The diester vinyl unit can be represented by the resonance hybrid between the diene (A) and the $2\sigma-\pi$ complex (B).

CH_3OCO OCOCH₃ CH_3OCO OCOCH₃

Fe   Fe

(CO)₃   (CO)₃

(A)   (B)

The canonical form (B) makes a large contribution as indicated by the C(5)—C(6) bond length which is shorter by 0·022 and 0·029 Å than those of C(4)—C(5) and C(6)—C(7).

The Fe—C bond distances vary over a small range [2·059 (4) to 2·112 (4) Å] reflecting the fact that the metal–ligand bonding is nearly the same for the four C atoms of the η^4 system.

The two CH₃COO— ester groups are cis to each other about the C(5)—C(6) bond. Both ester groups [C(11)—C(10)—O(6),O(4) and C(9)—C(8)—O(5),O(7)] are planar [to within ±0·004 (6) and ±0·015 (6) Å, respectively]. The dihedral angle between the two ester groups is 21·4 (6)°. The C(8)—O(7) and C(10)—O(6) bonds are shorter by 0·024 and 0·022 Å than the accepted value of 1·215 (5) Å for the C=O bond (Sutton, 1965); they are oriented cis to the C(4)—H and C(7)—H bonds, respectively (Mathieson, 1965; Chothia & Pauling, 1970).

The butadiene residue is planar within ±0·005 Å. The dihedral angles between the butadiene residue and the ester groups at C(4) and C(7) are 10·1 (5) and 11·3 (6)°, respectively.

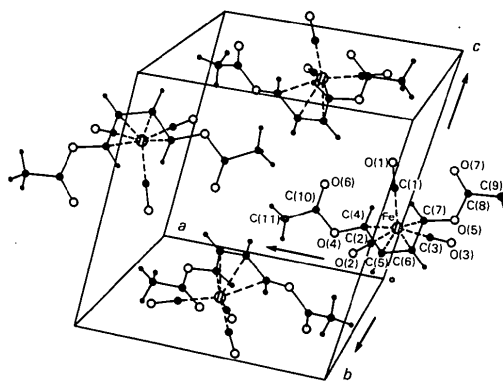The discrete molecules, as shown in Fig. 2, are held in the crystal by van der Waals forces.

Fig. 2. A perspective drawing of the contents of one unit cell.

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Structure of a Copper(II) Complex with a Chiral Schiff Base and a Chiral Aminoalcohol

BY KAZUNORI YANAGI AND MASAO MINOBE*

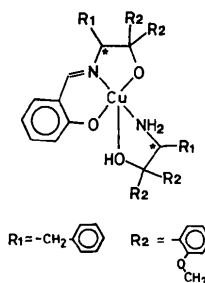Takatsuki Research Laboratory, Sumitomo Chemical Co. Ltd, 2-10-1, Tsukahara, Takatsuki, Osaka 569, Japan

Abstract. [(R)-2-Amino-1,1-bis(2-methoxyphenyl)-3-phenyl-1-propanolato][(R)-1,1-bis(2-methoxyphenyl)-3-phenyl-2-salicylideneamino-1-propanolato]copper(II), $[Cu(C_{30}H_{27}NO_4)(C_{23}H_{25}NO_3)]$, $M_r = 892\cdot6$, monoclinic, $P2_1$, $a = 11\cdot527$ (1), $b = 21\cdot081$ (1), $c = 9\cdot564$ (1) Å, $\beta = 99\cdot01$ (1)°, $V = 2295\cdot3$ (6) Å³, $Z = 2$, $D_x = 1\cdot29$ Mg m⁻³, $\lambda(Cu\ K\alpha) = 1\cdot5418$ Å, $\mu(Cu\ K\alpha) = 1\cdot073$ mm⁻¹, $T = 295$ K, $F(000) = 938$, $R = 0\cdot029$ for 3852 observed reflections. The co-ordination geometry of the Cu atom is a distorted square pyramid (4 + 1). The tridentate Schiff-base group occupies three of the basal square-planar coordination sites and an N atom of the aminoalcohol

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group completes the plane. A protonated O atom of the aminoalcohol group occupies the axial position [Cu—O = 2·650 (2) Å].

Introduction. Reaction of an alkyl diazoacetate with an olefin catalyzed by a chiral copper complex gives an optically active alkyl cyclopropanecarboxylate (Nozaki, Takaya, Moriuti & Noyori, 1968). This reaction was applied to the synthesis of cyclopropane-carboxylic acids of practical value: (1R)-trans-chrysanthemic acid, (1R)-cis-permethrinic acid and (1S)-2,2-dimethylcyclopropanecarboxylic acid (Aratani, Yoneyoshi & Nagase, 1975, 1977, 1982; Aratani, 1985). The binuclear structure of an effective catalyst in which the chiral Schiff base was incorporated as a tridentate ligand was established by X-ray analysis (Yanagi & Minobe, 1987). In order to characterize the geometries of the chiral Schiff base–copper complexes, the crystal structure of the title mononuclear complex has been determined.

Experimental. Dark brown prismatic crystals obtained by slow evaporation from a chloroform/methanol solution. Crystal $0.3 \times 0.2 \times 0.2$ mm. Enraf–Nonius CAD-4 diffractometer. Cell dimensions refined by least-squares fitting of θ values of 25 reflections with $20 < \theta < 27°$. $\omega–2\theta$ scan technique, scan angle $0.8° + 0.15°$ tan θ, three reference reflections monitored every 60 min throughout data collection showed no significant deterioration. Data corrected for Lorentz and polarization effects, but not for absorption. 4479 unique reflections measured with $1 < \theta < 70°$; 3852 with $I > 3\sigma(I)$ used in structure determination. h: -15 to 15, k: 0 to 27, l: 0 to 12. The Cu-atom position was obtained from a three-dimensional Patterson map. The remaining non-H atoms were found on successive Fourier syntheses. Structure refined by full-matrix least squares; $\sum w(|F_o| - |F_c|)^2$ minimized. All non-H atoms refined anisotropically. H-atom positions refined with a fixed isotropic thermal parameter (6 Å²), except those in methyl groups which were fixed in the calculated positions. Final $R = 0.029$, $wR = 0.041$ for 688 variables, $w = 4I/[\sigma^2(I) + (0.05I)^2]$, $S = 1.372$, $(\Delta/\sigma)_{max} = 0.29$. Extinction coefficient refined to 1.4 (1) $\times 10^{-6}$. Max. and min. peaks in final difference Fourier map 0.17 and -0.45 e Å^{-3}. Atomic scattering factors from International Tables for X-ray Crystallography (1974).

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters for non-hydrogen atoms*

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

	x	y	z	$B_{eq}(\text{Å}^2)$
Cu	0·66671 (3)	0·5	0·66326 (4)	3·025 (6)
O(1)	0·5362 (2)	0·4435 (1)	0·6428 (2)	3·26 (4)
O(2)	0·7951 (2)	0·5563 (1)	0·6473 (3)	4·84 (6)
O(3)	0·1977 (2)	0·5058 (2)	0·4770 (3)	5·48 (6)
O(4)	0·4033 (3)	0·5692 (1)	0·3368 (3)	5·25 (6)
O(5)	0·6943 (2)	0·4784 (1)	0·9395 (2)	3·72 (4)
O(6)	1·0140 (2)	0·3834 (2)	1·0882 (3)	5·28 (6)
O(7)	0·7806 (3)	0·5694 (1)	1·1086 (3)	5·77 (6)
N(1)	0·5516 (2)	0·5657 (1)	0·6139 (3)	3·12 (5)
N(2)	0·7974 (2)	0·4360 (1)	0·7157 (3)	3·05 (5)
C(1)	0·7895 (3)	0·6161 (2)	0·6094 (4)	4·03 (7)
C(2)	0·8963 (3)	0·6485 (2)	0·6023 (5)	5·05 (8)
C(3)	0·8967 (4)	0·7106 (2)	0·5589 (5)	5·93 (9)
C(4)	0·7919 (4)	0·7440 (2)	0·5236 (5)	6·4 (1)
C(5)	0·6889 (4)	0·7143 (2)	0·5306 (5)	5·30 (9)
C(6)	0·6842 (3)	0·6499 (2)	0·5716 (4)	3·85 (6)
C(7)	0·5700 (3)	0·6228 (2)	0·5777 (3)	3·71 (6)
C(8)	0·4342 (2)	0·5430 (1)	0·6253 (3)	2·99 (5)
C(9)	0·4170 (3)	0·5483 (2)	0·7819 (3)	3·52 (6)
C(10)	0·4239 (3)	0·6159 (2)	0·8353 (3)	3·59 (6)
C(11)	0·5310 (4)	0·6421 (2)	0·8983 (4)	5·20 (9)
C(12)	0·5361 (5)	0·7049 (2)	0·9451 (5)	6·8 (1)
C(13)	0·4346 (5)	0·7409 (2)	0·9302 (5)	7·2 (1)
C(14)	0·3289 (4)	0·7159 (2)	0·8678 (5)	6·8 (1)
C(15)	0·3238 (3)	0·6537 (2)	0·8204 (4)	5·16 (8)
C(16)	0·4320 (2)	0·4722 (2)	0·5766 (3)	3·11 (5)
C(17)	0·3256 (3)	0·4381 (2)	0·6234 (3)	3·52 (6)
C(18)	0·2097 (3)	0·4556 (2)	0·5704 (4)	4·35 (7)
C(19)	0·1159 (3)	0·4237 (2)	0·6149 (4)	5·36 (8)
C(20)	0·1350 (3)	0·3753 (2)	0·7104 (5)	5·96 (9)
C(21)	0·2495 (4)	0·3577 (2)	0·7652 (4)	5·42 (9)
C(22)	0·3432 (3)	0·3895 (2)	0·7210 (4)	4·27 (7)
C(23)	0·0850 (4)	0·5214 (3)	0·4073 (7)	8·6 (1)
C(24)	0·4232 (3)	0·4610 (2)	0·4136 (3)	3·57 (6)
C(25)	0·4128 (2)	0·5058 (2)	0·3037 (3)	4·25 (7)
C(26)	0·4128 (3)	0·4872 (3)	0·1645 (4)	5·7 (1)
C(27)	0·4186 (4)	0·4228 (3)	0·1324 (4)	6·5 (1)
C(28)	0·4263 (3)	0·3783 (2)	0·2366 (4)	5·71 (9)
C(29)	0·4287 (3)	0·3983 (2)	0·3751 (4)	4·48 (7)
C(30)	0·4005 (5)	0·6152 (3)	0·2301 (5)	7·8 (1)
C(31)	0·8179 (2)	0·4045 (1)	0·8561 (3)	3·05 (5)
C(32)	0·7265 (3)	0·3513 (2)	0·8553 (4)	3·80 (6)
C(33)	0·7409 (3)	0·3005 (2)	0·7492 (3)	3·61 (6)
C(34)	0·6621 (3)	0·2961 (2)	0·6228 (4)	4·16 (7)
C(35)	0·6770 (4)	0·2506 (2)	0·5231 (4)	4·95 (8)
C(36)	0·7709 (4)	0·2084 (2)	0·5470 (5)	5·9 (1)
C(37)	0·8503 (4)	0·2134 (2)	0·6714 (5)	6·1 (1)
C(38)	0·8359 (4)	0·2585 (2)	0·7711 (5)	5·05 (8)
C(39)	0·8098 (2)	0·4531 (2)	0·9736 (3)	3·09 (5)
C(40)	0·8258 (3)	0·4195 (2)	1·1197 (3)	3·36 (6)
C(41)	0·9288 (3)	0·3862 (2)	1·1721 (3)	3·80 (6)
C(42)	0·9406 (3)	0·3570 (2)	1·3033 (4)	4·38 (7)
C(43)	0·8522 (3)	0·3598 (2)	1·3831 (4)	4·60 (8)
C(44)	0·7513 (3)	0·3912 (2)	1·3351 (4)	4·67 (8)
C(45)	0·7383 (3)	0·4210 (2)	1·2033 (4)	4·21 (7)
C(46)	1·1264 (4)	0·3637 (4)	1·1431 (5)	9·7 (2)
C(47)	0·9001 (2)	0·5072 (2)	0·9810 (3)	3·64 (6)
C(48)	0·8815 (3)	0·5647 (2)	1·0500 (4)	4·53 (7)
C(49)	0·9607 (4)	0·6148 (2)	1·0548 (5)	6·3 (1)
C(50)	1·0622 (4)	0·6076 (2)	0·9955 (6)	6·9 (1)
C(51)	1·0852 (3)	0·5518 (2)	0·9326 (5)	6·2 (1)
C(52)	1·0034 (3)	0·5018 (2)	0·9247 (4)	4·46 (6)
C(53)	0·7785 (5)	0·6035 (4)	1·2335 (6)	11·4 (2)

Calculations were carried out using the SDP system (Frenz, 1978) on a micro VAX II.

Discussion. Final atomic coordinates and equivalent isotropic thermal parameters are listed in Table 1.*

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

Cu—O(1)	1·905 (2)	C(16)—C(24)	1·565 (4)
Cu—O(2)	1·922 (2)	C(17)—C(18)	1·402 (4)
Cu—O(5)	2·650 (2)	C(17)—C(22)	1·380 (5)
Cu—N(1)	1·925 (2)	C(18)—C(19)	1·395 (5)
Cu—N(2)	2·026 (2)	C(19)—C(20)	1·364 (7)
O(1)—C(16)	1·404 (3)	C(20)—C(21)	1·392 (7)
O(2)—C(1)	1·310 (4)	C(21)—C(22)	1·392 (5)
O(3)—C(18)	1·377 (5)	C(24)—C(25)	1·403 (5)
O(3)—C(23)	1·403 (4)	C(24)—C(29)	1·376 (5)
O(4)—C(25)	1·384 (5)	C(25)—C(26)	1·388 (5)
O(4)—C(30)	1·404 (5)	C(26)—C(27)	1·396 (8)
O(5)—C(39)	1·423 (3)	C(27)—C(28)	1·362 (8)
O(6)—C(41)	1·364 (4)	C(28)—C(29)	1·386 (6)
O(6)—C(46)	1·384 (5)	C(31)—C(32)	1·538 (4)
O(7)—C(48)	1·371 (5)	C(31)—C(39)	1·536 (4)
O(7)—C(53)	1·397 (6)	C(32)—C(33)	1·502 (4)
N(1)—C(7)	1·279 (5)	C(33)—C(34)	1·397 (4)
N(1)—C(8)	1·456 (4)	C(33)—C(38)	1·400 (5)
N(2)—C(31)	1·483 (3)	C(34)—C(35)	1·381 (5)
C(1)—C(2)	1·419 (4)	C(35)—C(36)	1·392 (7)
C(1)—C(6)	1·404 (5)	C(36)—C(37)	1·387 (6)
C(2)—C(3)	1·375 (5)	C(37)—C(38)	1·374 (6)
C(3)—C(4)	1·394 (7)	C(39)—C(40)	1·552 (4)
C(4)—C(5)	1·353 (7)	C(39)—C(47)	1·539 (4)
C(5)—C(6)	1·417 (4)	C(40)—C(41)	1·403 (5)
C(6)—C(7)	1·445 (4)	C(40)—C(45)	1·382 (5)
C(8)—C(9)	1·545 (4)	C(41)—C(42)	1·385 (4)
C(8)—C(16)	1·562 (4)	C(42)—C(43)	1·367 (5)
C(9)—C(10)	1·511 (5)	C(43)—C(44)	1·355 (6)
C(10)—C(11)	1·400 (5)	C(44)—C(45)	1·395 (5)
C(10)—C(15)	1·391 (5)	C(47)—C(48)	1·412 (5)
C(11)—C(12)	1·396 (6)	C(47)—C(52)	1·386 (4)
C(12)—C(13)	1·385 (8)	C(48)—C(49)	1·393 (6)
C(13)—C(14)	1·375 (8)	C(49)—C(50)	1·387 (8)
C(14)—C(15)	1·385 (7)	C(50)—C(51)	1·366 (7)
C(16)—C(17)	1·548 (4)	C(51)—C(52)	1·409 (5)

O(1)—Cu—O(2)	169·7 (1)	O(3)—C(18)—C(19)	124·3 (3)
O(1)—Cu—O(5)	87·94 (8)	C(17)—C(18)—C(19)	120·3 (4)
O(1)—Cu—N(1)	85·55 (9)	C(18)—C(19)—C(20)	120·9 (4)
O(1)—Cu—N(2)	98·8 (1)	C(19)—C(20)—C(21)	119·7 (3)
O(2)—Cu—O(5)	102·2 (2)	C(20)—C(21)—C(22)	119·5 (4)
O(2)—Cu—N(1)	92·7 (1)	C(17)—C(22)—C(21)	121·6 (4)
O(2)—Cu—N(2)	83·06 (9)	C(16)—C(24)—C(25)	129·0 (3)
O(5)—Cu—N(1)	109·81 (8)	C(16)—C(24)—C(29)	114·5 (3)
O(5)—Cu—N(2)	70·74 (8)	C(25)—C(24)—C(29)	116·6 (3)
N(1)—Cu—N(2)	175·6 (2)	O(4)—C(25)—C(24)	118·6 (3)
Cu—O(1)—C(16)	112·4 (2)	O(4)—C(25)—C(26)	120·2 (4)
Cu—O(2)—C(1)	127·7 (2)	C(24)—C(25)—C(26)	121·1 (4)
C(18)—O(3)—C(23)	118·6 (3)	C(25)—C(26)—C(27)	119·5 (4)
C(25)—O(4)—C(30)	119·6 (3)	C(26)—C(27)—C(28)	120·6 (4)
Cu—O(5)—C(39)	104·8 (2)	C(27)—C(28)—C(29)	118·6 (4)
C(41)—O(6)—C(46)	120·5 (3)	C(24)—C(29)—C(28)	123·6 (4)
C(48)—O(7)—C(53)	121·1 (4)	N(2)—C(31)—C(32)	108·0 (2)
Cu—N(1)—C(7)	127·4 (2)	N(2)—C(31)—C(39)	110·2 (2)
Cu—N(1)—C(8)	111·0 (2)	C(32)—C(31)—C(39)	111·7 (2)
C(7)—N(1)—C(8)	121·6 (3)	C(31)—C(32)—C(33)	112·1 (2)
Cu—N(2)—C(31)	122·0 (2)	C(32)—C(33)—C(34)	120·4 (3)
O(2)—C(1)—C(2)	118·1 (4)	C(32)—C(33)—C(38)	121·2 (3)
O(2)—C(1)—C(6)	124·2 (3)	C(34)—C(33)—C(38)	118·3 (4)
C(2)—C(1)—C(6)	117·7 (3)	C(33)—C(34)—C(35)	120·7 (3)
C(1)—C(2)—C(3)	121·1 (4)	C(34)—C(35)—C(36)	120·6 (3)
C(2)—C(3)—C(4)	120·7 (4)	C(35)—C(36)—C(37)	118·9 (4)
C(3)—C(4)—C(5)	119·4 (4)	C(36)—C(37)—C(38)	120·8 (4)
C(4)—C(5)—C(6)	121·9 (4)	C(33)—C(38)—C(37)	120·7 (3)
C(1)—C(6)—C(5)	119·2 (4)	O(5)—C(39)—C(31)	104·1 (3)
C(1)—C(6)—C(7)	123·1 (3)	O(5)—C(39)—C(40)	110·6 (3)
C(5)—C(6)—C(7)	117·6 (3)	O(5)—C(39)—C(47)	109·6 (2)
N(1)—C(7)—C(6)	125·0 (3)	C(31)—C(39)—C(40)	110·0 (2)
N(1)—C(8)—C(9)	108·1 (2)	C(31)—C(39)—C(47)	114·2 (2)
N(1)—C(8)—C(16)	105·3 (2)	C(40)—C(39)—C(47)	108·3 (3)
C(9)—C(8)—C(16)	111·1 (2)	C(39)—C(40)—C(41)	121·7 (2)
C(8)—C(9)—C(10)	112·8 (2)	C(39)—C(40)—C(45)	121·0 (3)
C(9)—C(10)—C(11)	120·9 (4)	C(41)—C(40)—C(45)	117·3 (3)
C(9)—C(10)—C(15)	120·5 (3)	O(6)—C(41)—C(40)	117·3 (3)
C(11)—C(10)—C(15)	118·7 (3)	O(6)—C(41)—C(42)	122·4 (3)
C(10)—C(11)—C(12)	120·2 (4)	C(40)—C(41)—C(42)	120·3 (3)
C(11)—C(12)—C(13)	119·7 (5)	C(41)—C(42)—C(43)	120·6 (4)
C(12)—C(13)—C(14)	120·7 (4)	C(42)—C(43)—C(44)	120·5 (3)
C(13)—C(14)—C(15)	119·6 (4)	C(43)—C(44)—C(45)	119·4 (3)
C(10)—C(15)—C(14)	121·1 (4)	C(40)—C(45)—C(44)	121·8 (3)
O(1)—C(16)—C(8)	107·8 (2)	C(39)—C(47)—C(48)	120·4 (3)
O(1)—C(16)—C(17)	109·2 (2)	C(39)—C(47)—C(52)	122·5 (3)
O(1)—C(16)—C(24)	107·5 (2)	C(48)—C(47)—C(52)	117·1 (3)
C(8)—C(16)—C(17)	109·5 (2)	O(7)—C(48)—C(47)	117·1 (3)

Table 2 (cont.)

C(8)—C(16)—C(24)	115·9 (2)	O(7)—C(48)—C(49)	121·6 (3)
C(17)—C(16)—C(24)	106·7 (2)	C(47)—C(48)—C(49)	121·3 (4)
C(16)—C(17)—C(18)	121·8 (3)	C(48)—C(49)—C(50)	119·6 (5)
C(16)—C(17)—C(22)	120·2 (3)	C(49)—C(50)—C(51)	120·6 (4)
C(18)—C(17)—C(22)	118·1 (3)	C(50)—C(51)—C(52)	119·6 (4)
O(3)—C(18)—C(17)	115·4 (3)	C(47)—C(52)—C(51)	121·7 (4)

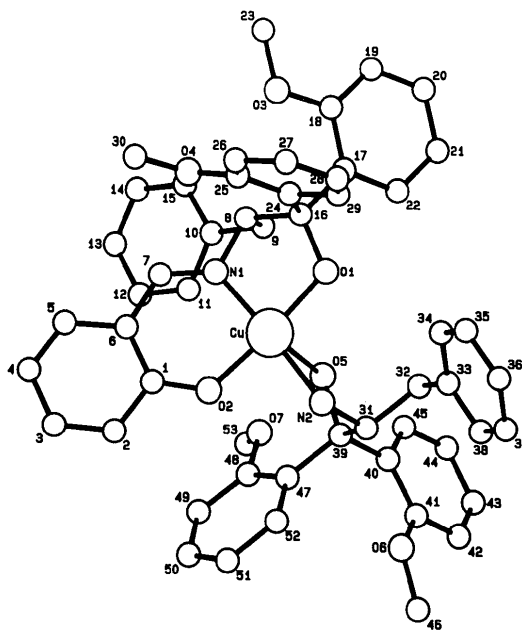|			
N(1)—C(8)—C(9)—C(10)	62·4 (3)	C(31)—C(32)—C(33)—C(34)	−105·7 (3)
N(2)—C(31)—C(32)—C(33)	63·8 (3)	O(1)—C(16)—C(17)—C(18)	−178·0 (3)
N(1)—C(8)—C(16)—O(1)	45·5 (3)	O(5)—C(39)—C(40)—C(41)	174·7 (3)
N(2)—C(31)—C(39)—O(5)	58·9 (3)	O(1)—C(16)—C(24)—C(25)	−123·1 (3)
C(8)—C(9)—C(10)—C(11)	−90·6 (4)	O(5)—C(39)—C(47)—C(48)	43·6 (4)

Fig. 1. The molecular structure of the title complex showing the atom numbering.

Bond distances and angles are given in Table 2. The molecular structure with the atom numbering is shown in Fig. 1. The coordination geometry of the Cu atom is a distorted square pyramid (4 + 1). The tridentate Schiff-base group occupies three of the basal square-planar coordination sites [Cu—O(1) = 1·905 (2), Cu—O(2) = 1·922 (2) and Cu—N(1) = 1·925 (2) Å] and an N atom of the aminoalcohol group [Cu—N(2) = 2·026 (2) Å] completes the plane. This basal plane is roughly planar. The deviations of the atoms from the least-squares plane are: Cu −0·0832 (4), O(1) 0·083 (2), O(2) 0·089 (3), N(1) −0·090 (2) and N(2) −0·083 (2) Å. A protonated O atom of the amino-alcohol group occupies the axial position [Cu—O(5) = 2·650 (2) Å].

Bond distances and angles of the two ligands have normal values. Selected torsion angles are also listed in Table 2. The conformations of the aminoalcohol moieties of the two ligands are similar to each other except for one of the R_2 groups. The torsion angle O(1)—C(16)—C(24)—C(25) is −123·1 (3)°, whereas
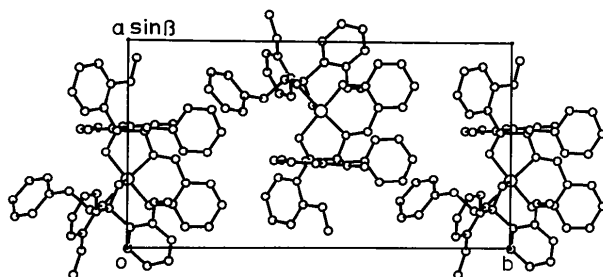
Fig. 2. The crystal packing of the title complex viewed along the c axis.

O(5)—C(39)—C(47)—C(48) is 43·6 (4)°. Other torsion angles are nearly the same for the two aminoalcohol moieties. It should be noted that the structural features of the title complex are similar to those of the phenolic-oxygen-bridged binuclear copper(II) complex (Yanagi & Minobe, 1987). This indicates that the structure of the tridentate Schiff-base ligand plays an important role in the catalytic asymmetric induction. The absolute configuration of the two ligands must be R since they were synthesized from D-phenylalanine.

The crystal packing is shown in Fig. 2. The crystal structure is stabilized mainly by van der Waals forces; the shortest intermolecular distances are $C(28)\cdots C(46)$

$(x-1, y, z-1)$ 3·446 (6) and $C(35)\cdots C(43)$ $(x, y, z-1)$ 3·466 (5) Å.

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Structural Study of Tris(tetrabutylammonium) Hexaisothiocyanatopraseodymate(III)

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Abstract. $3C_4H_9N^+.[Pr(NCS)_6]^{3-}$, $M_r = 1216\cdot8$, triclinic, $P\bar{1}$, $a = 12\cdot419$ (5), $b = 12\cdot927$ (3), $c = 22\cdot848$ (6) Å, $\alpha = 90\cdot94$ (2), $\beta = 92\cdot423$ (4), $\gamma = 96\cdot75$ (4)°, $V = 3638\cdot26$ Å³, $Z = 2$, $D_x = 1\cdot11$ g cm⁻³, $\lambda(Mo\ K\alpha) = 0\cdot71069$ Å, $\mu = 8\cdot13$ cm⁻¹, $F(000) = 1300$, $T = 293$ K, $R = 0\cdot077$ for 6236 observed unique reflexions $[F_o > 6\sigma(F_o)]$. The structure consists of praseodymium atoms coordinated to six N atoms from thiocyanate groups. The coordination polyhedron approaches an ideal octahedron with only minor distortions. The thiocyanate groups are nearly linear. The coordination of n-butyl groups to the ammonium N atom is tetrahedral and the butyl groups are partly disordered.

Introduction. For the last few years there has been a steadily growing interest in the coordination chemistry of non-oxygen-bonded rare-earth compounds. In particular, their optical properties have been studied.

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