| | | | |
|---|---|---|---|
| Sn—Cl2 | 2.3818 (10) | P2—C13 | 1.790 (3) |
| Sn—Cl1 | 2.3894 (9) | P2—C19 | 1.794 (3) |
| P1—O1 | 1.505 (2) | P2—C30 | 1.773 (3) |
| O2—Sn—O1 | 85.31 (8) | O1—P1—C25 | 112.97 (13) |
| O2—Sn—Cl4 | 86.22 (6) | O1—P1—C1 | 111.30 (14) |
| O1—Sn—Cl4 | 86.09 (6) | C25—P1—C1 | 106.58 (14) |
| O2—Sn—Cl3 | 84.77 (6) | O1—P1—C7 | 108.06 (14) |
| O1—Sn—Cl3 | 85.88 (6) | C25—P1—C7 | 106.83 (14) |
| Cl4—Sn—Cl3 | 168.38 (3) | C1—P1—C7 | 111.03 (14) |
| O2—Sn—Cl2 | 90.94 (6) | O2—P2—C30 | 113.54 (13) |
| O1—Sn—Cl2 | 176.15 (6) | O2—P2—C13 | 108.46 (13) |
| Cl4—Sn—Cl2 | 94.55 (4) | C30—P2—C13 | 108.09 (14) |
| Cl3—Sn—Cl2 | 92.91 (4) | O2—P2—C19 | 112.87 (13) |
| O2—Sn—Cl1 | 174.65 (6) | C30—P2—C19 | 106.37 (13) |
| O1—Sn—Cl1 | 89.39 (6) | C13—P2—C19 | 107.24 (14) |
| Cl4—Sn—Cl1 | 92.71 (4) | P1—O1—Sn | 161.52 (14) |
| Cl3—Sn—Cl1 | 95.58 (4) | P2—O2—Sn | 158.88 (14) |
| Cl2—Sn—Cl1 | 94.37 (4) | | |

The title structure was solved by direct methods and refined by full-matrix least-squares techniques. All H atoms were located from difference maps and refined isotropically.

Data collection: *XSCANS* (Siemens, 1994). Cell refinement: *XSCANS*. Data reduction: *XSCANS*. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990*a*). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL/PC* (Sheldrick, 1990*b*). Software used to prepare material for publication: *SHELXL*93. Geometric calculations: *PARST* (Nardelli, 1983).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: KH1088). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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*Acta Cryst.* (1996). **C52**, 1968–1971

# Chlorobis[2-(diphenylphosphino)phenolato-*O*,*P*]oxorhenium(V)

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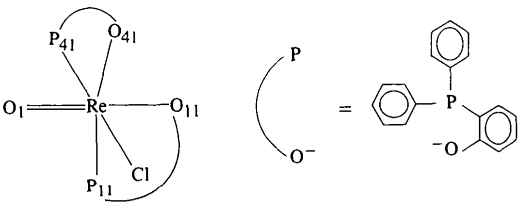
## Abstract

The title compound, $[ReClO(C_{18}H_{14}OP)_2]$, contains severely distorted octahedra with a *cis,cis,cis* configuration. One of the phenolate O atoms is *trans* to the Re═O bond, whereas the two P atoms occupy *cis* sites. Departure from octahedral geometry can be interpreted in terms of the steric hindrance between the phosphine groups, the small bite of the P—O chelating agent and the tendency of the Re═O bond to repel the adjacent bonds. Bond lengths are Re═O 1.686 (4), Re—Cl 2.394 (2), Re—P 2.443 (2) and 2.451 (2), and Re—O(phenolate) 2.003 (4) (*trans* to Re═O) and 1.987 (4) Å (*trans* to P).

## Comment

Chlorobis[2-(diphenylphosphino)phenolato-*O*,*P*]oxorhenium(V), (I), was prepared as part of our ongoing research into rhenium complexes with various P—O chelating agents of potential interest in radiopharmacy. While this work was in progress, the same complex was prepared *via* a different route by Luo, Setyawati, Rettig & Orvig (1995). The present crystallographic study confirms the geometry proposed by those authors from NMR data.



(I)

The crystal structure of (I) contains highly distorted *cis*,*cis*,*cis*-octahedral molecules (Fig. 1). The metal is a chiral centre and all molecules in the crystal studied have an absolute *C* configuration. The bulk sample is racemic, however, as evidenced from the zero rotatory power measured in $CH_2Cl_2$.

Departure from idealized octahedral geometry (Table 2) can be rationalized from the three factors discussed

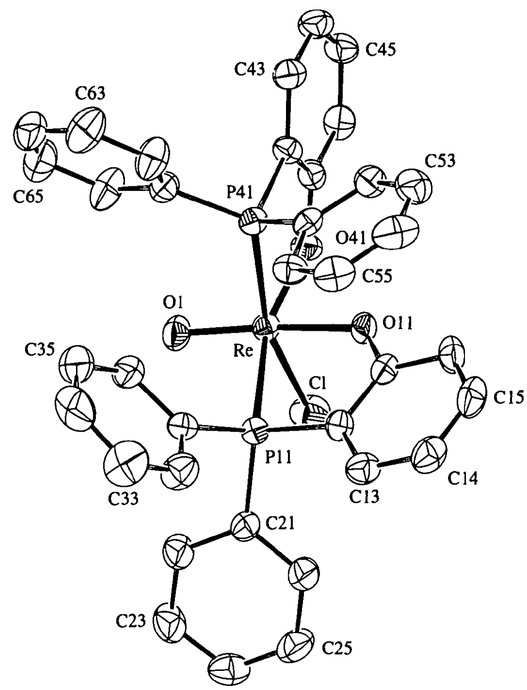


Fig. 1. *ORTEP*II (Johnson, 1976) drawing of the title molecule. In the atomic symbols for ring atoms, the last digit corresponds to the position around the ring and the first two digits (first for the phenol ring) are used to identify the ring. H atoms have been omitted for clarity and ellipsoids correspond to 40% probability.

by Luo *et al.* (1995) for complexes with a related tridentate O—P—O ligand, *i.e.* P—O chelation imposes an O—Re—P angle of *ca* 80° in the ring, bulky $Ph_2P$ groups in *cis* positions open the P11—Re—P41 angle to *ca* 100° and the Re═O bond tends to repel the *cis* ligands. The latter effect increases the O1═Re—Cl and O1═Re—O41 angles to 99.5 (2) and 107.8 (2)°, respectively, but for phosphines, this effect is either less important [O1—Re—P41 93.7 (2)°] or non-existent [O1—Re—P11 89.4 (2)°].

The Re═O1 distance [1.686 (4) Å] is typical of mono-oxo compounds (Nugent & Mayer, 1988). The Re—Cl distance [2.394 (2) Å] is also in the normal range (2.37–2.44 Å) for this type of compound (Lebuis & Beauchamp, 1994). The Re—P bonds [2.443 (2) and 2.451 (2) Å] are approximately equal, but somewhat longer than that reported [2.428 (1) Å] for the same P—O ligand in [ReO(P–O)(O–P–O)] (Luo *et al.*, 1995). The Re—O11 bond [2.003 (4) Å], which is *trans* to Re═O1, is significantly longer than Re—O41 [1.987 (4) Å], which is *trans* to a $PPh_2$ group. This difference can be ascribed to the *trans* influence of Re═O. Both these distances are not very different from the one reported for the same phenolate ligand [1.994 (3) Å; Luo *et al.*, 1995], but definitely longer than those found in O═Re—O*R* units with aliphatic *R* groups (Lebuis, Roux & Beauchamp, 1993; Lebuis & Beauchamp, 1994).

The metal atom does not lie exactly along the expected lone-pair direction of the phosphine; chelation imposes an Re—P—C(phenolate) angle of *ca* 100°, whereas the two Re—P—C(phenyl) angles are *ca* 18° greater. The Re—P41—C42—C41—O41 chelate ring is planar within 0.017 (4) Å (mean deviation 0.011 Å), but the Re—P11—C12—C11—O11 chelate ring is more puckered [mean deviation 0.035 Å, maximum deviation 0.053(3) Å for O11]. The phenyl rings display no unusual features. It is worth noting that the C51–C56 ring is nearly parallel to the phenolate C11–C16 unit and is probably involved in intramolecular stacking interactions with it.

Compounds containing the O═Re—O*R* unit are common in $Re^V$ chemistry and the present structure provides extra support for this marked preference. The presence of phosphine groups in *cis* positions is not the best way to minimize steric hindrance. However, the fact that the $Ni(P\text{–}O)_2$ complex with the same ligand adopts the *cis* square-planar arrangement rather than the less crowded *trans* geometry (Dartiguenave *et al.*, 1996) indicates that the steric effect is not the predominant factor here. The phosphine group does not seem to be bulky enough to overcome an electronic preference for phosphines to position themselves *trans* to O or Cl atoms, instead of *trans* with respect to one another.

## Experimental

The title compound was obtained by mixing a solution of $[ReOCl_3(PPh_3)_2]$ (0.50 g, 0.6 mmol) in toluene (25 ml) with the ligand (0.334 g, 1.20 mmol) and triethylamine (0.121 g, 1.20 mmol) also dissolved in toluene (25 ml). The solutions were stirred separately at 353 K for 30 min and the rhenium solution was transferred into the other by means of a cannula. Upon mixing, the solution turned bottle green and became progressively darker. The mixture was stirred for a further 15 min at 353 K and the khaki-green precipitate was filtered, washed with ethanol and diethyl ether, and dried *in vacuo* (84% yield). The same compound was obtained from $(AsPh_4)[ReOCl_4]$ (0.50 g, 0.69 mmol) dissolved in refluxing ethanol (50 ml), to which the ligand (0.383 g, 1.38 mmol) was added. The yellow-green solution quickly turned khaki green and a green precipitate appeared. The mixture was refluxed for 5 h and the khaki-green precipitate was filtered, washed with diethyl ether and dried *in vacuo* (82% yield). Crystals were obtained by recrystallization from $CH_2Cl_2$ at 273 K.

*Crystal data*

$[ReClO(C_{18}H_{14}OP)_2]$
$M_r = 792.18$
Orthorhombic
$P2_12_12_1$
$a = 10.223\ (3)$ Å
$b = 14.096\ (3)$ Å
$c = 21.454\ (8)$ Å
$V = 3091.6\ (16)$ Å$^3$
$Z = 4$
$D_x = 1.702$ Mg m$^{-3}$
$D_m$ not measured

Cu $K\alpha$ radiation
$\lambda = 1.54056$ Å
Cell parameters from 25 reflections
$\theta = 20.0\text{–}25.0°$
$\mu = 9.51$ mm$^{-1}$
$T = 293\ (2)$ K
Parallelepiped
0.16 × 0.16 × 0.11 mm
Khaki green

*Data collection*

Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: by integration from crystal shape
$T_{min} = 0.29$, $T_{max} = 0.48$
22 362 measured reflections
5871 independent reflections
4936 observed reflections $[I > 2\sigma(I)]$
$R_{int} = 0.101$
$\theta_{max} = 69.93°$
$h = 0 \rightarrow 12$
$k = 0 \rightarrow 17$
$l = -26 \rightarrow 26$
5 standard reflections
frequency: 30 min
intensity decay: 9.0%

*Refinement*

Refinement on $F^2$
$R(F) = 0.0310$
$wR(F^2) = 0.0650$
$S = 0.740$
5871 reflections
389 parameters
H atoms riding (C—H = 0.93 Å)
$w = 1/\sigma^2(F_o^2)$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.876$ e Å$^{-3}$
$\Delta\rho_{min} = -0.963$ e Å$^{-3}$
Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.000211 (14)
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
Absolute configuration: Flack (1983) parameter = −0.033 (10)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

| | $x$ | $y$ | $z$ | $U_{eq}$ |
|---|---|---|---|---|
| Re | 0.87048 (3) | 0.95958 (2) | 0.14206 (1) | 0.03362 (7) |
| Cl | 0.7371 (2) | 0.90959 (14) | 0.22769 (9) | 0.0569 (5) |
| O1 | 0.7542 (5) | 1.0083 (3) | 0.0964 (2) | 0.0480 (13) |
| O11 | 1.0308 (4) | 0.9369 (3) | 0.1937 (2) | 0.0384 (11) |
| C11 | 1.0997 (6) | 1.0018 (5) | 0.2262 (3) | 0.036 (2) |
| C12 | 1.0522 (6) | 1.0940 (5) | 0.2332 (3) | 0.036 (2) |
| C13 | 1.1244 (8) | 1.1597 (5) | 0.2679 (3) | 0.049 (2) |
| C14 | 1.2409 (7) | 1.1337 (6) | 0.2939 (3) | 0.055 (2) |
| C15 | 1.2900 (7) | 1.0433 (7) | 0.2851 (3) | 0.058 (2) |
| C16 | 1.2205 (7) | 0.9756 (5) | 0.2523 (3) | 0.048 (2) |
| P11 | 0.9027 (2) | 1.11394 (12) | 0.19234 (7) | 0.0357 (4) |
| C21 | 0.7836 (6) | 1.1558 (5) | 0.2490 (3) | 0.039 (2) |
| C22 | 0.6707 (6) | 1.1981 (5) | 0.2287 (3) | 0.049 (2) |
| C23 | 0.5755 (7) | 1.2262 (6) | 0.2701 (4) | 0.058 (2) |
| C24 | 0.5933 (7) | 1.2122 (6) | 0.3329 (4) | 0.058 (2) |
| C25 | 0.7050 (7) | 1.1707 (6) | 0.3538 (4) | 0.063 (2) |
| C26 | 0.7990 (7) | 1.1420 (6) | 0.3122 (3) | 0.059 (2) |
| C31 | 0.9216 (6) | 1.2173 (4) | 0.1426 (3) | 0.0406 (14) |
| C32 | 0.9668 (8) | 1.3022 (6) | 0.1639 (3) | 0.059 (2) |
| C33 | 0.9886 (9) | 1.3783 (6) | 0.1241 (4) | 0.078 (3) |
| C34 | 0.9641 (10) | 1.3672 (6) | 0.0619 (5) | 0.076 (3) |
| C35 | 0.9176 (9) | 1.2852 (6) | 0.0402 (4) | 0.075 (3) |
| C36 | 0.8940 (8) | 1.2093 (5) | 0.0790 (3) | 0.057 (2) |
| O41 | 0.8826 (5) | 0.8227 (3) | 0.1209 (2) | 0.0407 (10) |
| C41 | 0.9625 (6) | 0.7859 (5) | 0.0772 (3) | 0.0375 (15) |
| C42 | 1.0450 (6) | 0.8450 (4) | 0.0418 (3) | 0.0353 (15) |
| C43 | 1.1204 (8) | 0.8055 (5) | −0.0058 (3) | 0.046 (2) |
| C44 | 1.1187 (8) | 0.7108 (5) | −0.0180 (3) | 0.050 (2) |
| C45 | 1.0385 (7) | 0.6516 (5) | 0.0178 (3) | 0.052 (2) |
| C46 | 0.9616 (7) | 0.6883 (5) | 0.0645 (3) | 0.047 (2) |
| P41 | 1.0388 (2) | 0.96815 (15) | 0.06143 (7) | 0.0348 (4) |
| C51 | 1.2022 (7) | 1.0046 (5) | 0.0861 (3) | 0.038 (2) |
| C52 | 1.2984 (7) | 0.9385 (5) | 0.0958 (3) | 0.046 (2) |
| C53 | 1.4188 (7) | 0.9665 (7) | 0.1183 (3) | 0.061 (2) |
| C54 | 1.4424 (7) | 1.0586 (7) | 0.1315 (4) | 0.067 (3) |
| C55 | 1.3483 (7) | 1.1251 (6) | 0.1228 (3) | 0.055 (2) |
| C56 | 1.2257 (7) | 1.0974 (5) | 0.1004 (3) | 0.044 (2) |
| C61 | 1.0088 (7) | 1.0274 (5) | −0.0126 (3) | 0.041 (2) |
| C62 | 1.1070 (8) | 1.0757 (5) | −0.0432 (3) | 0.060 (2) |
| C63 | 1.0835 (10) | 1.1159 (6) | −0.1005 (4) | 0.076 (3) |
| C64 | 0.9627 (10) | 1.1108 (6) | −0.1269 (4) | 0.071 (3) |
| C65 | 0.8631 (10) | 1.0652 (6) | −0.0971 (3) | 0.074 (3) |
| C66 | 0.8853 (8) | 1.0235 (6) | −0.0395 (3) | 0.062 (2) |

Table 2. *Selected geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Re—Cl | 2.394 (2) | P11—C12 | 1.784 (6) |
| Re—P11 | 2.451 (2) | P11—C21 | 1.819 (7) |
| Re—P41 | 2.443 (2) | P11—C31 | 1.816 (7) |
| Re—O1 | 1.686 (4) | O41—C41 | 1.347 (7) |
| Re—O11 | 2.003 (4) | C41—C42 | 1.408 (8) |
| Re—O41 | 1.987 (4) | P41—C42 | 1.787 (6) |
| O11—C11 | 1.348 (7) | P41—C61 | 1.820 (6) |
| C11—C12 | 1.396 (8) | P41—C51 | 1.826 (7) |
| O1—Re—Cl | 99.5 (2) | O11—C11—C12 | 120.4 (6) |
| O1—Re—P11 | 89.4 (2) | C11—C12—P11 | 113.0 (5) |
| O1—Re—P41 | 93.7 (2) | C12—P11—C31 | 108.9 (3) |
| O1—Re—O11 | 164.3 (2) | C12—P11—C21 | 107.2 (3) |
| O1—Re—O41 | 107.8 (2) | C31—P11—C21 | 101.8 (3) |
| Cl—Re—P11 | 90.01 (6) | C12—P11—Re | 101.1 (2) |
| Cl—Re—P41 | 163.57 (7) | C31—P11—Re | 117.9 (2) |
| Cl—Re—O11 | 89.70 (13) | C21—P11—Re | 119.5 (2) |
| Cl—Re—O41 | 85.71 (13) | C41—O41—Re | 124.8 (4) |
| P11—Re—P41 | 99.96 (6) | O41—C41—C42 | 120.7 (6) |
| P11—Re—O11 | 77.77 (13) | C41—C42—P41 | 115.2 (5) |
| P11—Re—O41 | 162.72 (13) | C42—P41—C51 | 108.0 (3) |
| P41—Re—O11 | 79.82 (12) | C61—P41—C51 | 106.1 (3) |
| P41—Re—O41 | 80.92 (14) | C42—P41—Re | 98.3 (2) |
| O11—Re—O41 | 85.5 (2) | C61—P41—Re | 121.4 (2) |
| C11—O11—Re | 127.2 (4) | C51—P41—Re | 117.0 (2) |

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *NRC*-2, *NRC*-2*A* (Ahmed, Hall, Pippy & Huber, 1973). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*II (Johnson (1976); *NRCVAX* (Gabe, Le Page, Charland, Lee & White, 1989). Software used to prepare material for publication: *SHELXL*93.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and torsion angles have been deposited with the IUCr (Reference: FG1173). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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# A Five-Coordinate Bis(*p*-bromophenylsalicylaldimino)chloroiron(III) Complex

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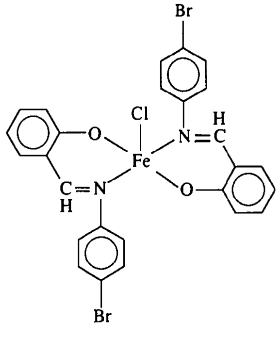
## Abstract

In the title complex, bis[2-(4-bromophenyliminomethyl)-phenolato-*N*,*O*]chloroiron(III), [FeCl(C$_{13}$H$_9$BrNO)$_2$], the Fe$^{3+}$ ion shows a distorted square-pyramidal geometry, with the N and O ligand atoms forming the base [Fe—O 1.857 (3) and 1.864 (3) Å, and Fe—N 2.144 (3) and 2.164 (3) Å] and the Cl atom at the apex [Fe—Cl 2.238 (1) Å].

## Comment

The complexes of transition metal ions with Schiff bases are a large and growing class of compounds of both stereochemical and magnetochemical interest (Garnovskii, Nivorozhkin & Minkin, 1973; Maggio, Pizzino & Romano, 1974; Morassi, Bertini & Sacconi, 1973). Characteristically, several distinct compounds may be isolated from one reaction mixture. The products may differ in the coordination number of the metal ion, the stereochemistry of ligand isomers or the degree of molecular complexity. The nature of the products appears to depend on many factors which include the solvent system, steric constraints imposed by ligand side groups, crystal-packing considerations and hybridization which, if any, is the predominant effect (Elmalı, Elerman, Svoboda & Fuess, 1993; Elmalı, Atakol, Svoboda & Fuess, 1993; Gerloch & Mabbs, 1967).

The reaction of iron(III) chloride with the Schiff base *p*-bromophenylsalicylaldimine is one from which several complexes with similar steric and magnetic properties may be derived. The present five-coordinate monomeric iron(III) complex, (I), is a distorted square pyramid with the Cl atom at the apex. The Fe atom is 0.495 (2) Å above the least-squares plane defined by the Schiff base N- and O-donor atoms, which show a small tetrahedral distortion with an r.m.s. displacement of 0.199 (3) Å.



(I)

The bond lengths of Fe$^{3+}$ (Table 2) are close to those in the related five-coordinate salen [salen is *N*,*N*-ethylenebis(salicylideneaminato)] complexes [FeCl(salen)] (Garnovskii *et al.*, 1973) and [Fe$_2$(salen)$_2$O] (Maggio et al., 1974), and also in chloro(1,1′-diphenyl-3,3′-ethylenediiminodi-1-butanonato)iron(III) (Morassi *et al.*, 1973). The Fe1 atom is located 0.268 (3) and 0.499 (3) Å above the least-squares planes through O1, C7, C13, N1 (chelate 1) and O2, C14, C20, N2 (chelate 2), respectively. The chelate planes are inclined at angles of

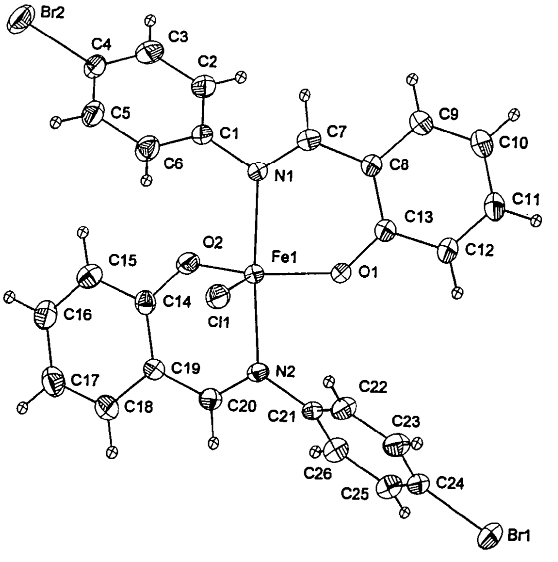


Fig. 1. The molecular structure and atomic numbering of the title compound (*ORTEP*II; Johnson, 1976). The displacement ellipsoids are drawn at the 50% probability level.

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