Acta Crystallographica Section C
**Crystal Structure Communications**
ISSN 0108-2701

# Dicarbonyldi-$\mu$-chloro-*cis,cis*-$\eta^4$-1,5-cyclooctadienedirhodium(I)

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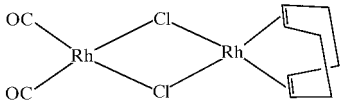
Received 6 October 2000
Accepted 11 December 2000

The title compound, dicarbonyl-1$\kappa^2$*C*-di-$\mu$-chloro-1:2$\kappa^4$*Cl*-[*cis,cis*-2($\eta^4$)-1,5-cyclooctadiene]dirhodium(I), $[Rh_2Cl_2(C_8H_{12})(CO)_2]$, consists of a dichloro-bridged dimer of rhodium, with a non-bonded Rh···Rh distance of 3.284 (2) Å. One Rh atom is coordinated to two carbonyl ligands, while the other Rh atom is coordinated to the cyclooctadiene moiety.

## Comment

The crystal structures of the compounds $[Rh_2Cl_2(CO)_4]$ (Dahl *et al.*, 1961; Walz & Scheer, 1991) and $[Rh_2Cl_2(C_8H_{12})_2]$ (Ibers & Snyder, 1962; Boeyens *et al.*, 1986; De Ridder & Imhoff, 1994) have been reported. However, the structure of the mixed-ligand rhodium dimer, with two carbonyl ligands coordinated to one Rh atom and a cyclooctadiene ligand coordinated to the other Rh atom, *i.e.* (I), has only been determined by X-ray powder diffraction (Corradi *et al.*, 1997).




(I)

The structure of (I) (Fig. 1) consists of two square-planar Rh atoms linked by two bridging Cl atoms. The bond lengths and angles of the Rh1 moiety are very similar to those found in the $[Rh_2Cl_2(C_8H_{12})_2]$ molecule, while those of the Rh2 moiety are similar to those found in the $[Rh_2Cl_2(CO)_4]$ molecule. This is particularly remarkable with regard to the different Rh—Cl bond lengths. Thus, Rh1—Cl1 of 2.406 (2) Å and Rh1—Cl2 of 2.412 (2) Å correspond to the equivalent bond lengths found in $[Rh_2Cl_2(C_8H_{12})_2]$ (average 2.410 Å; De Ridder & Imhoff, 1994), while the shorter bond lengths, Rh2—Cl1 of 2.371 (2) Å and Rh2—Cl2 of 2.372 (2) Å, correspond to the equivalent bond lengths found in $[Rh_2Cl_2(CO)_4]$ (average 2.384 Å; Walz & Scheer, 1991). As expected also, the Rh···Rh distance in the title compound [3.284 (2) Å] approximates to the average of the corresponding values for $[Rh_2Cl_2(C_8H_{12})_2]$ [3.509 (1) Å; Boeyens *et al.*, 1986] and $[Rh_2Cl_2(CO)_4]$ [3.138 (1) Å; Walz & Scheer, 1991]. The dihedral angle about the Cl···Cl vector of the $Rh_2Cl_2$ core is 139.6°, somewhat larger than that of $[Rh_2Cl_2(CO)_4]$ (128.6°; Dahl *et al.*, 1961; Walz & Scheer, 1991), but markedly different from the planar $Rh_2Cl_2$ core in $[Rh_2Cl_2(C_8H_{12})_2]$ (Ibers & Snyder, 1962; Boeyens *et al.*, 1986; De Ridder & Imhoff, 1994). There are relatively short Rh···Rh intermolecular contacts (Rh2···Rh2′ 3.50 Å) between the Rh atoms bearing the carbonyl ligands. The structure obtained from powder diffraction methods (Corradi *et al.*, 1997) showed a rather short packing contact between O1 and O1′ [2.67 (6) Å] which was recognized to be susceptible to small structural changes. The present data show this contact to be much longer at 3.19 Å, otherwise there are no major differences in the structural parameters.

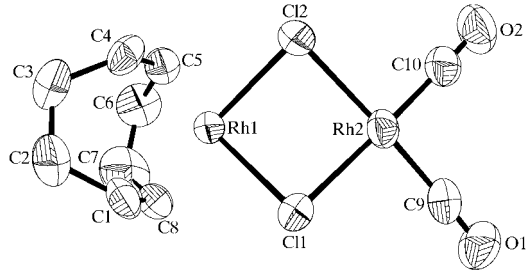



**Figure 1**
The molecular structure of the title compound with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level.

## Experimental

The title compound was extracted as a minor product from the solution resulting from the reaction between $[RuCl(C_5H_5)(C_8H_{12})]$ and $[Rh_2Cl_2(CO)_4]$. Orange crystals were grown from a $CH_2Cl_2$–hexane solution.

*Crystal data*

$[Rh_2Cl_2(C_8H_{12})(CO)_2]$
$M_r$ = 440.92
Monoclinic, $P2_1/c$
$a$ = 6.6500 (12) Å
$b$ = 12.261 (3) Å
$c$ = 16.058 (3) Å
$\beta$ = 92.19 (3)°
$V$ = 1308.3 (5) Å$^3$
$Z$ = 4
$D_x$ = 2.238 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 15389 reflections
$\theta$ = 2.09–30.02°
$\mu$ = 2.912 mm$^{-1}$
$T$ = 293 (2) K
Block, orange
0.15 × 0.10 × 0.10 mm

*Data collection*

Nonius KappaCCD diffractometer
Area-detector scans
15389 measured reflections
3699 independent reflections
2261 reflections with $I > 2\sigma(I)$
$R_{int}$ = 15389
$\theta_{min}$ = 2.09°
$\theta_{max}$ = 30.02°
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 17$
$l = -22 \rightarrow 22$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.196
$S$ = 1.118
3699 reflections
145 parameters
H atoms constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.01 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.28 e Å$^{-3}$

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**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Rh1—C1 | 2.099 (8) | O2—C10 | 1.125 (10) |
| Rh1—C4 | 2.118 (7) | O1—C9 | 1.121 (10) |
| Rh1—C5 | 2.094 (7) | C1—C8 | 1.395 (14) |
| Rh1—C8 | 2.101 (8) | C1—C2 | 1.516 (12) |
| Rh1—Cl1 | 2.406 (2) | C2—C3 | 1.476 (12) |
| Rh1—Cl2 | 2.412 (2) | C3—C4 | 1.512 (12) |
| Rh2—C9 | 1.844 (9) | C4—C5 | 1.365 (11) |
| Rh2—C10 | 1.850 (9) | C5—C6 | 1.493 (13) |
| Rh2—Cl1 | 2.371 (2) | C6—C7 | 1.487 (13) |
| Rh2—Cl2 | 2.372 (2) | C7—C8 | 1.504 (14) |
| | | | |
| Cl1—Rh1—Cl2 | 85.03 (8) | C10—Rh2—Cl2 | 91.3 (3) |
| C9—Rh2—C10 | 91.4 (4) | Cl1—Rh2—Cl2 | 86.71 (8) |
| C9—Rh2—Cl1 | 90.5 (3) | Rh2—Cl1—Rh1 | 86.88 (8) |
| C10—Rh2—Cl1 | 176.7 (3) | Rh2—Cl2—Rh1 | 86.71 (7) |
| C9—Rh2—Cl2 | 176.8 (3) | | |

H atoms were constrained during the refinement with C—H distances in the range 0.93–0.97 Å.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1990); software used to prepare material for publication: *SHELXCIF*-97 (Sheldrick, 1997).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: GD1124). Services for accessing these data are described at the back of the journal.

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