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$_2$O (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.

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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

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Abstract. [Cu$_2$(C$_{44}$H$_{55}$NO$_4$)$_2$], $M_r = 1451\cdot0$, monoclinic, $P2_1$, $a = 17\cdot657\ (1)$, $b = 25\cdot573\ (2)$, $c = 9\cdot165\ (1)$ Å, $\beta = 91\cdot58\ (1)^\circ$, $V = 4136\cdot9$ Å^3, $Z = 2$, $D_x = 1\cdot17$ Mg m^{-3}, $\lambda(\mathrm{Cu}\ K\alpha) = 1\cdot5418$ Å, $\mu(\mathrm{Cu}\ K\alpha) = 1\cdot017$ mm^{-1}, $T = 295$ K, $F(000) = 1548$, $R = 0\cdot057$ for 5133 observed reflections. The complex consists of a phenolic-oxygen-bridged binuclear copper(II) unit,

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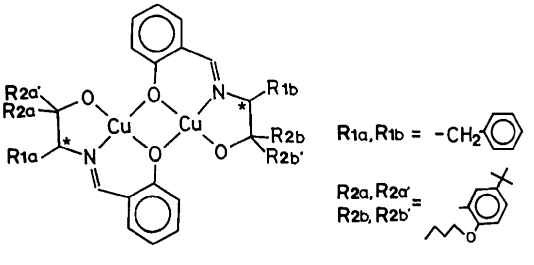
and the chiral Schiff base is incorporated as a tridentate ligand. The Cu···Cu distance is 3·023 (1) Å. The two 2-butoxy-5-*tert*-butylphenyl groups are perpendicular to the oxygen-bridged binuclear copper unit plane and make a groove in the axial positions of the two copper atoms.

Introduction. Reaction of an alkyl diazoacetate with an olefin catalyzed by a copper complex gives an optically active alkyl cyclopropanecarboxylate (Nozaki, Takaya, Moriuti & Noyori, 1968). A series of effective catalysts, chiral Schiff base–copper complexes, was prepared to achieve high e.e. of the products. These complexes have two substituents R_1 and R_2. R_1 comes from the α-amino acid and R_2 comes from the Grignard reagent (Aratani, Yoneyoshi & Nagase, 1982). This chiral copper carbenoid reaction was successfully applied to the synthesis of cyclopropanecarboxylic acids of practical value (Aratani, 1985). Recently, crystals suitable for X-ray work were obtained for the title complex which has benzyl and 2-butoxy-5-*tert*-butylphenyl groups as R_1 and R_2, respectively. As part of a series of studies on the steric course of the reaction (Yanagi, Minobe & Aratani, 1986; Yanagi & Aratani, 1987), the structure has been determined by X-ray analysis.



Experimental. Dark green prismatic crystals obtained by slow evaporation from a chloroform/methanol solution. Crystal used 0·3 × 0·3 × 0·2 mm. Enraf–Nonius CAD-4 diffractometer. Cell dimensions refined by least-squares fitting of θ values of 25 reflections with $20 < \theta < 27°$. ω–2θ scan technique, scan angle $0{\cdot}85° + 0{\cdot}15° \tan\theta$, three reference reflections monitored every 80 min throughout data collection showed no significant changes in intensity. Data corrected for Lp effects and absorption (based on ψ scan; transmission-factor range 0·895–0·997). 8020 unique reflections measured with $1 < \theta < 70°$; 5133 with $I > 2{\cdot}5\sigma(I)$ used in structure determination. h: −22 to 22, k: −33 to 0, l: 0 to 11. Cu atoms located by direct methods with *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982), remaining non-H atoms found on successive Fourier synthesis. Structure refined by full-matrix least squares; $\sum w(|F_o| - |F_c|)^2$ minimized. All non-H atoms refined anisotropically. H atoms are not included in the calculation. Final $R = 0{\cdot}057$, $wR = 0{\cdot}076$ for 901 variables, $w = 4I/[\sigma^2(I) + (0{\cdot}05I)^2]$, $S = 2{\cdot}307$. Because of the disorder, the butoxy and *tert*-butyl groups are not well defined, and further improvements were not possible. $(\Delta/\sigma)_{\max} = 0{\cdot}33$ in the final cycle. Max. and min. peaks in final difference Fourier map 0·48 and −0·24 e Å^{-3}, respectively. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Calculations were carried out on a micro VAX II using the *SDP* system (Frenz, 1978).

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters*

$$B_{eq} = \tfrac{4}{3}\textstyle\sum_i\sum_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}(Å^2)
Cu(1)	0·50670 (5)	0·25	0·8003 (1)	4·18 (2)
Cu(2)	0·36147 (5)	0·24134 (5)	0·6193 (1)	4·15 (2)
O(1)	0·6046 (2)	0·2231 (2)	0·8101 (5)	4·6 (1)
O(2)	0·4070 (2)	0·2806 (2)	0·7833 (5)	4·4 (1)
O(3)	0·2735 (2)	0·2791 (2)	0·5760 (5)	4·9 (1)
O(4)	0·4567 (2)	0·2047 (2)	0·6489 (5)	4·2 (1)
O(5)	0·7714 (3)	0·2851 (3)	1·0962 (6)	7·0 (1)
O(6)	0·5933 (3)	0·2756 (2)	1·2326 (6)	6·6 (1)
O(7)	0·1001 (3)	0·2190 (2)	0·2991 (6)	6·5 (1)
O(8)	0·1296 (3)	0·2836 (3)	0·7212 (7)	7·1 (2)
N(1)	0·5446 (3)	0·3049 (2)	0·9255 (6)	4·4 (1)
N(2)	0·3327 (3)	0·1983 (2)	0·4555 (6)	4·1 (1)
C(1)	0·3790 (4)	0·3181 (3)	0·8718 (7)	4·2 (1)
C(2)	0·2991 (4)	0·3276 (4)	0·8680 (9)	5·5 (2)
C(3)	0·2694 (5)	0·3662 (4)	0·9551 (11)	7·1 (2)
C(4)	0·3178 (5)	0·3962 (4)	1·0500 (10)	7·3 (2)
C(5)	0·3940 (5)	0·3869 (4)	1·0492 (10)	6·4 (2)
C(6)	0·4265 (4)	0·3473 (3)	0·9673 (8)	4·6 (2)
C(7)	0·5061 (4)	0·3412 (3)	0·9866 (8)	4·5 (2)
C(8)	0·6294 (4)	0·3035 (3)	0·9448 (8)	4·8 (2)
C(9)	0·6627 (5)	0·3359 (3)	0·8186 (10)	5·6 (2)
C(10)	0·6539 (5)	0·3940 (4)	0·8446 (10)	6·3 (2)
C(11)	0·5923 (6)	0·4216 (4)	0·7922 (12)	8·1 (3)
C(12)	0·5898 (9)	0·4786 (5)	0·8331 (16)	14·7 (4)
C(13)	0·6420 (15)	0·4987 (8)	0·9242 (22)	23·9 (9)
C(14)	0·06987 (13)	0·4681 (8)	0·9730 (21)	21·9 (8)
C(15)	0·7086 (8)	0·4182 (5)	0·9300 (16)	13·0 (4)
C(16)	0·6490 (3)	0·2452 (4)	0·9273 (7)	4·7 (1)
C(17)	0·7337 (4)	0·2375 (3)	0·8882 (8)	4·9 (2)
C(18)	0·7928 (4)	0·2556 (4)	0·9813 (8)	5·3 (2)
C(19)	0·8662 (4)	0·2452 (5)	0·9514 (9)	7·0 (2)
C(20)	0·8846 (4)	0·2152 (4)	0·8308 (11)	6·9 (2)
C(21)	0·8273 (4)	0·1964 (4)	0·7332 (10)	5·9 (2)
C(22)	0·7503 (4)	0·2093 (3)	0·7683 (9)	5·1 (2)
C(23)	0·8298 (5)	0·3055 (5)	1·1898 (12)	9·0 (3)
C(24)	0·7844 (7)	0·3352 (6)	1·3142 (12)	11·2 (4)
C(25)	0·8443 (11)	0·3658 (9)	1·4097 (17)	16·6 (6)
C(26)	0·7907 (15)	0·3915 (13)	1·5402 (22)	27 (1)
C(27)	0·8434 (5)	0·1629 (5)	0·5974 (10)	7·7 (3)
C(28)	0·9234 (7)	0·1416 (7)	0·5941 (17)	16·4 (5)
C(29)	0·7865 (7)	0·1168 (6)	0·5824 (14)	11·7 (4)
C(30)	0·8237 (9)	0·1959 (6)	0·4607 (14)	13·1 (5)
C(31)	0·6377 (4)	0·2092 (3)	1·0634 (7)	4·8 (2)
C(32)	0·6137 (4)	0·2244 (3)	1·2040 (8)	5·6 (2)
C(33)	0·6100 (5)	0·1852 (4)	1·3190 (9)	6·8 (2)
C(34)	0·6260 (5)	0·1340 (4)	1·2886 (10)	7·1 (2)
C(35)	0·6512 (5)	0·1189 (4)	1·1459 (10)	6·1 (2)
C(36)	0·6546 (4)	0·1572 (3)	1·0418 (8)	5·0 (2)
C(37)	0·5687 (7)	0·2867 (4)	1·3762 (10)	8·9 (3)
C(38)	0·5292 (9)	0·3403 (6)	1·3656 (13)	12·5 (4)
C(39)	0·4785 (10)	0·3500 (7)	1·4814 (19)	14·2 (5)
C(40)	0·4258 (11)	0·3949 (8)	1·4881 (21)	19·7 (6)
C(41)	0·6681 (6)	0·0630 (4)	1·1137 (11)	8·0 (3)
C(42)	0·7441 (10)	0·0597 (6)	1·0507 (27)	21·3 (6)
C(43)	0·6696 (13)	0·0276 (6)	1·2456 (18)	18·5 (7)
C(44)	0·6090 (13)	0·0444 (6)	1·0210 (21)	20·5 (7)
C(45)	0·4711 (4)	0·1557 (3)	0·6047 (7)	4·4 (2)
C(46)	0·5331 (4)	0·1286 (3)	0·6686 (9)	5·2 (2)
C(47)	0·5486 (5)	0·0773 (4)	0·6239 (10)	6·9 (2)
C(48)	0·5021 (6)	0·0515 (4)	0·5193 (11)	7·3 (2)
C(49)	0·4412 (5)	0·0776 (3)	0·4585 (10)	6·4 (2)
C(50)	0·4253 (4)	0·1304 (3)	0·4978 (8)	4·6 (2)
C(51)	0·3612 (4)	0·1537 (3)	0·4250 (8)	4·5 (2)
C(52)	0·2673 (4)	0·2209 (3)	0·3709 (7)	4·3 (1)
C(53)	0·2981 (4)	0·2556 (3)	0·2477 (7)	4·7 (2)

Table 1 (*cont.*)

	x	*y*	*z*	B_{eq}(Å²)
C(54)	0·3321 (4)	0·2213 (3)	0·1322 (8)	4·7 (2)
C(55)	0·2838 (5)	0·1980 (4)	0·0292 (8)	6·2 (2)
C(56)	0·3103 (6)	0·1626 (4)	−0·0672 (10)	7·4 (3)
C(57)	0·3875 (5)	0·1483 (4)	−0·0646 (9)	6·5 (2)
C(58)	0·4365 (5)	0·1713 (4)	0·0320 (9)	6·7 (2)
C(59)	0·4091 (4)	0·2078 (3)	0·1312 (9)	5·6 (2)
C(60)	0·2216 (3)	0·2500 (3)	0·4861 (7)	4·4 (1)
C(61)	0·1666 (4)	0·2901 (3)	0·4117 (8)	4·9 (2)
C(62)	0·1053 (4)	0·2706 (3)	0·3200 (9)	5·4 (2)
C(63)	0·0539 (4)	0·3074 (4)	0·2562 (10)	7·0 (2)
C(64)	0·0663 (5)	0·3608 (4)	0·2852 (12)	7·7 (3)
C(65)	0·1264 (5)	0·3799 (4)	0·3717 (10)	6·4 (2)
C(66)	0·1771 (4)	0·3425 (3)	0·4349 (9)	5·3 (2)
C(67)	0·0336 (5)	0·2010 (4)	0·2204 (9)	6·2 (2)
C(68)	0·0417 (5)	0·1435 (4)	0·2098 (10)	7·4 (2)
C(69)	−0·0261 (6)	0·1180 (5)	0·1304 (13)	9·1 (3)
C(70)	−0·0254 (10)	0·0613 (6)	0·1113 (17)	13·5 (5)
C(71)	0·1409 (6)	0·4391 (4)	0·3947 (12)	8·4 (3)
C(72)	0·2189 (8)	0·4500 (6)	0·4427 (16)	13·0 (4)
C(73)	0·0775 (9)	0·4604 (6)	0·4830 (7)	13·7 (5)
C(74)	0·1284 (9)	0·4671 (6)	0·2242 (17)	13·3 (5)
C(75)	0·1789 (4)	0·2116 (4)	0·5872 (8)	5·2 (2)
C(76)	0·1379 (4)	0·2314 (4)	0·7034 (8)	6·6 (2)
C(77)	0·1035 (5)	0·1947 (4)	0·8073 (9)	6·7 (2)
C(78)	0·1114 (5)	0·1426 (5)	0·7860 (11)	8·0 (3)
C(79)	0·1504 (5)	0·1207 (4)	0·6655 (10)	6·6 (2)
C(80)	0·1831 (4)	0·1568 (3)	0·5682 (10)	6·0 (2)
C(81)	0·0702 (7)	0·3024 (6)	0·8003 (24)	21·3 (7)
C(82)	0·0534 (8)	0·3538 (6)	0·7843 (22)	15·5 (6)
C(83)	−0·0225 (10)	0·3679 (8)	0·8499 (22)	17·8 (6)
C(84)	−0·0358 (14)	0·4208 (10)	0·8792 (24)	25·2 (9)
C(85)	0·1594 (6)	0·0631 (4)	0·6406 (13)	8·3 (3)
C(86)	0·2410 (9)	0·0489 (5)	0·6500 (26)	16·8 (7)
C(87)	0·1207 (11)	0·0461 (6)	0·5078 (18)	19·3 (6)
C(88)	0·1169 (11)	0·0320 (7)	0·7624 (30)	22·8 (8)

Discussion. Final atomic coordinates and equivalent isotropic thermal parameters are listed in Table 1.[*] Selected bond distances and angles are given in Table 2. The molecular structure with atom numbering is shown in Fig. 1. The title complex consists of a phenolic-oxygen-bridged binuclear copper(II) unit, and the chiral Schiff base was incorporated as a tridentate ligand. The coordination sphere around Cu(2) is roughly planar within 0·049 (1) Å, while that around Cu(1) deviates significantly from planarity, maximum deviation from the mean plane being 0·249 (5) Å. The Cu$\cdots$Cu distance is 3·023 (1) Å. The Cu—O—Cu bridge angles are 102·0 (2) and 100·4 (2)°.

The conformations of the two Schiff base ligands are similar to each other except for the $R_{2a'}$ group which is rotated about 180° around the C(16)—C(31) bond. The two benzene rings of the salicylidene moieties are planar within 0·022 (9) Å, and the dihedral angle is 33·0 (4)°. R_{1a} and R_{1b} lie on the same side of the copper coordination plane. $R_{2a'}$ and $R_{2b'}$ lie on the opposite side to the R_1 groups and approximately perpendicular to the copper coordination plane to make a groove in the axial position of the two copper atoms.

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

Cu(1)–O(1)	1·861 (3)	Cu(2)–O(3)	1·863 (4)
Cu(1)–O(2)	1·929 (3)	Cu(2)–O(4)	1·938 (3)
Cu(1)–O(4)	1·996 (4)	Cu(2)–O(2)	1·961 (4)
Cu(1)–N(1)	1·921 (5)	Cu(2)–N(2)	1·920 (4)
O(1)–C(16)	1·429 (6)	O(3)–C(60)	1·426 (6)
O(2)–C(1)	1·358 (6)	O(4)–C(45)	1·341 (7)
O(5)–C(18)	1·358 (8)	O(7)–C(62)	1·336 (7)
O(5)–C(23)	1·422 (8)	O(7)–C(67)	1·437 (7)
O(6)–C(32)	1·385 (8)	O(8)–C(76)	1·353 (9)
O(6)–C(37)	1·426 (8)	O(8)–C(81)	1·377 (12)
N(1)–C(7)	1·288 (7)	N(2)–C(51)	1·279 (7)
N(1)–C(8)	1·504 (6)	N(2)–C(52)	1·490 (6)
C(1)–C(2)	1·432 (7)	C(45)–C(46)	1·411 (7)
C(1)–C(6)	1·408 (7)	C(45)–C(50)	1·410 (7)
C(2)–C(3)	1·383 (9)	C(46)–C(47)	1·402 (9)
C(3)–C(4)	1·426 (10)	C(47)–C(48)	1·409 (10)
C(4)–C(5)	1·367 (9)	C(48)–C(49)	1·369 (9)
C(5)–C(6)	1·394 (8)	C(49)–C(50)	1·428 (8)
C(6)–C(7)	1·421 (7)	C(50)–C(51)	1·428 (8)
C(8)–C(9)	1·552 (9)	C(52)–C(53)	1·547 (8)
C(8)–C(16)	1·539 (10)	C(52)–C(60)	1·539 (8)
C(9)–C(10)	1·514 (9)	C(53)–C(54)	1·512 (8)
C(16)–C(17)	1·560 (7)	C(60)–C(61)	1·555 (8)
C(16)–C(31)	1·568 (8)	C(60)–C(75)	1·561 (8)

O(1)–Cu(1)–O(2)	171·1 (2)	O(3)–Cu(2)–O(4)	174·9 (2)
O(1)–Cu(1)–O(4)	102·2 (2)	O(2)–Cu(2)–O(3)	102·7 (2)
O(1)–Cu(1)–N(1)	86·2 (2)	O(3)–Cu(2)–N(2)	86·0 (2)
O(2)–Cu(1)–O(4)	78·1 (1)	O(2)–Cu(2)–O(4)	78·8 (1)
O(2)–Cu(1)–N(1)	93·1 (2)	O(4)–Cu(2)–N(2)	92·4 (2)
O(3)–Cu(1)–N(1)	168·5 (2)	O(2)–Cu(2)–N(2)	170·9 (2)
Cu(1)–O(1)–C(16)	112·3 (3)	Cu(2)–O(3)–C(60)	111·8 (3)
Cu(1)–O(2)–Cu(2)	102·0 (2)	Cu(1)–O(4)–Cu(2)	100·4 (2)
Cu(1)–O(2)–C(1)	125·7 (3)	Cu(2)–O(4)–C(45)	125·5 (3)
Cu(2)–O(2)–C(1)	132·2 (3)	Cu(1)–O(4)–C(45)	131·9 (3)
Cu(1)–N(1)–C(7)	127·4 (4)	Cu(2)–N(2)–C(51)	125·8 (4)
Cu(1)–N(1)–C(8)	112·5 (4)	Cu(2)–N(2)–C(52)	111·7 (3)
C(7)–N(1)–C(8)	120·1 (5)	C(51)–N(2)–C(52)	122·4 (5)
O(2)–C(1)–C(2)	118·6 (5)	O(4)–C(45)–C(46)	119·0 (5)
O(2)–C(1)–C(6)	121·7 (5)	O(4)–C(45)–C(50)	121·9 (5)
C(1)–C(6)–C(7)	126·2 (5)	C(45)–C(50)–C(51)	124·3 (5)
C(5)–C(6)–C(7)	115·6 (5)	C(49)–C(50)–C(51)	115·9 (5)
N(1)–C(7)–C(6)	123·7 (5)	N(2)–C(51)–C(50)	125·6 (5)
N(1)–C(8)–C(9)	107·2 (4)	N(2)–C(52)–C(53)	108·6 (4)
N(1)–C(8)–C(16)	103·7 (4)	N(2)–C(52)–C(60)	104·2 (4)
C(9)–C(8)–C(16)	110·4 (5)	C(53)–C(52)–C(60)	115·1 (5)
C(8)–C(9)–C(10)	111·4 (6)	C(52)–C(53)–C(54)	109·4 (5)
O(1)–C(16)–C(8)	110·0 (4)	O(3)–C(60)–C(52)	108·0 (4)
O(1)–C(16)–C(17)	106·7 (5)	O(3)–C(60)–C(61)	107·1 (5)
O(1)–C(16)–C(31)	106·7 (5)	O(3)–C(60)–C(75)	107·4 (4)
C(8)–C(16)–C(17)	111·5 (5)	C(52)–C(60)–C(61)	110·6 (4)
C(8)–C(16)–C(31)	116·8 (5)	C(52)–C(60)–C(75)	111·9 (6)
C(17)–C(16)–C(31)	104·6 (4)	C(61)–C(60)–C(75)	111·6 (4)

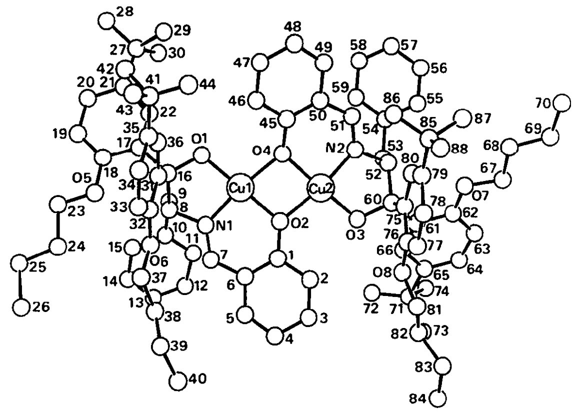


Fig. 1. The molecular structure of the title complex showing the atom numbering. [R_{1a}: C(9) to C(15); R_{1b}: C(53) to C(59); R_{2a}: O(5), C(17) to C(30); $R_{2a'}$: O(6), C(31) to C(44); R_{2b}: O(7), C(61) to C(74); $R_{2b'}$: O(8), C(75) to C(88).]

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[*] Lists of structure factors, anisotropic thermal parameters, supplementary bond distances and angles and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43650 (38 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

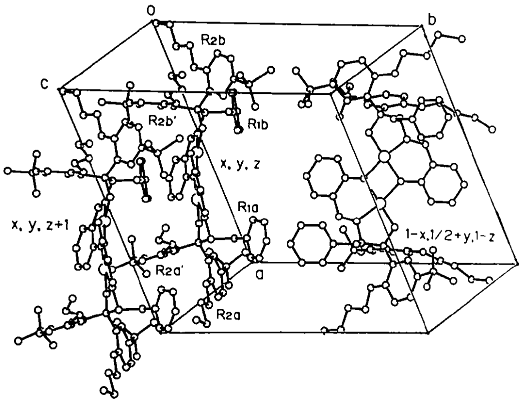

Fig. 2. The crystal packing of the title complex.

Some carbon atoms in the *tert*-butyl and butoxy groups have rather high thermal factors. This is possibly a sign of structural disorder, which could not be resolved into major disorder sites. Bond distances and angles within these groups are not reliable because of the disorder problem. The absolute configuration of the Schiff base must be *R* since the Schiff base was synthesized from D-phenylalanine.

The crystal packing is shown in Fig. 2. The grooves formed by the $R_{2a'}$ and $R_{2b'}$ groups are occupied by the R_{1b} group of the neighbouring molecule along the *c* axis. The atoms of the R_{1b} group have relatively small thermal factors compared with those of the R_{1a} group. There are no unusually close intermolecular contacts.

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Chlorure Hexachloroplatinate(IV) de Bis(pentanediammonium-1,5) (Chlorure Hexachloroplatinate de Cadavérine)

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Abstract. $[C_5H_{16}N_2]_2Cl_2[PtCl_6]$, $M_r = 687\cdot1$, orthorhombic, $Fmmm$, $a = 9\cdot624$ (2), $b = 13\cdot966$ (3), $c = 19\cdot076$ (4) Å, $V = 2564$ (1) Å^3, $Z = 4$, $D_m = 1\cdot80$ (2), $D_x = 1\cdot78$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0\cdot7107$ Å, $\mu = 6\cdot37$ mm^{-1}, $F(000) = 1336$, $T = 294$ (1) K, $R = 0\cdot020$ for 1052 independent reflections $[I > 2\sigma(I)]$. The Pt atom exhibits an almost regular octahedral surrounding. The C and N atoms of $[C_5H_{16}N_2]^{2+}$ are in the same plane. The cation shows 2 and *m* symmetries. Its bond lengths and angles are normal. The structure can be regarded as constituted of cation layers separated alternately by layers of Cl^- and layers of $[PtCl_6]^{2-}$. N—H···Cl hydrogen bonds take part in the cohesion of the structure.

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