

# Bis[di- $\eta^5$ -cyclopentadienylcobalt(I)] dicarbonyl-trichloro(chlorodiphenylsilyl)ruthenium(II)

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## Key indicators

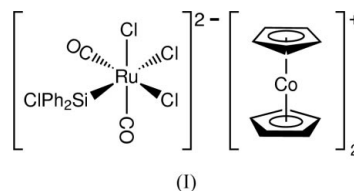
Single-crystal X-ray study  
 T = 150 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.018 \text{ \AA}$   
 R factor = 0.064  
 wR factor = 0.127  
 Data-to-parameter ratio = 14.2

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The asymmetric unit of the title compound,  $[\text{Co}(\text{C}_5\text{H}_5)_2]_2^- [\text{RuCl}_3(\text{C}_{12}\text{H}_{10}\text{ClSi})(\text{CO})_2]_2$ , consists of a discrete  $\text{ClPh}_2\text{Si}-\text{Ru}(\text{CO})_2\text{Cl}_3$  dianion and two  $(\eta\text{-C}_5\text{H}_5)_2\text{Co}$  cations. The dianion has octahedral coordination geometry, with the three Cl atoms in *cis* positions. In addition, two carbonyl groups (*cis*) and a  $\text{Ph}_2\text{ClSi}$  group (bonded through Si) complete the coordination. The Ru—Si bond length is 2.362 (3) Å and the longest Ru—Cl bond [2.566 (2) Å] is *trans* to the Si atom. In one cobaltocene cation, the cyclopentadienyl (*Cp*) rings are staggered, while in the other, the *Cp* rings are almost eclipsed.

## Comment

Metal complexes with functional groups are of potential interest as precursors to metallopolymers. As part of our work in this area (Nguyen *et al.*, 1999), we report the characterization of an unexpected product, (I).



## Experimental

The reaction between two equivalents of  $(\eta\text{-C}_5\text{H}_5)_2\text{Co}$  and  $[\text{ClPh}_2\text{SiRu}(\text{CO})_4]_2$  was carried out at 298 K in tetrahydrofuran under an atmosphere of  $\text{N}_2$ . After *ca* 16 h, the solvent was removed under high vacuum and  $\text{CD}_2\text{Cl}_2$  was added to the residue. A vigorous reaction was observed with evolution of gas. Red–orange crystals of (I) were obtained upon slow room-temperature concentration of the resultant product mixture under an  $\text{N}_2$  atmosphere.

### Crystal data

$[\text{Co}(\text{C}_5\text{H}_5)_2]_2^-$	$D_x = 1.679 \text{ Mg m}^{-3}$
$[\text{RuCl}_3(\text{C}_{12}\text{H}_{10}\text{ClSi})(\text{CO})_2]$	Mo $K\alpha$ radiation
$M_r = 859.40$	Cell parameters from 3060 reflections
Orthorhombic, $P2_12_12_1$	$\theta = 2.6\text{--}25.0^\circ$
$a = 9.7462 (5) \text{ \AA}$	$\mu = 1.78 \text{ mm}^{-1}$
$b = 10.2277 (6) \text{ \AA}$	$T = 150 (1) \text{ K}$
$c = 34.099 (2) \text{ \AA}$	Plate, dark orange
$V = 3399.0 (3) \text{ \AA}^3$	$0.20 \times 0.20 \times 0.02 \text{ mm}$
$Z = 4$	

### Data collection

Nonius KappaCCD diffractometer	5652 independent reflections
$\varphi$ scans and $\omega$ scans with $\kappa$ offsets	3558 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan ( <i>DENZO-SMN</i> ; Otwinowski & Minor, 1997)	$R_{\text{int}} = 0.109$
$T_{\text{min}} = 0.717$ , $T_{\text{max}} = 0.965$	$\theta_{\text{max}} = 25.0^\circ$
12 795 measured reflections	$h = -11 \rightarrow 11$
	$k = -12 \rightarrow 12$
	$l = -37 \rightarrow 36$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.064$   
 $wR(F^2) = 0.128$   
 $S = 1.01$   
 5652 reflections  
 397 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0371P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.84 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.54 \text{ e } \text{\AA}^{-3}$   
 Absolute structure: (Flack, 1983),  
 2319 Friedel pairs  
 Flack parameter = 0.03 (3)

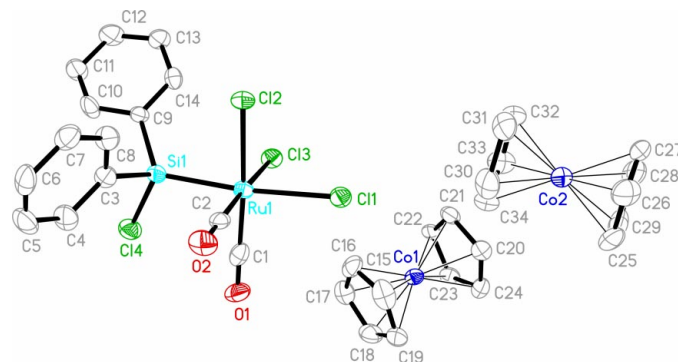
**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Ru1—Si1	2.362 (3)	Ru1—Cl1	2.566 (2)
Ru1—Cl2	2.456 (3)	Cl4—Si1	2.134 (4)
Ru1—Cl3	2.462 (3)		
Si1—Ru1—Cl1	173.57 (10)	Cl4—Si1—Ru1	111.99 (15)
Cl1—Ru1—Si1—Cl4	−11.3 (4)		

All H atoms were included in calculated positions with distances of 0.95  $\text{\AA}$  for phenyl C—H and 1.00  $\text{\AA}$  for cyclopentadienyl C—H. In the refinement, H atoms were included in a riding-motion approximation, with  $U_{\text{iso}} = 1.2U_{\text{eq}}$  of the carrier atom.

Data collection: *COLLECT* (Nonius, 1997–2001); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.



**Figure 1**

View of molecule (I), with displacement ellipsoids drawn at the 30% probability level.

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## References

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