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Orthorhombic Modification of Dichlorotetrakis(dimethyl sulfoxide)ruthenium(II)

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Abstract. $[RuCl_2(C_2H_6OS)_4]$, $M_r = 484{\cdot}54$, orthorhombic, *Pccn*, $a = 28{\cdot}328\ (5)$, $b = 10{\cdot}831\ (3)$, $c = 11{\cdot}751\ (3)$ Å, $V = 3606\ (2)$ Å^3, $Z = 8$, $D_x = 1{\cdot}78$ Mg m^{-3}, graphite-monochromatized Mo $K\alpha$ radiation, $\lambda = 0{\cdot}7107$ Å, $\mu = 1{\cdot}59$ mm^{-1}, $F(000) = 1968$, room temperature, $R = 0{\cdot}042$ for 2904 unique observed reflections. The coordination geometry around ruthenium is essentially octahedral with *cis*-chlorine atoms. Of the four dimethyl sulfoxide (Me_2SO) molecules, three are S- and one is O-bonded to Ru. The O-bonded ligand is *trans* to an S-bonded Me_2SO.

Experimental. Crystal $0{\cdot}4 \times 0{\cdot}3 \times 0{\cdot}2$ mm grown by cooling of a hot Me_2SO solution. Enraf–Nonius CAD-4 diffractometer controlled by a PDP11/44 computer; $\omega/2\theta$ scan technique. Cell parameters from least-squares procedure on 25 reflections ($14 \le \theta \le 19°$). Max. and min. transmission factors for absorption correction: 0·9996 and 0·7857. 6128 reflections measured in range $2{\cdot}5 \le \theta \le 30°$. Indices ranged from 0 to $h = 39$, $k = 15$ and $l = 16$. Three standard reflections ($\bar{1}3,4,4$, $\bar{8}\bar{7}2$, 24,0,0) monitored every 3600 s did not vary significantly throughout data collection. 5852 unique reflections, 2904 satisfied $I \ge 3{\cdot}0\sigma(I)$. Structure solved from Patterson map and refinement of 172 parameters based on F (Enraf–Nonius, 1979). Anisotropic thermal parameters for non-H atoms, H atoms included at their tetrahedral estimates with fixed isotropic thermal factors ($B = 5{\cdot}0$ Å^2) and not refined. $R = 0{\cdot}042$, $wR = 0{\cdot}051$, $S = 4{\cdot}12$ for $w = 1$, $(\Delta/\sigma)_{max} \le 0{\cdot}07$, $(\Delta\rho)_{max} = 0{\cdot}61$, $(\Delta\rho)_{min} = -0{\cdot}72$ e Å^{-3}; no extinction correction. Atomic scattering factors and anomalous-dispersion terms taken from *International Tables for X-ray Crystallography* (1974). Computing with *SDP* (Enraf–Nonius, 1979) on a PDP11/44. Crystallographic results are summarized in Tables 1 and 2 and Fig. 1.†

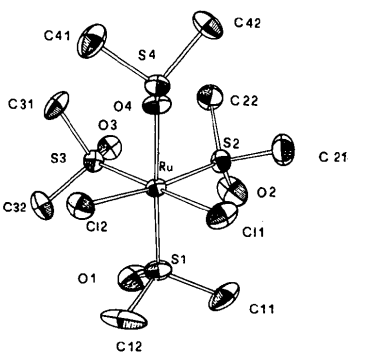

Fig. 1. View of the molecule, showing the atomic numbering (H atoms omitted for clarity).

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† Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43836 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Final positional parameters of the non-H atoms with e.s.d.'s in parentheses*

	x	y	z	B_{eq}(Å^2)
Ru	0·12557 (2)	0·45800 (5)	0·33090 (4)	1·703 (7)
Cl(1)	0·08912 (8)	0·4047 (2)	0·5099 (2)	3·45 (4)
Cl(2)	0·20048 (7)	0·4050 (2)	0·4194 (2)	3·00 (3)
S(1)	0·12788 (8)	0·6568 (2)	0·3854 (2)	2·80 (3)
S(2)	0·05397 (6)	0·4790 (2)	0·2446 (2)	2·43 (3)
S(3)	0·16670 (6)	0·4915 (2)	0·1681 (2)	2·12 (3)
S(4)	0·13014 (7)	0·1614 (2)	0·3617 (1)	2·11 (3)
O(1)	0·1412 (2)	0·7525 (6)	0·3023 (6)	4·3 (1)
O(2)	0·0361 (2)	0·6023 (6)	0·2146 (6)	4·6 (1)
O(3)	0·1417 (2)	0·5389 (5)	0·0655 (4)	2·8 (1)
O(4)	0·1206 (2)	0·2689 (4)	0·2801 (4)	2·40 (9)
C(11)	0·0738 (4)	0·7077 (8)	0·4495 (9)	5·0 (2)
C(12)	0·1694 (5)	0·6758 (9)	0·500 (1)	6·5 (3)
C(21)	0·0083 (3)	0·4039 (9)	0·3240 (9)	4·2 (2)
C(22)	0·0503 (3)	0·388 (1)	0·1191 (7)	4·2 (2)
C(31)	0·1963 (3)	0·3533 (8)	0·1255 (7)	3·3 (2)
C(32)	0·2173 (3)	0·5872 (8)	0·1883 (8)	3·5 (2)
C(41)	0·1779 (3)	0·0792 (8)	0·2997 (9)	4·0 (2)
C(42)	0·0851 (3)	0·0560 (7)	0·3228 (8)	3·3 (2)

Anisotropically refined atoms are given in the form of the isotropic equivalent thermal parameter defined as:

$B_{eq} = \frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

Table 2. *Bond lengths* (Å) *and angles* (°) *with their e.s.d.'s*

Ru–Cl(1)	2·413 (2)	S(1)–C(11)	1·793 (11)
Ru–Cl(2)	2·432 (2)	S(1)–C(12)	1·804 (13)
Ru–S(1)	2·248 (2)	S(2)–C(21)	1·789 (10)
Ru–S(2)	2·279 (2)	S(2)–C(22)	1·779 (9)
Ru–S(3)	2·269 (2)	S(3)–C(31)	1·787 (9)
Ru–O(4)	2·138 (4)	S(3)–C(32)	1·785 (9)
S(1)–O(1)	1·473 (7)	O(4)–S(4)	1·533 (5)
S(2)–O(2)	1·472 (7)	S(4)–C(41)	1·777 (9)
S(3)–O(3)	1·489 (6)	S(4)–C(42)	1·772 (8)
Cl(1)–Ru–Cl(2)	86·8 (1)	Ru–S(3)–C(31)	110·1 (3)
Cl(1)–Ru–S(1)	89·6 (1)	Ru–S(3)–C(32)	113·1 (3)
Cl(1)–Ru–S(2)	91·8 (1)	Ru–S(1)–O(1)	119·5 (3)
Cl(1)–Ru–S(3)	173·1 (1)	Ru–S(2)–O(2)	120·3 (3)
Cl(1)–Ru–O(4)	89·2 (1)	Ru–S(3)–O(3)	119·6 (2)
Cl(2)–Ru–S(1)	94·5 (1)	C(11)–S(1)–C(12)	101·9 (5)
Cl(2)–Ru–S(2)	172·0 (1)	C(21)–S(2)–C(22)	97·9 (5)
Cl(2)–Ru–S(3)	87·2 (1)	C(31)–S(3)–C(32)	98·4 (4)
Cl(2)–Ru–O(4)	87·2 (1)	C(11)–S(1)–O(1)	106·3 (4)
S(1)–Ru–S(2)	93·3 (1)	C(12)–S(1)–O(1)	104·4 (5)
S(1)–Ru–S(3)	94·1 (1)	C(21)–S(2)–O(2)	106·7 (4)
S(1)–Ru–O(4)	177·9 (2)	C(22)–S(2)–O(2)	106·6 (4)
S(2)–Ru–S(3)	93·8 (1)	C(31)–S(3)–O(3)	106·6 (4)
S(2)–Ru–O(4)	85·0 (2)	C(32)–S(3)–O(3)	106·8 (4)
S(3)–Ru–O(4)	87·2 (1)	Ru–O(4)–S(4)	122·8 (3)
Ru–S(1)–C(11)	112·9 (3)	O(4)–S(4)–C(41)	105·0 (4)
Ru–S(1)–C(12)	110·0 (4)	O(4)–S(4)–C(42)	101·6 (4)
Ru–S(2)–C(21)	111·5 (3)	C(41)–S(4)–C(42)	96·9 (4)
Ru–S(2)–C(22)	111·5 (3)		

Related literature. The structure represents a second modification of $(Me_2SO)_4RuCl_2$ with interatomic parameters in essential agreement with those of the previously reported monoclinic, $P2_1/n$, modification (Mercer & Trotter, 1975).

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A Chloro-Bridged Palladium Dimer: *trans*-Di-μ-chloro-bis[(2,2-dimethyl-2-phenylethyl)-(triphenylphosphine)palladium] Bis(dichloromethylate)

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Abstract. $[Pd_2Cl_2\{(C_6H_5)_3P\}_2(C_{10}H_{13})_2].2CH_2Cl_2$, M_r = 1244·6, triclinic, $P\bar{1}$, a = 9·361 (2), b = 12·982 (3), c = 13·873 (3) Å, α = 114·13 (1), β = 103·55 (1), γ = 99·17 (1)°, V = 1432·7 (5) Å^3, Z = 1, D_x = 1·442 g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, μ = 9·9 cm^{-1}, $F(000)$ = 632, 296 K, R_F = 3·59% for 3807 reflections with $F_o \geq 3\sigma(F_o)$ and 259 parameters. The compound is a chlorine-bridged *trans* dimer centered on a site of inversion. The coordination geometry is approximately square-planar about Pd with asymmetric chloro bridges; in keeping with expected *trans*-labilization trends, the Pd–Cl bond *trans* to the alkyl group, 2·416 (1) Å, is considerably shorter than that *trans* to the phosphine, 2·494 (1) Å.

Experimental. Yellow block-shaped crystals (0·30 × 0·35 × 0·40 mm) were recrystallized from CH_2Cl_2. Nicolet $R3m/\mu$, Wyckoff scans, lattice parameters from

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