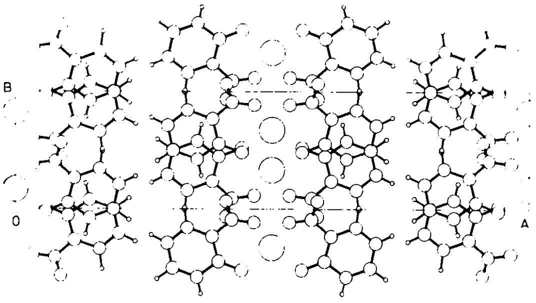

Fig. 2. Projection of the crystal structure along **c**, showing alternating polar and apolar zones.

Accordingly, there are two short bonds [C(3)–C(4) 1·352 (8) and C(5)–C(6) 1·359 (8) Å] and four longer bonds [av. 1·414 (8) Å] and the C–O [1·289 (6) Å] and C–N [1·414 (7) Å] bonds are also shorter than the corresponding bonds in aromatic phenols and nitro compounds (Bush & Truter, 1971; Hough, 1976). As in other *o*-nitrophenolates (Hough, 1976) the C–C–C angle subtended at C(1) is small [113·8 (5)°] at the expense of the angles at the *ortho* C atoms [123·1 (5) and 122·7 (5)°], whereas the other angles are close to 120°.

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Structure of Bis(2,4-dinitrophenolato)bis(triethanolamine)barium(II),* $[Ba(C_6H_3N_2O_5)_2(C_6H_{15}NO_3)_2]$

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Abstract. $M_r = 801{\cdot}91$, monoclinic, $P2_1/c$, $a = 7{\cdot}418\,(8)$, $b = 17{\cdot}884\,(10)$, $c = 25{\cdot}007\,(13)$ Å, $\beta = 100{\cdot}25\,(7)°$, $V = 3265\,(4)$ Å^3, $Z = 4$, $D_x = 1{\cdot}63$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 11{\cdot}93$ cm^{-1}, $F(000) = 1616$, $T = 294$ K, $R = 0{\cdot}039$ for 5930 observed reflections. Ba is bonded to six O atoms and two N atoms of the two triethanolamines (tea's) and to one *o*-nitro-group O of one of the dinitrophenolates (dnp1). The dnp2 molecule is not coordinated at all. All tea O atoms are hydrogen-bond donors; the phenolic O atoms of dnp1 and dnp2 accept two and three hydrogen bonds respectively.

Introduction. Recently we reported the structure analyses of two Ba complexes, in which Ba is coordinated to picric acid and phenanthroline (Postma, Kanters, Duisenberg, Venkatasubramanian & Poonia, 1983) and to 2,4-dinitrophenol and phenanthroline (phen) (Kanters, Postma, Duisenberg, Venkatasubramanian & Poonia, 1983). In order to study the coordination properties of Ba with respect to other powerful ligands and particularly to compare the coordinating capacity of nitrophenols, we undertook the structure determination of the title complex.

Experimental. Crystals obtained from the Chemistry Department, University of Indore, India. Rod-shaped

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

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crystal 0·2 × 0·2 × 1·1 mm. Nonius CAD-4 diffractometer, Zr-filtered Mo $K\alpha$ radiation. ω–2θ scan with $\omega = (0{\cdot}50+0{\cdot}35\ \mathrm{tg}\theta)^\circ$. Lattice parameters from 25 reflections. 7504 intensities measured in the quadrant $0 \le h \le 9$, $0 \le k \le 23$, $-32 \le l \le 32$ with $2\theta_{\max} = 55^\circ$; 5930 reflections with $I > 2{\cdot}5\sigma(I)$ considered observed. Three standard reflections (082, 200, 0,0,10) measured every 60 reflections showed an average decay of 8% which was corrected for by a polynomial scaling function. Absorption corrections (max. 2·148, min. 1·246) applied. Structure solved with Patterson and difference Fourier methods. All H atoms located from difference syntheses and included in the refinement with fixed isotropic thermal parameters; 6 of the 36 H atoms were refined with a bond-length constraint. Anisotropic, weighted least-squares refinement on F gave $R = 0{\cdot}0390$, $wR = 0{\cdot}0353$ with $w = [\sigma^2(F_o) + 0{\cdot}000033F_o^2]^{-1}$, and $S = 2{\cdot}17$. Max. Δ/σ ratios 0·167 for non-hydrogen atoms and 0·283 for H. Final difference synthesis revealed two regions of positive and negative electron densities of about 1·3 e Å^{-3} at 2·4 Å from Ba and four peaks of about 0·8 e Å^{-3} at 0·75 Å from Ba. Scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974). Calculations performed with *SHELX*76 (Sheldrick, 1976), *DIFABS* (Walker & Stuart, 1983) and the *EUCLID* package (Spek, 1982) on the CDC Cyber-175 of the University of Utrecht.

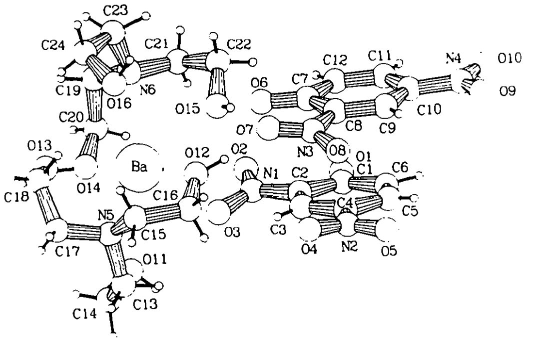

Fig. 1. A perspective view of the complex with the atom numbering.

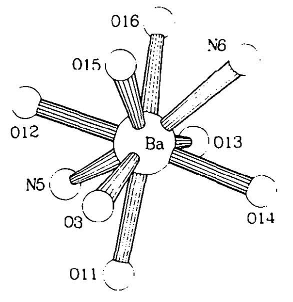

Fig. 2. View of the Ba coordination showing the cube and its cap O(15).

Discussion. The atomic coordinates and equivalent isotropic thermal parameters are listed in Table 1.* A view of the molecular complex is shown in Fig. 1. The structure consists of Ba^{2+} ions surrounded by two tea molecules and two dnp fragments. Ba is ninefold coordinated to the six O and both N atoms of the tea ligands and to an O atom of the *o*-nitro group of dnp1. The dnp2 molecule is not coordinated; the atom nearest to Ba is phenolic O(6) at 4·376 (5) Å. It is noteworthy that none of the phenolic O atoms is involved in the coordination of the metal as is usual in complexes containing mono-, di- and trinitrophenolates. However, this loss of interaction is compensated for by the extensive participation of these phenolic O atoms in hydrogen bonding (Table 3). The coordination sphere of Ba can be classified as a monocapped distorted cube (Fig. 2) as follows from the averages of the three types of internal coordination angles 158 (12), 71 (13), 109 (18)°, compared to the ideal values of 180, 70·5 and 109·5° respectively (Table 2). In the complex, the two quadridentate tea ligands are in nearly opposite positions, the angle between their least-squares planes being 35·2 (2)°; the dnp fragments are nearly parallel with an interplanar angle of 5·3 (1)°. The distances between Ba and the ethanolic O atoms are in the range 2·703 (4)–2·894 (3) Å with an average of 2·77 (6) Å; the tea N atoms have coordination distances of 3·000 (4) and 3·036 (5) Å whereas the dnp1 nitro-group O is at 2·785 (4) Å from Ba. Similar observations have been made in the complex Ba(tea)$_2$(CH$_3$COO$^-$)$_2$ (Voegele, Thierry & Weiss, 1974) where the six Ba—O distances range from 2·703 (4)–2·894 (3) Å with an average of 2·77 (6) Å; Ba—N distances are 3·025 (4) and 3·108 (5) Å and an acetate O at 2·726 (2) Å completes the coordination. The averages of the N—Ba—O angles within the coordination sphere are 60·9 (5)° for tea1 and 60 (2)° for tea2. In the Ba acetate complex these values are 58·9 (7) and 58·6 (4)°. The bond lengths and angles of dnp1 and dnp2 (Table 2) show a good mutual correspondence, the maximal differences are 0·02 Å and 1·3° respectively. The C—O bond lengths of 1·273 (5) and 1·283 (6) Å are slightly larger than the values of 1·265 (5) and 1·260 (6) Å observed in the complex Ba(dnp)$_2$(phen)$_3$ (Kanters, Postma, Duisenberg, Venkatasubramanian & Poonia, 1983). The bond-length and bond-angle variation in the benzene rings of the dnp residues is similar to that observed in the Ba(dnp)$_2$(phen)$_3$ complex and also to that reported for a number of *o*-nitrophenolate-containing complexes

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* Lists of structure factors, anisotropic thermal parameters, least-squares planes, H-atom coordinates and the complete geometry data have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39546 (46 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* ($\text{Å}^2 \times 10^2$)

Least-squares-derived standard deviations of the least significant figures are given in parentheses in all tables.

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

	x	y	z	U_{eq}
Ba	0·12875 (3)	0·06455 (1)	0·20580 (1)	2·91 (1)
O(1)	0·0244 (5)	0·4211 (2)	0·1730 (1)	5·2 (1)
O(2)	0·0161 (8)	0·2867 (2)	0·2198 (2)	8·9 (2)
O(3)	−0·0560 (5)	0·1938 (2)	0·1652 (2)	5·3 (1)
O(4)	0·1328 (7)	0·1896 (2)	−0·0051 (2)	7·7 (2)
O(5)	0·1576 (8)	0·2922 (3)	−0·0477 (2)	8·6 (2)
O(6)	0·5170 (4)	0·1734 (2)	0·1180 (1)	4·6 (1)
O(7)	0·5671 (8)	0·1012 (2)	0·0284 (2)	9·0 (2)
O(8)	0·5554 (7)	0·1651 (3)	−0·0445 (2)	8·6 (2)
O(9)	0·7105 (7)	0·4219 (2)	−0·0379 (2)	7·8 (2)
O(10)	0·6936 (6)	0·4879 (2)	0·0335 (2)	6·9 (2)
O(11)	−0·2573 (4)	0·0492 (2)	0·1616 (1)	4·3 (1)
O(12)	0·2481 (5)	0·0709 (2)	0·1090 (1)	4·6 (1)
O(13)	0·1323 (6)	−0·0799 (2)	0·2376 (2)	6·4 (1)
O(14)	−0·0122 (5)	0·0648 (2)	0·3001 (1)	4·4 (1)
O(15)	0·3589 (5)	0·1860 (2)	0·2060 (1)	5·2 (1)
O(16)	0·4828 (5)	0·0077 (2)	0·2323 (1)	5·5 (1)
N(1)	0·0013 (6)	0·2590 (2)	0·1743 (2)	4·8 (1)
N(2)	0·1332 (6)	0·2583 (3)	−0·0077 (2)	5·2 (2)
N(3)	0·5694 (6)	0·1608 (3)	0·0052 (2)	5·4 (2)
N(4)	0·6810 (6)	0·4285 (3)	0·0086 (2)	5·4 (2)
N(5)	0·0084 (5)	−0·0531 (2)	0·1215 (2)	3·4 (1)
N(6)	0·3740 (5)	0·1166 (3)	0·3095 (2)	5·0 (1)
C(1)	0·0573 (6)	0·3828 (2)	0·1329 (2)	3·9 (1)
C(2)	0·0447 (6)	0·3022 (2)	0·1298 (2)	3·6 (1)
C(3)	0·0684 (6)	0·2632 (3)	0·0838 (2)	3·5 (1)
C(4)	0·1080 (6)	0·3007 (3)	0·0402 (2)	3·7 (1)
C(5)	0·1275 (7)	0·3791 (3)	0·0408 (2)	4·1 (2)
C(6)	0·1028 (7)	0·4173 (3)	0·0856 (2)	4·4 (2)
C(7)	0·5531 (6)	0·2309 (3)	0·0911 (2)	3·8 (1)
C(8)	0·5818 (6)	0·2301 (3)	0·0361 (2)	4·0 (1)
C(9)	0·6211 (7)	0·2944 (3)	0·0093 (2)	4·1 (1)
C(10)	0·6324 (6)	0·3615 (3)	0·0358 (2)	4·0 (1)
C(11)	0·6034 (7)	0·3666 (3)	0·0893 (2)	4·6 (2)
C(12)	0·5640 (7)	0·3036 (3)	0·1156 (2)	4·6 (2)
C(13)	−0·1786 (7)	−0·0362 (3)	0·0922 (2)	4·4 (2)
C(14)	−0·3110 (7)	−0·0166 (3)	0·1295 (2)	4·7 (2)
C(15)	0·1396 (7)	−0·0523 (3)	0·0835 (2)	4·3 (2)
C(16)	0·1809 (8)	0·0239 (3)	0·0637 (2)	4·5 (2)
C(17)	0·0147 (7)	−0·1282 (3)	0·1473 (2)	5·0 (2)
C(18)	0·1576 (8)	−0·1318 (3)	0·1988 (2)	5·6 (2)
C(19)	0·2782 (8)	0·1013 (4)	0·3552 (2)	5·6 (2)
C(20)	0·0733 (8)	0·1135 (3)	0·3423 (2)	5·4 (2)
C(21)	0·3991 (9)	0·1974 (4)	0·3031 (2)	6·4 (2)
C(22)	0·4698 (10)	0·2190 (5)	0·2523 (3)	7·0 (2)
C(23)	0·5512 (8)	0·0757 (5)	0·3178 (3)	6·9 (2)
C(24)	0·5323 (9)	0·0008 (4)	0·2909 (3)	6·7 (2)

(Hughes, 1973, 1975; Bush & Truter, 1971; Krogh Andersen & Krogh Andersen, 1975; Hough, 1976). In both dnp residues the two C–C bonds at the phenolic site are long [average 1·434 (9) Å] and two of the remaining bonds are short [average 1·359 (6) Å] whereas the bond angles at the phenolic site are small [average 114·3 (2)°]. These differences are consistent with the contributions of quinonoid resonance forms to the molecular structure (Bush & Truter, 1971) and second-order hybridization at the ring C atoms bearing neighboring substituents (Hughes, 1973). The *o*-nitro group of dnp1 is rotated 16·9 (3)° with respect to the plane of the aromatic ring; the rotation angle of the *p*-nitro group is 5·5 (3)°; for dnp2 these values are 14·5 (3) and 2·8 (3)°. The larger twisting of the *o*-nitro group is a common feature in *o*-nitrophenolates and must be ascribed to molecular overcrowding (Krogh Andersen & Krogh Andersen, 1975). The benzene rings of the dnp's are moderately planar, σ_{plane}, defined as $(\sum_i d_i^2/N-3)^{1/2}$, being 0·012 and 0·008 Å respectively.

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

Ba–O(13)	2·703 (4)	Ba–O(15)	2·761 (4)	Ba–O(11)	2·894 (3)
Ba–O(12)	2·724 (3)	Ba–O(16)	2·784 (4)	Ba–N(5)	3·000 (4)
Ba–O(14)	2·745 (3)	Ba–O(3)	2·785 (4)	Ba–N(6)	3·036 (5)

O(1)–C(1)	1·273 (5)	O(16)–C(24)	1·451 (8)	C(4)–C(5)	1·409 (8)
O(2)–N(1)	1·228 (7)	N(1)–C(2)	1·438 (7)	C(5)–C(6)	1·352 (7)
O(3)–N(1)	1·248 (5)	N(2)–C(4)	1·458 (7)	C(7)–C(8)	1·429 (7)
O(4)–N(2)	1·230 (6)	N(3)–C(8)	1·455 (7)	C(7)–C(12)	1·433 (7)
O(5)–N(2)	1·211 (7)	N(4)–C(10)	1·455 (7)	C(8)–C(9)	1·388 (7)
O(6)–C(7)	1·283 (6)	N(5)–C(13)	1·480 (6)	C(9)–C(10)	1·366 (7)
O(7)–N(3)	1·215 (7)	N(5)–C(17)	1·487 (7)	C(10)–C(11)	1·395 (7)
O(8)–N(3)	1·231 (7)	N(5)–C(15)	1·476 (7)	C(11)–C(12)	1·362 (7)
O(9)–N(4)	1·227 (7)	N(6)–C(19)	1·475 (7)	C(13)–C(14)	1·511 (7)
O(10)–N(4)	1·227 (7)	N(6)–C(21)	1·469 (9)	C(15)–C(16)	1·500 (7)
O(11)–C(14)	1·440 (6)	N(6)–C(23)	1·486 (8)	C(17)–C(18)	1·517 (7)
O(12)–C(16)	1·427 (6)	C(1)–C(6)	1·427 (7)	C(19)–C(20)	1·512 (8)
O(13)–C(18)	1·380 (7)	C(1)–C(2)	1·446 (5)	C(21)–C(22)	1·508 (9)
O(14)–C(20)	1·427 (6)	C(2)–C(3)	1·383 (7)	C(23)–C(24)	1·494 (11)
O(15)–C(22)	1·424 (8)	C(3)–C(4)	1·356 (7)		

O(13)–Ba–O(12)	108·3 (1)	O(14)–Ba–N(6)	61·8 (1)
O(13)–Ba–O(14)	74·6 (1)	O(15)–Ba–O(16)	74·4 (1)
O(13)–Ba–O(15)	141·1 (1)	O(15)–Ba–O(3)	67·2 (1)
O(13)–Ba–O(16)	67·7 (1)	O(15)–Ba–O(11)	130·2 (1)
O(13)–Ba–O(3)	151·5 (1)	O(15)–Ba–N(5)	131·3 (1)
O(13)–Ba–O(11)	88·8 (1)	O(15)–Ba–N(6)	58·8 (1)
O(13)–Ba–N(5)	61·4 (1)	O(16)–Ba–O(3)	140·6 (1)
O(13)–Ba–N(6)	93·9 (1)	O(16)–Ba–O(11)	152·1 (1)
O(12)–Ba–O(14)	175·8 (1)	O(16)–Ba–N(5)	93·5 (1)
O(12)–Ba–O(15)	70·8 (1)	O(16)–Ba–N(6)	60·8 (1)
O(12)–Ba–O(16)	77·6 (1)	O(3)–Ba–O(11)	63·3 (1)
O(12)–Ba–O(3)	81·9 (1)	O(3)–Ba–N(5)	105·1 (1)
O(12)–Ba–O(11)	96·9 (1)	O(3)–Ba–N(6)	103·8 (1)
O(12)–Ba–N(5)	60·5 (1)	O(11)–Ba–N(5)	60·9 (1)
O(12)–Ba–N(6)	120·4 (1)	O(11)–Ba–N(6)	139·2 (1)
O(14)–Ba–O(15)	109·1 (1)	N(5)–Ba–N(6)	150·8 (1)
O(14)–Ba–O(16)	106·5 (1)		
O(14)–Ba–O(3)	94·2 (1)		
O(14)–Ba–O(11)	80·0 (1)		
O(14)–Ba–N(5)	119·6 (1)		

O(2)–N(1)–O(3)	121·2 (5)	C(3)–C(4)–C(5)	121·3 (5)
O(2)–N(1)–C(2)	120·3 (4)	C(4)–C(5)–C(6)	118·9 (5)
O(3)–N(1)–C(2)	118·5 (5)	C(1)–C(6)–C(5)	123·7 (5)
O(4)–N(2)–O(5)	123·1 (5)	C(8)–C(7)–C(12)	114·4 (5)
O(4)–N(2)–C(4)	118·3 (5)	O(6)–C(7)–C(12)	120·3 (4)
O(5)–N(2)–C(4)	118·6 (5)	O(6)–C(7)–C(8)	125·3 (5)
O(8)–N(3)–C(8)	118·0 (5)	N(3)–C(8)–C(7)	120·9 (5)
O(7)–N(3)–O(8)	122·1 (5)	C(7)–C(8)–C(9)	122·5 (5)
O(7)–N(3)–C(8)	119·9 (5)	N(3)–C(8)–C(9)	116·6 (5)
O(9)–N(4)–C(10)	117·7 (5)	C(8)–C(9)–C(10)	119·6 (5)
O(9)–N(4)–O(10)	123·7 (5)	N(4)–C(10)–C(11)	119·2 (5)
O(10)–N(4)–C(10)	118·6 (5)	C(9)–C(10)–C(11)	121·1 (5)
C(15)–N(5)–C(17)	108·3 (4)	N(4)–C(10)–C(9)	119·7 (5)
C(13)–N(5)–C(15)	110·3 (4)	C(10)–C(11)–C(12)	119·5 (5)
C(13)–N(5)–C(17)	110·7 (4)	C(7)–C(12)–C(11)	123·0 (5)
C(21)–N(6)–C(23)	111·9 (5)	N(5)–C(13)–C(14)	113·4 (4)
C(19)–N(6)–C(23)	109·7 (5)	O(11)–C(14)–C(13)	112·8 (4)
C(19)–N(6)–C(21)	110·8 (5)	N(5)–C(15)–C(16)	114·7 (4)
O(1)–C(1)–C(6)	121·8 (4)	O(12)–C(16)–C(15)	109·6 (4)
C(2)–C(1)–C(6)	114·2 (4)	N(5)–C(17)–C(18)	111·7 (4)
O(1)–C(1)–C(2)	124·0 (4)	O(13)–C(18)–C(17)	114·0 (5)
C(1)–C(2)–C(3)	122·1 (4)	N(6)–C(19)–C(20)	114·4 (4)
N(1)–C(2)–C(3)	116·9 (4)	O(14)–C(20)–C(19)	111·6 (5)
N(1)–C(2)–C(1)	121·0 (4)	N(6)–C(21)–C(22)	114·4 (6)
C(2)–C(3)–C(4)	119·8 (5)	O(15)–C(22)–C(21)	110·0 (6)
N(2)–C(4)–C(5)	119·9 (5)	N(6)–C(23)–C(24)	111·6 (5)
N(2)–C(4)–C(3)	118·8 (5)	O(16)–C(24)–C(23)	111·4 (6)

C(15)–N(5)–C(17)–C(18)	89·3 (5)	C(21)–N(6)–C(19)–C(20)	78·5 (6)
C(17)–N(5)–C(13)–C(14)	74·8 (5)	C(23)–N(6)–C(19)–C(20)	−157·5 (5)
C(17)–N(5)–C(15)–C(16)	−166·8 (4)	C(21)–N(6)–C(23)–C(24)	−144·1 (6)
C(15)–N(5)–C(13)–C(14)	−165·3 (4)	N(5)–C(13)–C(14)–O(11)	61·4 (5)
C(13)–N(5)–C(17)–C(18)	−149·7 (4)	N(5)–C(15)–C(16)–O(12)	56·8 (6)
C(13)–N(5)–C(15)–C(16)	71·9 (5)	N(5)–C(17)–C(18)–O(13)	57·9 (6)
C(23)–N(6)–C(21)–C(22)	66·1 (7)	N(6)–C(19)–C(20)–O(14)	61·9 (7)
C(19)–N(6)–C(23)–C(24)	92·6 (7)	N(6)–C(21)–C(22)–O(15)	52·0 (8)
C(19)–N(6)–C(21)–C(22)	−171·2 (5)	N(6)–C(23)–C(24)–O(16)	64·3 (7)

Table 3. H-*bond distances* (Å) *and angles* (°)

O–H···O	O···O	O–H	H···O	O–H···O
O(11)–H(19)···O(6^{i})	2·877 (5)	0·88 (4)	2·00 (4)	171 (4)
O(12)–H(20)···O(6)	2·689 (5)	0·88 (3)	1·88 (4)	152 (4)
O(13)–H(21)···O(1^{ii})	2·697 (6)	0·89 (4)	2·01 (5)	133 (4)
O(13)–H(21)···O(2^{ii})	2·908 (6)	0·89 (4)	2·21 (5)	134 (4)
O(14)–H(34)···O(1^{ii})	2·662 (5)	1·05 (5)	1·63 (5)	167 (4)
O(15)–H(35)···O(6)	2·681 (4)	0·77 (5)	1·92 (5)	171 (6)
O(16)–H(36)···O(11^{iii})	2·934 (4)	0·88 (3)	2·18 (5)	144 (4)

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

The tea ligands have an extended conformation which is also encountered in $(tea)_2Sr(NO_3)_2$ (Voegele, Fischer & Weiss, 1974*b*), $(tea)_3NaI$ (Voegele, Fischer & Weiss, 1974*a*) and in $(tea)_2Ba(CH_3COO^-)_2$ (Voegele, Thierry & Weiss, 1974). This requires three nearly planar C—N—C—C fragments for each tea and a *gauche* conformation of the terminal OH groups with respect to the C—N bonds. The geometries of both tea's show a good mutual correspondence; the maximal differences in bond lengths and angles are 0·02 Å and 1·2° respectively and they compare well with the geometries observed in the Sr, Na and Ba complexes. The six N—C—C—O torsion angles range from 52·0 (8) to 64·3 (7)°, compared with an overall range of 46·8 (4) to 67·4 (4)° in the three complexes mentioned above.

All six tea hydroxyl groups, within the coordination sphere of Ba, take part in hydrogen bonds; one of the OH groups is a double donor (Table 3). The phenolic O atoms are strong acceptors as O(1) of dnp1 accepts two and O(6) of dnp2 three hydrogen bonds. The two remaining acceptors are a nitro-group O next to phenolic O in dnp1 and an O atom of a tea ligand. Each Ba cluster is connected by donor and acceptor hydrogen bonds to four other Ba clusters, thus forming a strong two-dimensional network parallel with the *ab* plane. Two of the hydrogen bonds which link tea O atoms to phenolic O of dnp2 are within the Ba cluster. Although dnp2 is not involved in the coordination to Ba, it effectively contributes to the interaction energy by its participation in three acceptor bonds of phenolic O.

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9,9-Bis(triphenylphosphine)-7,8-dicarba-9-rhoda-*nido*-undecaborane(11), $C_{38}H_{41}B_8P_2Rh$, an *endo-nido*-Carbarhodaborane Complex Containing an Acidic Bridging Hydrogen

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Abstract. $M_r = 749·2$, monoclinic, $P2_1/n$, $a = 18·950$ (6), $b = 12·057$ (3), $c = 15·585$ (5) Å, $\beta = 97·80$ (3)°, $V = 3527·9$ Å^3, $Z = 4$, $D_x = 1·41$ g cm^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 5·93$ cm^{-1}, $F(000) = 1536$, $T = 117$ K, final $R = 0·038$ for 5021 unique observed reflections. Rh can be considered to possess a pseudo square-planar coordination with $C_2B_8H_{11}$ as a bidentate ligand. Distances to Rh within the icosahedral fragment are Rh—C = 2·198 (4), Rh—B = 2·132 (4), 2·181 (4) and 2·238 (4) Å. An acidic hydrogen bridges B(10) and B(11) at distances of 1·25 (5) and 1·29 (5) Å, B—H—B = 95 (3)°.

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