trans-Dichlorotetrakis(dimethyl sulfide)ruthenium(II)

Alireza Abbasi,[a]* Fereshteh Azizi,[a] Lars Eriksson[b] and Magnus Sandström[b]

[a]School of Chemistry, University College of Science, University of Tehran, Tehran, Iran, and [b]Department of Physical, Inorganic and Structural Chemistry, Arrhenius Laboratory, Stockholm University, S-106 91 Stockholm, Sweden

Correspondence e-mail:
aabbasi@khayam.ut.ac.ir

In the title compound, trans-[RuCl$_2$(C$_2$H$_6$S)$_4$], the Ru^{II} ion, located on a special position (4a) with crystallographically imposed $\bar{1}$ symmetry, coordinates four S atoms from the dimethyl sulfide molecules and two chloride ions in an octahedral trans configuration. All atoms, except ruthenium, occupy general positions (8c).

Comment

One aim of the current study is to investigate the nature of Ru—S bonds by comparison with analogous compounds, including the corresponding sulfoxides. Some structures of dimethyl sulfide- and dimethyl sulfoxide-solvated ruthenium(II) ions have been studied in recent years (Calligaris, 2004; Alessio, 2004). Even though the ruthenium(II) ion is classified as borderline (Pearson, 1967), it preferably forms bonds to the S atom of sulfoxides (Calligaris, 2004). The title compound, (I), has been characterized previously by means of elemental analyses, ^{1}H NMR and IR spectroscopy (Riley & Oliver, 1986). The crystal structure of (I) is satisfactorily described in the space group Pbca. The ruthenium(II) ion is octahedrally coordinated by four S atoms from dimethyl sulfide molecules, with a mean Ru—S bond distance of 2.365 Å, and by two chloride ions in centrosymmetric trans configuration (Fig. 1).

(I)
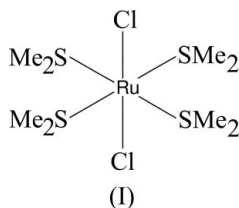
The Ru—S bond distances in mer-[RuCl$_3$(C$_2$H$_6$S)$_3$] for S trans to Cl [2.380 (1) Å] are shorter than for the Ru—S bonds to the trans S atoms [2.388 (1) Å], indicating the stronger trans influence of S than Cl (Bolton et al., 2004). The Ru—S bond distance for S trans to Cl in fac-trichlorotris(dimethyl sulfoxide)ruthenium(II), fac-[RuCl$_3$(C$_2$H$_6$SO)$_3$]$^-$ [2.268 (5) Å; Geremia et al., 2000], is also shorter. The reason is the π-backbonding from metal to ligand, which in sulfur-coordinated dimethyl sulfoxide solvates is stronger for d^6 Ru^{II} than for d^5 Ru^{III}. However, the mean Ru—S bond lengths in (I) and in trans-dichlorotetrakis(dimethyl sulfoxide)ruthenium(II), trans-[RuCl$_2$(C$_2$H$_6$SO)$_4$], are found to be nearly the same, because of the similar trans effect of the coordinated S atoms of dimethyl sulfide and dimethyl sulfoxide ligands (Alessio et al., 1988).

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Experimental

Compound (I) was synthesized by dissolving ruthenium(III) chloride hydrate (Aldrich, 99.98%) in excess of dimethyl sulfide (Merck, 99%). The solution was heated and kept at 343 K for 8 h. Crystals suitable for X-ray crystallographic analysis were obtained after a few days.

Crystal data

$[RuCl_2(C_2H_6S)_4]$
$M_r = 420.48$
Orthorhombic, $Pbca$
$a = 8.4312 (5)$ Å
$b = 14.1135 (7)$ Å
$c = 14.7463 (7)$ Å
$V = 1754.72 (16)$ Å^3

$Z = 4$
$D_x = 1.592$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.65$ mm^{-1}
$T = 290 (2)$ K
Block, brown
$0.3 \times 0.2 \times 0.1$ mm

Data collection

Oxford Diffraction X-calibur 3 CCD detector diffractometer
ω scans
Absorption correction: numerical (*X-RED*; Stoe & Cie, 1997) $T_{min} = 0.610$, $T_{max} = 0.848$

15450 measured reflections
2786 independent reflections
2354 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 31.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.085$
$S = 1.12$
2786 reflections
71 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0275P)^2 + 2.0516P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.76$ e Å^{-3}
$\Delta\rho_{min} = -0.62$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0062 (6)

Table 1
Selected bond lengths (Å).

Ru1—S2^i	2.3624 (7)	S1—C11	1.785 (4)
Ru1—S1^i	2.3678 (7)	S2—C21	1.803 (4)
Ru1—Cl1^i	2.4207 (7)	S2—C22	1.804 (4)
S1—C12	1.781 (4)		

Symmetry code: (i) $-x + 1, -y, -z + 1$.

H atoms were placed in calculated positions, with C—H = 0.96 Å for CH$_3$ groups and $U_{iso}(H) = 1.5U_{eq}(C)$, and constrained to ride on the parent C atom.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2003); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg,
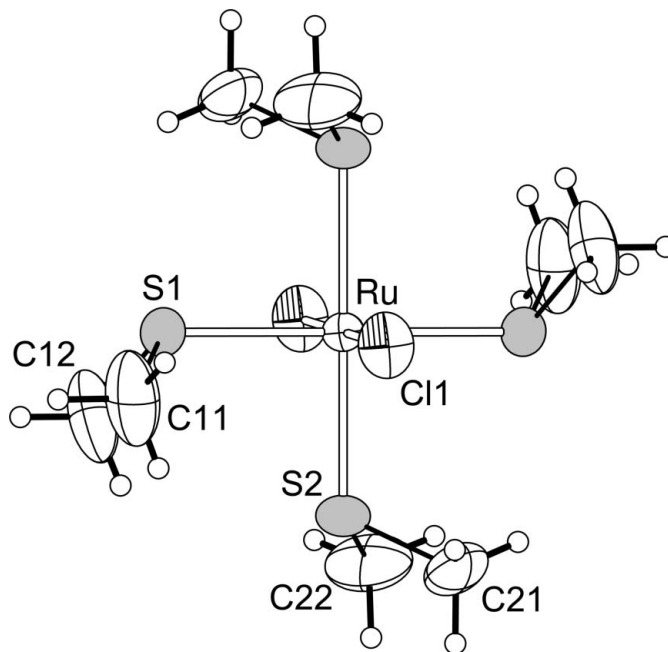

Figure 1
The molecular structure of (I), shown with 50% probability displacement ellipsoids. H atoms are shown with arbitrary radii. Unlabelled atoms are related to labelled atoms by $(1 - x, -y, 1 - z)$.

1999); software used to prepare material for publication: *SHELXL97*.

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