6097 (4)	−0·6242 (3)	−0·4411 (3)	0·081 (1)
O(15)	−0·7643 (4)	−0·2890 (3)	−0·4721 (4)	0·059 (1)
O(16)	−0·5920 (4)	−0·1387 (3)	−0·4051 (3)	0·065 (2)
C(21)	−0·6513 (4)	−0·3979 (4)	−0·1416 (3)	0·041 (1)
C(22)	−0·6625 (5)	−0·5133 (4)	−0·1758 (3)	0·046 (1)
C(23)	−0·7854 (5)	−0·5831 (4)	−0·2649 (4)	0·049 (2)
C(24)	−0·8985 (5)	−0·5434 (4)	−0·3199 (4)	0·050 (1)
C(25)	−0·8836 (5)	−0·4294 (4)	−0·2834 (3)	0·046 (1)
C(26)	−0·7636 (5)	−0·3555 (4)	−0·1950 (3)	0·045 (1)
C(27)	−0·5100 (5)	−0·3180 (4)	−0·0504 (3)	0·048 (1)
N(21)	−0·7953 (5)	−0·7046 (4)	−0·3058 (3)	0·057 (1)
N(22)	−0·9978 (5)	−0·3844 (4)	−0·3441 (3)	0·068 (1)
O(21)	−0·5073 (3)	−0·2155 (3)	−0·0243 (3)	0·079 (1)
O(22)	−0·4068 (3)	−0·3621 (3)	−0·0133 (3)	0·084 (1)
O(23)	−0·6808 (4)	−0·7372 (3)	−0·2738 (3)	0·104 (2)
O(24)	−0·9173 (5)	−0·7648 (3)	−0·3701 (3)	0·099 (2)
O(25)	−1·1088 (4)	−0·4498 (3)	−0·4156 (3)	0·062 (2)
O(26)	−0·9785 (5)	−0·2857 (4)	−0·3195 (3)	0·063 (1)
C(35)	0·3475 (6)	−0·1217 (6)	0·3180 (5)	0·098 (3)
C(36)	0·3523 (6)	−0·2005 (5)	0·2111 (5)	0·084 (3)
C(37)	0·1218 (5)	−0·3409 (4)	0·1479 (4)	0·064 (2)
C(38)	−0·0408 (5)	−0·3698 (4)	0·0737 (4)	0·055 (2)
O(31)	−0·2461 (3)	−0·0671 (3)	0·0819 (2)	0·053 (1)
O(32)	−0·0224 (3)	0·0045 (3)	0·2820 (2)	0·066 (1)
O(33)	0·2660 (4)	−0·0406 (3)	0·2984 (3)	0·082 (1)
O(34)	0·2016 (3)	−0·2471 (3)	0·1364 (3)	0·065 (1)
O(35)	−0·1101 (3)	−0·2755 (3)	0·1112 (3)	0·053 (1)
O(4)	0·2899 (4)	−0·0743 (3)	0·0407 (3)	0·066 (2)
Disordered atoms with occupation 0·64				
C(311)	−0·2707 (8)	0·0127 (6)	0·1776 (3)	0·064 (2)
C(321)	−0·1826 (5)	−0·0047 (8)	0·2770 (5)	0·070 (3)
Disordered atoms with occupation 0·55				
C(331)	0·1073 (7)	0·0755 (6)	0·3755 (6)	0·076 (3)
C(341)	0·2204 (9)	0·0016 (9)	0·3958 (4)	0·081 (4)
Disordered atoms with occupation 0·36				
C(312)	−0·2868 (8)	−0·035 (1)	0·1827 (4)	0·060 (4)
C(322)	−0·1542 (9)	0·0543 (9)	0·2724 (8)	0·073 (5)
Disordered atoms with occupation 0·45				
C(332)	0·0723 (7)	0·018 (1)	0·3872 (5)	0·072 (4)
C(342)	0·2392 (8)	0·0476 (8)	0·3880 (6)	0·075 (4)

* $U_{eq} = \frac{1}{3}\{\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j\}$.

---

* Lists of structure factors, anisotropic thermal parameters, coordinates of H atoms and bond lengths, angles and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43631 (31 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Selected bond distances* (Å), *angles* (°), *and torsional angles* (°)

O(11)–C(17)	1·257 (6)	O(21)–C(27)	1·254 (7)	O(31)–C(311)	1·442 (6)
O(12)–C(17)	1·238 (6)	O(22)–C(27)	1·247 (6)	O(32)–C(321)	1·429 (6)
O(13)–N(11)	1·205 (6)	O(23)–N(21)	1·207 (6)	O(32)–C(331)	1·449 (8)
O(14)–N(11)	1·219 (6)	O(24)–N(21)	1·218 (6)	O(33)–C(341)	1·432 (7)
O(15)–N(12)	1·212 (6)	O(25)–N(22)	1·209 (6)	O(33)–C(35)	1·417 (9)
O(16)–N(12)	1·199 (6)	O(26)–N(22)	1·194 (8)	O(34)–C(36)	1·416 (7)
N(11)–C(13)	1·470 (6)	N(21)–C(23)	1·469 (8)	O(34)–C(37)	1·436 (7)
N(12)–C(15)	1·493 (6)	N(22)–C(25)	1·472 (7)	O(35)–C(38)	1·429 (6)
C(11)–C(17)	1·517 (6)	C(21)–C(27)	1·526 (6)	O(31)–C(312)	1·446 (6)
				O(32)–C(322)	1·42 (1)
				O(32)–C(332)	1·430 (7)
				O(33)–C(342)	1·447 (9)
				C(311)–C(321)	1·511 (9)
				C(331)–C(341)	1·52 (1)
				C(312)–C(322)	1·52 (1)
				C(332)–C(342)	1·52 (1)
				C(35)–C(36)	1·477 (9)
				C(37)–C(38)	1·499 (7)

Ring	⟨C–C⟩	⟨C–C–C⟩
DNB1	1·380 (6)	120 (3)
DNB2	1·384 (7)	120 (2)

O(11)–C(17)–C(11)	118·0 (4)	O(21)–C(27)–C(21)	116·6 (4)
O(11)–C(17)–O(12)	124·9 (4)	O(21)–C(27)–O(22)	127·2 (4)
O(12)–C(17)–C(11)	117·1 (4)	O(22)–C(27)–C(21)	116·2 (5)
O(13)–N(11)–C(13)	117·8 (4)	O(23)–N(21)–C(23)	117·3 (4)
O(13)–N(11)–O(14)	123·6 (5)	O(23)–N(21)–O(24)	124·9 (5)
O(14)–N(11)–C(13)	118·6 (4)	O(24)–N(21)–C(23)	117·9 (5)
O(15)–N(12)–C(15)	116·8 (4)	O(25)–N(22)–O(26)	123·1 (5)
O(15)–N(12)–O(16)	124·5 (4)	O(25)–N(22)–C(25)	117·9 (5)
O(16)–N(12)–C(15)	118·7 (4)	O(26)–N(22)–C(25)	118·9 (4)
C(12)–C(11)–C(17)	118·4 (4)	C(22)–C(21)–C(27)	120·1 (4)
C(16)–C(11)–C(17)	121·6 (4)	C(26)–C(21)–C(27)	119·7 (5)
N(11)–C(13)–C(14)	118·5 (4)	N(21)–C(23)–C(24)	117·8 (4)
N(11)–C(13)–C(12)	118·7 (4)	N(21)–C(23)–C(22)	119·5 (4)
N(12)–C(15)–C(14)	118·5 (4)	N(22)–C(25)–C(24)	118·2 (4)
N(12)–C(15)–C(16)	117·8 (4)	N(22)–C(25)–C(26)	118·8 (5)
O(31)–C(311)–C(321)	109·0 (6)	C(36)–O(34)–C(37)	113·8 (4)
O(32)–C(321)–C(311)	109·2 (5)	O(34)–C(37)–C(38)	106·6 (4)
C(321)–O(32)–C(331)	125·9 (4)	O(35)–C(38)–C(37)	107·4 (4)
O(32)–C(331)–C(341)	106·8 (6)	O(31)–C(312)–C(322)	108·4 (7)
O(33)–C(341)–C(331)	105·5 (6)	O(32)–C(322)–C(312)	106·6 (8)
C(35)–O(33)–C(341)	100·8 (5)	C(322)–O(32)–C(332)	120·2 (5)
O(33)–C(35)–C(36)	107·1 (5)	O(32)–C(332)–C(342)	106·0 (6)
O(34)–C(36)–C(35)	111·6 (5)	O(33)–C(342)–C(332)	108·4 (7)
		C(342)–O(33)–C(35)	120·3 (5)

O(13)–N(11)–C(13)–C(12)	−2·7 (6)	O(23)–N(21)–C(23)–C(22)	−14·2 (7)
O(16)–N(12)–C(15)–C(14)	−166·5 (4)	O(26)–N(22)–C(25)–C(24)	−173·3 (5)
C(12)–C(11)–C(17)–O(11)	177·0 (4)	C(22)–C(21)–C(27)–O(21)	179·6 (4)

C(331)–O(32)–C(321)–C(311)	128·0 (6)	O(31)–C(311)–C(321)–O(32)	56·5 (8)
C(321)–O(32)–C(331)–C(341)	128·6 (7)	O(31)–C(312)–C(322)–O(32)	−62 (1)
C(35)–O(33)–C(341)–C(331)	−170·3 (6)	O(32)–C(331)–C(341)–O(33)	60·8 (8)
C(341)–O(33)–C(35)–C(36)	159·5 (6)	O(32)–C(332)–C(342)–O(33)	−57 (1)
C(37)–O(34)–C(36)–C(35)	−82·9 (6)	O(33)–C(35)–C(36)–O(34)	−55·3 (7)
C(36)–O(34)–C(37)–C(38)	172·8 (4)	O(34)–C(37)–C(38)–O(35)	−62·4 (5)
C(332)–O(32)–C(322)–C(312)	−133·3 (8)		
C(322)–O(32)–C(332)–C(342)	−134·1 (8)		
C(35)–O(33)–C(342)–C(332)	−102·1 (8)		

Table 3. *Strontium coordination* (*distances in* Å)

Sr···O(31)	2·687 (3)	Sr···O(11)	2·984 (3)
Sr···O(32)	2·623 (3)	Sr···O(12)	2·557 (3)
Sr···O(33)	2·740 (4)	Sr···O(11^{i})	2·478 (3)
Sr···O(34)	2·627 (4)	Sr···O(4)	2·569 (4)
Sr···O(35)	2·654 (4)		

Symmetry code: (i) $-x, -y, -z$.

Table 4. *Hydrogen bonds*

	O–H (Å)	O···O (Å)	O–H···O (°)
O(31)–H···O(21)	0·84 (5)	2·627 (5)	172 (5)
O(35)–H···O(22)	0·63 (5)	2·691 (5)	163 (8)
O(4)–H···O(31^{i})	0·90 (5)	2·903 (5)	174 (4)
O(4)–H···O(21^{ii})	0·74 (5)	2·810 (5)	161 (5)

Symmetry code: (i) $-x, -y, -z$; (ii) $x + 1, y, z$.

Of the two DNB residues in the asymmetric unit, only DNB1 is coordinated to Sr^{2+}; DNB2 is involved in hydrogen bonding. The cation is coordinated to nine O atoms, five of TEG, two of the carboxyl group of DNB1, one of the carboxyl group of DNB1 related by the centre of inversion and one of water. As the symmetry-related Sr^{2+} cations have a short separation [4·401 (1) Å] this coordination pattern gives rise to a tightly packed centrosymmetric cluster (Fig. 2). The TEG residues are on opposite sides of the Sr atom and the same holds for the DNB1 residues which are triply coordinated to the Sr^{2+} ions.

The terminal OH groups of TEG are hydrogen-bond donors to O(21) and O(22) of the carboxyl group of DNB2. The water molecule donates one hydrogen bond to the terminal O(31) of TEG at $-x, -y, -z$ and one to O(21) of DNB2 at $1 + x, y, z$. As this last water–DNB2 hydrogen bond connects a DNB2–TEG hydrogen-bonded dimer of which the TEG residue belongs to a coordination cluster at $1 + x, y, z$, the water molecule serves as a link between the centrosymmetric clusters *via* the non-coordinated DNB2. This results in a one-dimensional cluster chain in the direction of the *a*

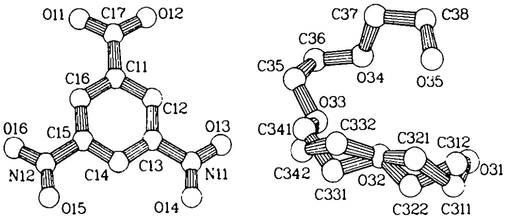

Fig. 1. Atom numbering of dinitrobenzoate (DNB) and tetraethyleneglycol (TEG), and a perspective view of the disorder of TEG. DNB1 has first digit 1 in the numbering, DNB2 has first digit 2. Atoms C(31), C(32), C(33), C(34) of TEG are disordered. Atoms C(311), C(321), C(331), C(341) have the higher s.o.f.'s, atoms C(312), C(322), C(332), C(342) the lower s.o.f.'s.

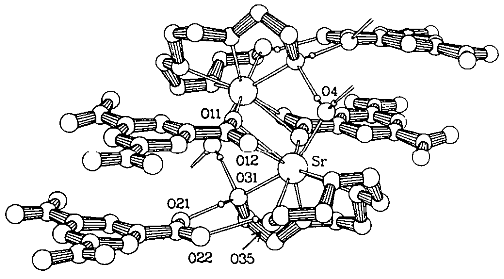

Fig. 2. Perspective view, approximately along [010], of the centrosymmetric strontium cluster showing metal coordination and hydrogen bonds. For the disordered tetraethyleneglycol only the C atoms with the higher s.o.f.'s are shown. All H atoms, except those of water and terminal OH groups of TEG, have been omitted for clarity.

axis. So DNB1 is coordinated to two centrosymmetrically related cations, while DNB2 is effectively charge separated by the TEG molecule which displays double action through its terminal hydroxyl groups in keeping DNB2 separated from its counter ion. A similar situation has been observed in $Ca(PIC)_2(TEG).H_2O$ (Singh, Reinhardt & Poonia, 1980) where TEG causes charge separation of one PIC anion.

Bond lengths and angles of the DNB's are normal; the phenyl rings are planar. The average deviations from planarity for DNB1 and DNB2 are 0·004 and 0·005 Å, respectively. The nitro groups of DNB1 are rotated with respect to the least-squares planes by 4·1 (6) and 13·7 (5)°. For DNB2 these values are 15·0 (5) and 6·8 (6)°. The carboxyl groups are almost coplanar with the phenyl rings with interplanar angles of 4·6 (5) and 8·1 (5)° for DNB1 and DNB2, respectively. The DNB's are nearly parallel [angle between least-squares planes 8·8 (2)°] and have the same orientation.

The TEG chain has an irregular form and is wrapped around the Sr ion resulting in a short O···O distance of 3·120(7) Å for the terminal O atoms. In the TEG chain the O atoms have *gauche* conformations with respect to the common C—C bonds. Two of these C—C bonds [C(31)—C(32) and C(33)—C(34)] are disordered over two positions (Fig. 1). This disordering represents a flip-flop model which has also been proposed for one of the C—C bonds of heptaethyleneglycol–$Sr(SCN)_2$ (Ohmoto, Kai, Yasuoka, Kasai, Yanagida & Okahara, 1979). The conformation with respect to the C—O bonds in the ordered part are either *gauche* or *anti*, in the disordered part some of these torsion angles deviate appreciably from the ideal values. The large deviation of C—C and C—O distances from their normal values observed in the complexes triethyleneglycol–$Nd(NO_3)_3$ (Hirashima, Tsutsiu & Shiokawa, 1982), tetraethyleneglycol–$Nd(NO_3)_3$ (Hirashima, Tsutsiu, Shiokawa, 1981), tetraethyleneglycol–$La(NO_3)_3$ (Casellato, Tomat, Di Bernardo & Graziani, 1982) and pentaethyleneglycol–$Nd(NO_3)_3$ (Hirashima, Kanetsuki, Shiokawa & Tanaka, 1981) are very probably caused by a similar type of disorder which illustrates the great flexibility of the polyethyleneglycol chain.

References

CASELLATO, U., TOMAT, G., DI BERNARDO, P. & GRAZIANI, R. (1982). *Inorg. Chim. Acta*, **61**, 181–187.

CROMER, D. T. & LIBERMAN, D. (1970). *J. Chem. Phys.* **53**, 1891–1898.

CROMER, D. T. & MANN, J. B. (1968). *Acta Cryst.* A**24**, 321–324.

HIRASHIMA, Y., KANETSUKI, K., SHIOKAWA, J. & TANAKA, N. (1981). *Bull. Chem. Soc. Jpn*, **54**, 1567–1568.

HIRASHIMA, Y., TSUTSIU, T. & SHIOKAWA, J. (1981). *Chem. Lett.* pp. 1501–1504.

HIRASHIMA, Y., TSUTSIU, T. & SHIOKAWA, J. (1982). *Chem. Lett.* pp. 1405–1408.

OHMOTO, H., KAI, Y., YASUOKA, N., KASAI, N., YANAGIDA, S. & OKAHARA, M. (1979). *Bull. Chem. Soc. Jpn*, **52**, 1209–1210.

POONIA, N. S. (1981). *Curr. Sci.* **50**, 881–886.

POONIA, N. S., BAGDI, P. & SIDHU, K. S. (1986). *J. Inclusion Phenom.* **4**, 43–54.

POONIA, N. S. & BAJAJ, A. V. (1979). *Chem. Rev.* **79**, 389–445.

SHELDRICK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.

SINGH, T. P., REINHARDT, R. & POONIA, N. S. (1980). *Inorg. Nucl. Chem. Lett.*, **16**, 293–296.

SPEK, A. L. (1982). The *EUCLID* package. In *Computational Crystallography*, edited by D. SAYRE, p. 528. Oxford: Clarendon Press.

VENKATASUBRAMANIAN, K., POONIA, N. S., CLINGER, R., ERNST, S. R. & HACKERT, M. L. (1984). *J. Inclusion Phenom.* **1**, 319–327.

WALKER, N. & STUART, D. (1983). *Acta Cryst.* A**39**, 158–166.

WILLIAMS, R. J. S. (1970). *Q. Rev. Chem. Soc.* **24**, 331–365.

Acta Cryst. (1987). C**43**, 1045–1048

Bis[μ-{[(*R*)-1,1-bis(2-butoxy-5-*tert*-butylphenyl)-3-phenyl-2-salicylideneamino-1-propanolato]-*O*}copper(II)]: A Phenolic-Oxygen-Bridged Binuclear Copper(II) Complex with a Chiral Schiff Base

BY KAZUNORI YANAGI AND MASAO MINOBE*

Takatsuki Research Laboratory, Sumitomo Chemical Co. Ltd, 2–10–1, *Tsukahara, Takatsuki, Osaka* 569, *Japan*

(*Received* 11 *November* 1986; *accepted* 16 *December* 1986)

Abstract. $[Cu_2(C_{44}H_{55}NO_4)_2]$, $M_r = 1451·0$, monoclinic, $P2_1$, $a = 17·657\,(1)$, $b = 25·573\,(2)$, $c = 9·165\,(1)$ Å, $\beta = 91·58\,(1)°$, $V = 4136·9$ Å^3, $Z = 2$, $D_x = 1·17$ Mg m^{-3}, $\lambda(\mathrm{Cu}\,K\alpha) = 1·5418$ Å, $\mu(\mathrm{Cu}\,K\alpha) = 1·017$ mm^{-1}, $T = 295$ K, $F(000) = 1548$, $R = 0·057$ for 5133 observed reflections. The complex consists of a phenolic-oxygen-bridged binuclear copper(II) unit,

---

* Present address: Ehime Research Laboratory, Sumitomo Chemical Co. Ltd, 5–1, Sobiraki-cho, Niihama, Ehime 792, Japan.

0108-2701/87/061045-04$01.50