International Tables for X-ray Crystallography (1974). Vol. IV, Tables 2.2B and 2.3.1. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)
Mond, L., Langer, C. & Quinke, C. (1890). *J. Chem. Soc.* pp. 749–754.
Saillard, J.-Y. & Grandjean, D. (1976). *Acta Cryst.* B**32**, 2285–2289.
Saillard, J.-Y. & Grandjean, D. (1978). *Acta Cryst.* B**34**, 3772–3775.
Saillard, J.-Y., Grandjean, D., Caillet, P. & Le Beuze, A. (1980). *J. Organomet. Chem.* **190**, 371–379.
Saillard, J.-Y., Leborgne, G. & Grandjean, D. (1975). *J. Organomet. Chem.* **94**, 409–416.
Steudel, R. (1967). *Angew. Chem. Int. Ed. Engl.* **6**, 635.

Acta Cryst. (1985). C**41**, 1585–1588

Structure of Bis(triethanolamine)bis(2,4,6-trinitrophenolato)barium(II)*

By J. A. Kanters, A. de Koster and A. Schouten

Laboratorium voor Kristal- en Structuurchemie, Rijksuniversiteit Utrecht, Transitorium 3, *Padualaan* 8,
3508 *TB Utrecht, The Netherlands*

and K. Venkatasubramanian and N. S. Poonia

Chemistry Department, University of Indore, Indore 452-001, *India*

(*Received* 7 *January* 1985; *accepted* 11 *June* 1985)

Abstract. $[Ba(C_6H_2N_3O_7)_2(C_6H_{15}NO_3)_2]$, $M_r = 891\cdot9$, monoclinic, $C2/c$, $a = 21\cdot704\ (3)$, $b = 8\cdot0224\ (6)$, $c = 22\cdot650\ (4)$ Å, $\beta = 122\cdot30\ (1)^\circ$, $V = 3333\cdot5\ (9)$ Å^3, $Z = 4$, $D_x = 1\cdot777$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0\cdot71069$ Å, $\mu = 11\cdot83$ cm^{-1}, $F(000) = 1800$, $T = 294$ K, $R = 0\cdot0338$ for 2837 observed reflections. Ba lies on a twofold axis and is coordinated to eight O and two N atoms which form a bicapped distorted cube. The N atom and three O atoms of triethanolamine (tea) and one O of the *p*-nitro group of the picrate (tnp) are involved in the coordination. The tea ligand is disordered over two positions which are approximately related by pseudo mirror planes through N and each of the terminal C atoms, with occupancies of 0·637 (7) and 0·363 (7). Hydrogen bonds from the three tea OH groups to two neighbouring tnp ligands link the Ba complexes in extensive sheets. Two hydrogen bonds are bifurcated and the phenolate O accepts three hydrogen bonds.

Introduction. Recently we reported the structure analyses of two complexes of Ba^{II}: $Ba(dnp)_2(phen)_3$ (Kanters, Postma, Duisenberg, Venkatasubramanian & Poonia, 1983) and $Ba(tnp)_2(phen)_2$ (Postma, Kanters, Duisenberg, Venkatasubramanian & Poonia, 1983) (dnp = 2,4-dinitrophenolato, tnp = 2,4,6-trinitrophenolato, phen = 1,10-phenanthroline). In order to study the relative binding capacities of nitrophenolates and triethanolamine we also determined the structure of $Ba(dnp)_2(tea)_2$ (Kanters, Smeets, Venkatasubramanian & Poonia, 1984). In the latter compound the N and O atoms of both tea ligands are coordinated to Ba, whereas only one *o*-nitro-group O atom of one of the dnp ligands contributes to the coordination. The powerful binding capacity of triethanolamine in the presence of 2,4,6-trinitrophenolate is studied in the structure analysis of the title compound.

Experimental. Crystals obtained from the Chemistry Department, University of Indore, India. Rod-shaped, orange-reddish crystal 0·6 × 0·3 × 0·2 mm. Enraf–Nonius CAD-4 diffractometer. Cell constants from least-squares fit of positions of 25 reflections with θ range 11·2–18·6°. ω–2θ scan, $\omega = (0\cdot60 + 0\cdot35 \tan\theta)^\circ$, $\sigma(I)/(I) < 1\%$ or a maximum scan time of 60 s, horizontal and vertical slit widths 3 and 4 mm respectively, Zr-filtered Mo $K\alpha$ radiation. One quadrant, h 0–26, k 0–9, l −27–23, $\theta_{max} = 26^\circ$. 3143 unique reflections, 2837 above $2\cdot5\sigma(I)$ level. Three standard reflections, measured every hour of X-ray exposure, showed an average fluctuation of 0·9%. Intensities corrected for Lp effects, but not for absorption. Ba position from Patterson synthesis, non-H atoms of tnp, N and three terminal C atoms of tea from Fourier maps. Six maxima appeared around N, the densities of which fell into two groups with a ratio of about 2:1. The same feature was observed near the terminal C atoms where three pairs of close-lying maxima were found. This pattern was interpreted as a disorder of tea over two positions. Accordingly, the two groups of positions of the disordered C and O atoms were refined with occupancy factors p and $(1-p)$ [refined value, $p = 0\cdot637\ (7)$]. The two H atoms of tnp were located from difference maps. The H atoms of tea were placed

---

* Triethanolamine is 2,2′,2″-nitrilotriethanol.

0108-2701/85/111585-04$01.50

at calculated C(sp^3) positions, those bonded to the disordered C atoms with corresponding occupancies, whereas the four H atoms attached to each ordered terminal C atom were pair-wise allocated occupancies corresponding to those of the disordered C atoms. The H atoms bonded to O atoms with the greater occupancy could be located from a difference map.

The non-H atoms were refined anisotropically, the H atoms of tnp isotropically; all other H atoms were kept fixed at their calculated positions with a constant U of 0·05 Å^2. Because of the large number of parameters (308) the refinement was split into two blocks: one for Ba and tnp, the other for tea. At convergence $R = 0{\cdot}0338$, $wR = 0{\cdot}0355$ with $w = [\sigma^2(F_o) + 0{\cdot}00182F_o^2]^{-1}$, $S = 3{\cdot}12$, $(\Delta/\sigma)_{\max} = 0{\cdot}24$, $(\Delta/\sigma)_{\text{av}} = 0{\cdot}042$. The final difference map showed intensities of $\pm0{\cdot}8$ e Å^{-3} at about 1 Å from Ba, with other features below 0·4 e Å^{-3}. Scattering factors for non-H atoms from Cromer & Mann (1968), for H from Stewart, Davidson & Simpson (1965); anomalous-dispersion coefficients from Cromer & Liberman (1970). Calculations were performed with *SHELX*76 (Sheldrick, 1976) (structure determination and refinement) and the *EUCLID* package (Spek, 1982) (geometry and illustrations) on the CDC Cyber-175 of the University of Utrecht.

Discussion. Final atomic coordinates and equivalent isotropic thermal parameters are given in Table 1,* derived distances and angles in Table 2. The complex with the atom numbering scheme is shown in Fig. 1.

In the complex Ba is coordinated to two tnp and two (disordered) tea ligands. Each tnp ligand is only coordinated by one O atom of the *p*-nitro group and each tea ligand contributes N and all six disordered O atoms (Table 2). Considering only the O atoms of tea with the greater occupancy, each Ba is bonded to ten N and O atoms, which form a distorted bicapped cubic arrangement (Fig. 2) with the twofold axis passing through Ba; O(5) and O(5′) of tnp are the capping atoms. A similar (monocapped) coordination is present in $\text{Ba(dnp)}_2\text{(tea)}_2$ (Kanters, Smeets, Venkatasubramanian & Poonia, 1984). In that complex the two dnp ligands contribute only one *o*-nitro-group O atom and the phenolic O of dnp is also not involved in the coordination, whereas in nitrophenolate complexes with 1,10-phenanthroline as a ligand, $\text{Ba(tnp)}_2\text{(phen)}_2$ (Postma, Kanters, Duisenberg, Venkatasubramanian & Poonia, 1983) and $\text{Ba(dnp)}_2\text{(phen)}_3$ (Kanters, Postma, Duisenberg, Venkatasubramanian & Poonia, 1983) the distance Ba—O(phenolate) is the shortest contact, which illustrates the great coordination capacity of tea. This loss of coordination energy is compensated for by the extensive participation of phenolic O in hydrogen bonding (Table 3).

The cluster of Ba with its surrounding tnp and tea ligands is built in such a way that the two tea's with their eight coordinating atoms effectively screen Ba from the tnp fragments which approach the cluster from one side. The distances between Ba and the O atoms of tea with the greater occupancy range from 2·728 (5) to 2·809 (5) Å and the Ba—N(4) distance is

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters, with e.s.d.'s in parentheses*

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

	x	y	z	U_{eq}(Å^2)
Ba	0·5	0·21592 (4)	0·25	0·0520 (1)
Trinitrophenolate				
O(1)	0·4847 (1)	0·8144 (4)	−0·0698 (1)	0·079 (1)
O(2)	0·3660 (2)	1·0118 (5)	−0·1220 (2)	0·091 (1)
O(3)	0·2813 (2)	0·8633 (6)	−0·1295 (2)	0·125 (2)
O(4)	0·3329 (2)	0·6154 (4)	0·0870 (2)	0·092 (1)
O(5)	0·4441 (2)	0·5531 (4)	0·1672 (2)	0·093 (1)
O(6)	0·6259 (1)	0·5670 (5)	0·1141 (2)	0·093 (1)
O(7)	0·6140 (2)	0·6908 (5)	0·0265 (2)	0·097 (2)
N(1)	0·3447 (2)	0·8994 (5)	−0·1004 (2)	0·063 (1)
N(2)	0·3983 (2)	0·6077 (4)	0·1090 (2)	0·068 (1)
N(3)	0·5897 (1)	0·6474 (4)	0·0612 (2)	0·059 (1)
C(1)	0·4684 (2)	0·7778 (5)	−0·0261 (2)	0·054 (1)
C(2)	0·3971 (2)	0·8085 (4)	−0·0381 (2)	0·052 (1)
C(3)	0·3733 (2)	0·7513 (4)	0·0031 (2)	0·053 (1)
C(4)	0·4223 (2)	0·6687 (4)	0·0641 (2)	0·053 (1)
C(5)	0·4932 (2)	0·6388 (5)	0·0829 (2)	0·052 (1)
C(6)	0·5152 (2)	0·6906 (4)	0·0392 (2)	0·051 (1)
Triethanolamine				
O(8)	0·4172 (6)	0·151 (1)	0·1081 (6)	0·071 (3)
O(81)	0·4142 (9)	0·228 (2)	0·1062 (9)	0·047 (4)
O(9)	0·4564 (3)	−0·0365 (6)	0·3060 (2)	0·067 (2)
O(91)	0·4597 (5)	−0·108 (1)	0·2632 (8)	0·117 (5)
O(10)	0·4159 (2)	0·3418 (7)	0·2957 (2)	0·054 (1)
O(101)	0·4012 (5)	0·425 (1)	0·2583 (6)	0·082 (4)
N(4)	0·3411 (1)	0·1169 (3)	0·1788 (1)	0·046 (1)
C(7)	0·3138 (3)	0·059 (1)	0·1064 (3)	0·058 (2)
C(71)	0·3050 (5)	0·179 (2)	0·1063 (5)	0·054 (4)
C(8)	0·3425 (2)	0·1521 (6)	0·0694 (2)	0·063 (1)
C(9)	0·3275 (3)	−0·0156 (9)	0·2148 (4)	0·064 (2)
C(91)	0·3407 (9)	−0·069 (2)	0·1816 (7)	0·092 (5)
C(10)	0·3927 (3)	−0·1306 (6)	0·2547 (2)	0·080 (2)
C(11)	0·3007 (3)	0·2695 (8)	0·1747 (4)	0·062 (2)
C(111)	0·3113 (5)	0·193 (1)	0·2175 (6)	0·055 (4)
C(12)	0·3372 (2)	0·3567 (6)	0·2455 (2)	0·067 (1)

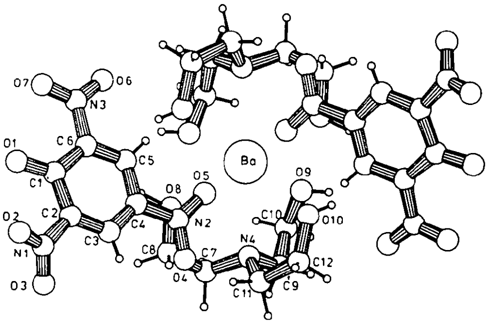

Fig. 1. Perspective drawing of the molecule with atom numbering. The tea molecule with the higher occupancy is shown.

---

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and least-squares-planes' data have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42326 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Interatomic distances* (Å), *bond angles* (°) *and selected torsion angles* (°)

Ba–O(10)	2·728 (5)	Ba–O(81)	2·76 (2)
Ba–O(8)	2·77 (1)	Ba–O(91)	2·808 (9)
Ba–O(9)	2·809 (5)	Ba–O(101)	2·81 (1)
Ba–N(4)	3·030 (2)		
Ba–O(5)	3·142 (2)		
N(4)–Ba–N(4′)	149·6 (6)	O(8)–Ba–O(9′)	60·4 (2)
N(4)–Ba–O(8′)	114·6 (2)	O(8)–Ba–O(10)	111·1 (3)
N(4)–Ba–O(9)	59·3 (1)	O(8)–Ba–O(10′)	77·3 (3)
N(4)–Ba–O(9′)	97·6 (1)	O(5)–Ba–O(5′)	61·2 (1)
N(4)–Ba–O(10)	59·8 (1)	O(9)–Ba–O(9′)	87·7 (2)
N(4)–Ba–O(10′)	134·2 (1)	O(9)–Ba–O(5)	140·8 (1)
N(4)–Na–O(8)	59·0 (3)	O(9)–Ba–O(5′)	117·8 (1)
N(4)–Ba–O(5)	86·6 (1)	O(9)–Ba–O(10)	68·9 (2)
N(4)–Ba–O(5′)	120·7 (1)	O(9)–Ba–O(10′)	153·3 (2)
O(8)–Ba–O(8′)	158·3 (2)	O(10)–Ba–O(10′)	136·5 (2)
O(8)–Ba–O(5′)	131·2 (2)	O(10)–Ba–O(5)	77·6 (1)
O(8)–Ba–O(5)	70·4 (2)	O(10)–Ba–O(5′)	65·0 (1)
O(8)–Ba–O(9)	102·9 (2)		

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

Trinitrophenolate

O(1)–C(1)	1·251 (6)	N(3)–O(6)	1·210 (5)
N(1)–C(2)	1·450 (6)	N(3)–O(7)	1·208 (6)
N(1)–O(2)	1·228 (6)	C(1)–C(2)	1·442 (6)
N(1)–O(3)	1·201 (5)	C(1)–C(6)	1·450 (6)
N(2)–C(4)	1·453 (7)	C(2)–C(3)	1·365 (7)
N(2)–O(4)	1·229 (5)	C(3)–C(4)	1·382 (6)
N(2)–O(5)	1·232 (6)	C(4)–C(5)	1·381 (5)
N(3)–C(6)	1·457 (4)	C(5)–C(6)	1·373 (7)
C(2)–N(1)–O(2)	119·4 (4)	C(1)–C(2)–N(1)	118·3 (4)
C(2)–N(1)–O(3)	119·1 (4)	C(1)–C(2)–C(3)	125·0 (4)
O(2)–N(1)–O(3)	121·6 (5)	N(1)–C(2)–C(3)	116·6 (4)
C(4)–N(2)–O(4)	117·9 (4)	C(2)–C(3)–C(4)	118·3 (4)
C(4)–N(2)–O(5)	118·9 (4)	C(3)–C(4)–N(2)	119·3 (4)
O(4)–N(2)–O(5)	123·3 (5)	C(3)–C(4)–C(5)	121·8 (4)
C(6)–N(3)–O(6)	118·7 (4)	N(2)–C(4)–C(5)	118·9 (4)
C(6)–N(3)–O(7)	120·0 (4)	C(4)–C(5)–C(6)	119·0 (4)
O(6)–N(3)–O(7)	121·3 (3)	C(1)–C(6)–C(5)	123·9 (4)
O(1)–C(1)–C(2)	122·6 (4)	C(1)–C(6)–N(3)	120·5 (4)
O(1)–C(1)–C(6)	125·5 (4)	C(5)–C(6)–N(3)	115·6 (4)
C(2)–C(1)–C(6)	111·8 (4)		
O(2)–N(1)–C(2)–C(1)	−35·2 (6)	O(5)–N(2)–C(4)–C(3)	−171·0 (4)
O(2)–N(1)–C(2)–C(3)	147·9 (4)	O(5)–N(2)–C(4)–C(5)	10·5 (5)
O(3)–N(1)–C(2)–C(1)	145·1 (5)	O(6)–N(3)–C(6)–C(1)	−176·1 (4)
O(3)–N(1)–C(2)–C(3)	−31·7 (6)	O(6)–N(3)–C(6)–C(5)	1·9 (5)
O(4)–N(2)–C(4)–C(3)	8·1 (5)	O(7)–N(3)–C(6)–C(1)	3·3 (6)
O(4)–N(2)–C(4)–C(5)	−170·4 (4)	O(7)–N(3)–C(6)–C(5)	−178·6 (4)

Triethanolamine (population 0·637)

O(8)–C(8)	1·37 (1)	N(4)–C(11)	1·480 (7)
O(9)–C(10)	1·454 (8)	C(7)–C(8)	1·485 (9)
O(10)–C(12)	1·466 (5)	C(9)–C(10)	1·518 (8)
N(4)–C(7)	1·489 (8)	C(11)–C(12)	1·53 (1)
N(4)–C(9)	1·463 (9)		
C(7)–N(4)–C(9)	107·9 (5)	N(4)–C(11)–C(12)	110·8 (5)
C(7)–N(4)–C(11)	108·4 (5)	O(8)–C(8)–C(7)	110·2 (7)
C(9)–N(4)–C(11)	110·3 (5)	O(9)–C(10)–C(9)	110·2 (4)
N(4)–C(7)–C(8)	115·1 (5)	O(10)–C(12)–C(11)	120·9 (4)
N(4)–C(9)–C(10)	111·8 (5)		
C(9)–N(4)–C(7)–C(8)	−162·1 (5)	C(9)–N(4)–C(11)–C(12)	74·8 (6)
C(11)–N(4)–C(7)–C(8)	78·4 (5)	N(4)–C(7)–C(8)–O(8)	55·0 (8)
C(7)–N(4)–C(9)–C(10)	93·1 (6)	N(4)–C(9)–C(10)–O(9)	58·9 (7)
C(11)–N(4)–C(9)–C(10)	−148·7 (5)	N(4)–C(11)–C(12)–O(10)	28·6 (8)
C(7)–N(4)–C(11)–C(12)	−167·3 (5)		

Triethanolamine (population 0·363)

O(81)–C(8)	1·45 (2)	N(4)–C(111)	1·47 (1)
O(91)–C(10)	1·37 (1)	C(71)–C(8)	1·46 (1)
O(101)–C(12)	1·37 (1)	C(91)–C(10)	1·50 (2)
N(4)–C(71)	1·48 (1)	C(111)–C(12)	1·44 (1)
N(4)–C(91)	1·49 (2)		
C(71)–N(4)–C(91)	111·9 (9)	N(4)–C(111)–C(12)	116·7 (8)
C(71)–N(4)–C(111)	112·4 (7)	O(81)–C(8)–C(71)	111 (1)
C(91)–N(4)–C(111)	112·0 (8)	O(91)–C(10)–C(91)	103 (1)
N(4)–C(71)–C(8)	117·3 (8)	O(101)–C(12)–C(111)	124·9 (7)
N(4)–C(91)–C(10)	111 (1)		
C(91)–N(4)–C(71)–C(8)	−70 (1)	C(91)–N(4)–C(111)–C(12)	152·7 (9)
C(111)–N(4)–C(71)–C(8)	162·6 (9)	N(4)–C(71)–C(8)–O(81)	−58 (1)
C(71)–N(4)–C(91)–C(10)	166·1 (9)	N(4)–C(91)–C(10)–O(91)	−75 (1)
C(111)–N(4)–C(91)–C(10)	−67 (1)	N(4)–C(111)–C(12)–O(101)	−21 (1)
C(71)–N(4)–C(111)–C(12)	−80 (1)		

3·030 (2) Å, whereas O(5) of the *p*-nitro group of tnp is at 3·142 (2) Å. The O atoms of tea with the smaller occupancy are also coordinated at distances ranging from 2·76 (2) to 2·81 (1) Å (Table 2). Corresponding ranges have been observed in Ba(CH$_3$COO$^-$)$_2$(tea)$_2$ (Voegele, Thierry & Weiss, 1974) and Ba(dnp)$_2$(tea)$_2$. The tea ligand is disordered over two positions such that the N atom and the three terminal C atoms are ordered and the remaining C and O atoms are disordered. The disordered atoms are related by pseudo mirror planes, each comprising a terminal C atom and the perpendicular through N on the plane of C(7), C(9), C(11) (Fig. 3). The differences between the distances of the seven mirror-related atom pairs to these three planes average to 0·2 (3), 0·16 (7) and 0·08 (6) Å for the three planes passing through N(4)···C(8), N(4)···C(10) and N(4)···C(12) respectively. The bond distances and angles of tea with the greater occupancy (Table 2) are in reasonable agreement with data observed in (tea)$_2$Sr(NO$_3$)$_2$ (Voegele, Fischer & Weiss, 1974*b*), (tea)$_3$NaI (Voegele, Fischer & Weiss, 1974*a*), Ba(CH$_3$COO$^-$)$_2$(tea)$_2$ (Voegele, Thierry & Weiss, 1974) and Ba(dnp)$_2$(tea)$_2$. For lower-occupancy tea some values show large deviations, which must be ascribed to the disorder. Therefore, only the geometry of tea with occupancy 0·637 will be discussed.

As in the other complexes, tea has three nearly planar C—N—C—C fragments. The conformation of two C—O bonds relative to C—N is almost *gauche* for C(8)—O(8) [55·2 (8)°] and C(10)—O(9) [58·9 (7)°], but deviates strongly for C(12)—O(10) [28·6 (8)°].

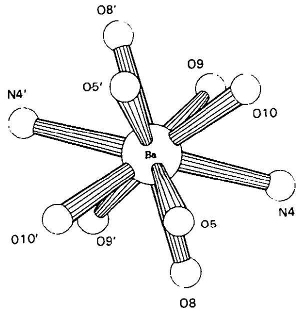

Fig. 2. View of the Ba coordination. Atoms N(4), O(8), O(9) and O(10) with the symmetry-related atoms of tea with the higher occupancy form a distorted cube, capped by O(5) and O(5′) of tnp. Symmetry code: (′) $1 - x, y, \frac{1}{2} - z$.

Table 3. *Hydrogen-bonding geometry* (*D: donor; A: acceptor*)

D–H···*A*	*D*–H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*–H···*A* (°)
O(8)–H(13)···O(1′)	1·10 (1)	1·76 (1)	2·71 (1)	141 (1)
O(8)–H(13)···O(7′)	1·10 (1)	2·19 (1)	3·03 (1)	131 (1)
O(9)–H(14)···O(1″)	0·90 (1)	2·29 (1)	3·101 (6)	151 (1)
O(9)–H(14)···O(2″)	0·90 (1)	2·46 (1)	3·157 (7)	135 (1)
O(10)–H(15)···O(1″)	0·87 (1)	2·00 (1)	2·867 (6)	174 (1)

Symmetry code: (′) $1 - x, 1 - y, -z$; (″) $x, 1 - y, \frac{1}{2} + z$.

This deviation is probably due to disorder, as in the other tea complexes the conformations are all close to *gauche*. As is usual in picrates the phenyl ring is moderately planar [$\sigma_{\rm av} = 0{\cdot}024\,(9)$ Å], with the immediate ring substitutents showing appreciable deviations from the best plane, the average distance of the three N atoms being 0·05 (1) Å and of phenolic O(1) 0·143 (8) Å. The three C—NO_2 fragments are planar and the nitro groups display various degrees of twisting, moderate for one of the *o*-nitro groups [3·1 (2)°] and the *p*-nitro group [10·1 (2)°] but large for the other *o*-nitro group [33·6 (3)°], which corresponds to the twisting in $Ba(tnp)_2(phen)_2$ where these twist angles are 0·4 (2), 5·1 (2) and 28·6 (2)° for tnp1 and 5·9 (2), 14·9 (2) and 38·9 (2)° for tnp2. The bond-length and bond-angle variation of the phenyl ring of tnp is similar to that observed in other picrates and mono- and di-*o*-nitrophenolates (Bush & Truter, 1971; Hughes, 1973, 1975; Hough, 1976; Postma, Kanters, Duisenberg, Venkatasubramanian & Poonia, 1983) in that both C—C bonds at the phenolic site are long [av. 1·446 (4) Å] and the four remaining bonds are short [av. 1·375 (7) Å], the bond angle at the phenolic site is small [111·8 (4)°], and the angles subtended at the *ortho* C atoms are enlarged to 123·9 (4) and 125·0 (4)°, whereas the remaining angles approach normal values (Table 2). The dimensions of tnp are consistent with significant contributions of resonance forms with an essentially normal C=O bond (Ferguson, Ruhl, Wieckowski, Lloyd & McNab, 1984).

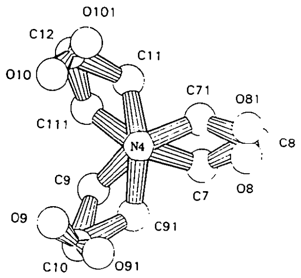

Fig. 3. The disordered triethanolamine ligand. The disordered atoms are related by pseudo mirror planes passing through the terminal C atoms and the perpendicular through N on the plane C(7), C(9), C(11).

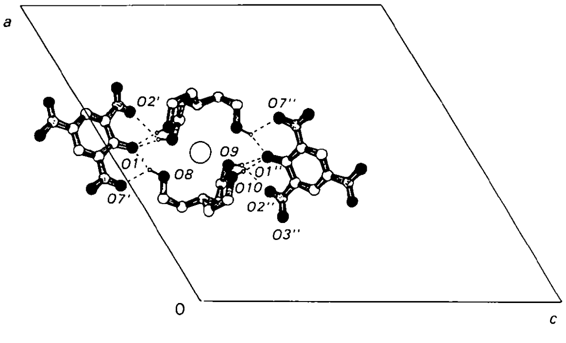

Fig. 4. View of the hydrogen-bond scheme down **b**. Hydrogen bonds, denoted by dashed lines, connect tea and tnp ligands of three different Ba coordination spheres, with Ba at $\frac{1}{2}, \frac{1}{2} + y, -\frac{1}{4}$; $\frac{1}{2}, y, \frac{1}{4}$; $\frac{1}{2}, \frac{1}{2} + y, \frac{3}{4}$ respectively. The tea residues are at x, y, z and $1 - x, y, \frac{1}{2} - z$. The tnp residues are at (′) $1 - x, 1 - y, -z$ and (″) $x, 1 - y, \frac{1}{2} + z$.

The OH groups of tea are involved in intermolecular hydrogen bonds, two of which are bifurcated, and they donate to acceptors O(1), O(2) and O(7) of the tnp fragments (Fig. 4). Only the hydrogen bonds relating to tea with occupancy 0·637 are given in Table 3, though the O atoms of tea with the smaller occupancy are within 3·40 Å of potential O acceptors. The phenolic O(1) accepts three hydrogen bonds and as in $Ba(dnp)_2(tea)_2$, where O(1) is also excluded from the Ba coordination, this acceptor therefore contributes effectively to the interaction energy. The hydrogen bonds connect each tea molecule to two tnp's belonging to two different Ba coordination spheres which are related by translations of $\frac{1}{2}(b + c)$ and $\frac{1}{2}(b - c)$ respectively. As these hydrogen bonds are all directed towards the phenolic site of the tnp's, whose *p*-nitro groups are coordinated to Ba, a strongly hydrogen-bonded sheet of Ba polyhedra is formed parallel to *bc*. The structure is built up by stacking of these infinite sheets along **a**.

References

BUSH, M. A. & TRUTER, M. R. (1971). *J. Chem. Soc. A*, pp. 745–750.

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.

FERGUSON, G., RUHL, B. L., WIECKOWSKI, T., LLOYD, D. & MCNAB, H. (1984). *Acta Cryst.* C**40**, 1740–1742.

HOUGH, E. (1976). *Acta Cryst.* B**32**, 1154–1162.

HUGHES, D. L. (1973). *J. Chem. Soc. Dalton Trans.* pp. 2347–2354.

HUGHES, D. L. (1975). *J. Chem. Soc. Dalton Trans.* pp. 2374–2378.

KANTERS, J. A., POSTMA, R., DUISENBERG, A. J. M., VENKATASUBRAMANIAN, K. & POONIA, N. S. (1983). *Acta Cryst.* C**39**, 1519–1522.

KANTERS, J. A., SMEETS, W. J. J., VENKATASUBRAMANIAN, K. & POONIA, N. S. (1984). *Acta Cryst.* C**40**, 1701–1704.

POSTMA, R., KANTERS, J. A., DUISENBERG, A. J. M., VENKATASUBRAMANIAN, K. & POONIA, N. S. (1983). *Acta Cryst.* C**39**, 1221–1225.

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

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

STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

VOEGELE, J. C., FISCHER, J. & WEISS, R. (1974*a*). *Acta Cryst.* B**30**, 62–65.

VOEGELE, J. C., FISCHER, J. & WEISS, R. (1974*b*). *Acta Cryst.* B**30**, 66–69.

VOEGELE, J. C., THIERRY, J. C. & WEISS, R. (1974). *Acta Cryst.* B**30**, 70–75.