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Crystal structure of di- μ -isobutyrate- κ^4 O:O'-bis[*cis*-dichlorido(dimethyl sulfoxide- κ S)rhenium(III)]

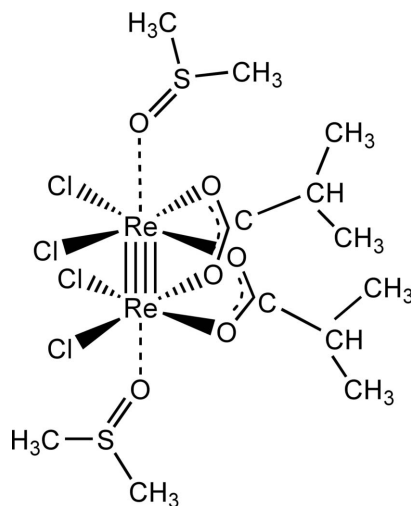
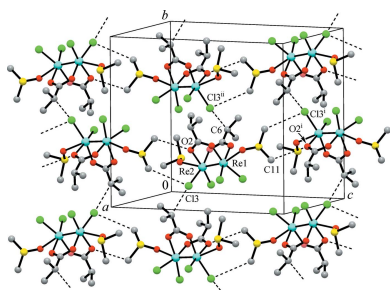
Alexander A. Golichenko* and Alexander V. Shtemenko

Department of Inorganic Chemistry, Ukrainian State University of Chemical Technology, Gagarin Ave. 8, Dnipropetrovsk 49005, Ukraine. *Correspondence e-mail: golichenko_alex@i.ua

The title compound, $[\text{Re}_2(\text{C}_3\text{H}_7\text{COO})_2\text{Cl}_4\{(\text{CH}_3)_2\text{SO}\}_2]$, comprises binuclear complex molecules [$\text{Re}-\text{Re} = 2.24502(13) \text{ \AA}$] involving *cis*-oriented double carboxylate bridges, four equatorial chloride ions and two weakly bonded O atoms from dimethyl sulfoxide ligands in the axial positions at the Re^{III} atoms. In the crystal, molecules are linked into corrugated layers parallel to (101) by very weak $\text{C}-\text{H}\cdots\text{Cl}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions. $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonding provides the links between layers to consolidate a three-dimensional framework.

1. Chemical context

Binuclear rhenium(III) clusters are classical complexes with a unique quadruple metal–metal bond (Cotton *et al.*, 2005, Golichenko & Shtemenko, 2006). In our previous work we have shown that such compounds with chloride and alkylcarboxylate equatorial ligands exhibit antitumor, antiradical and hepato- and nephroprotective biological activity with low toxicity (Dimitrov *et al.*, 1978, Shtemenko *et al.*, 2007, 2008, 2009, 2013).



Labile axial ligands and equatorial chloride groups are the reactive centers in interactions with other chemical compounds and biological macromolecules *in vitro* and *in vivo* (Shtemenko *et al.*, 2013). In this context, we present the synthesis and the structure of the title dirhenium(III) complex with isobutyrate equatorial ligands as biologically active groups, which can exhibit antitumor activity in the tetracarboxylate compound $\text{Re}_2(i\text{-C}_3\text{H}_7\text{COO})_4\text{Cl}_2$ (Shtemenko *et al.*, 2007).

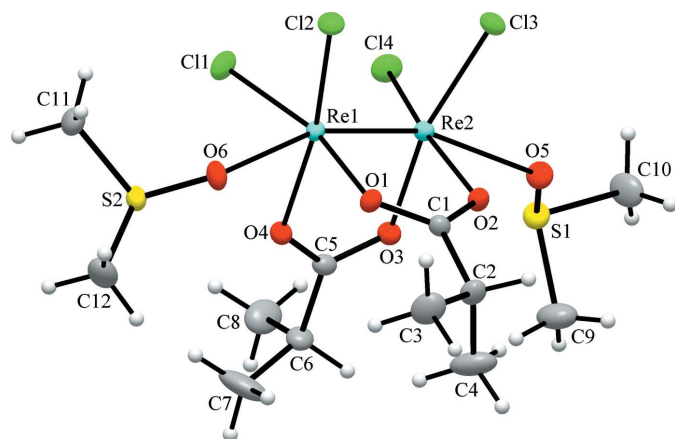


Figure 1
The structure of *cis*-Re₂Cl₄[*i*-C₃H₇COO]₂·2(CH₃)₂SO, showing displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radii.

2. Structural commentary

The quadruple Re–Re bond [2.24502 (13) Å] is typical for related dicarboxylato clusters (Cotton *et al.*, 2005, Shtemenko *et al.*, 2009) and the coordination of each of the rhenium ions also comprises two chlorides and two oxygen atoms of carboxylate ligands (Fig. 1). The distorted octahedral coordination geometry of Re1 and Re2 is completed by weakly bonded oxygen atoms from dimethyl sulfoxide ligands [Re1–O6 = 2.3282 (15) and Re2–O5 = 2.3938 (15) Å], in *trans*-positions to the Re–Re bond. This may be compared with a similar weak binding of N- or O-donors, which is characteristic of dicarboxylatodirhenium compounds (Bera *et al.*, 2003, Shtemenko *et al.*, 2009, Golichenko *et al.*, 2015).

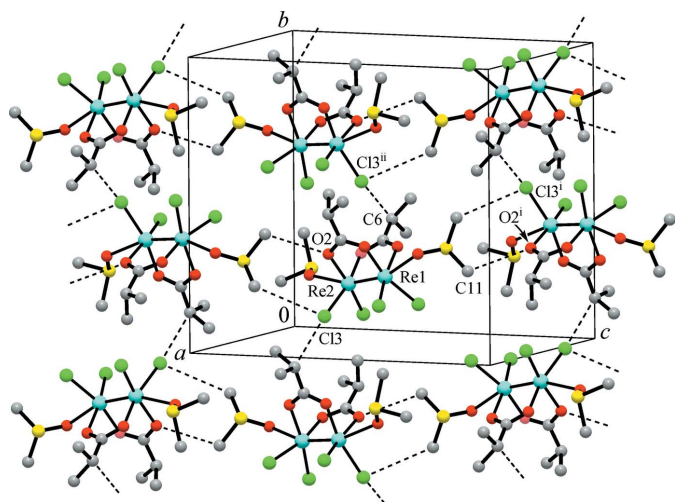


Figure 2
A fragment of the structure, showing weak C–H···O and C–H···Cl hydrogen-bond interactions (dashed lines), which assemble the molecules into corrugated layers parallel to (101). [Symmetry codes: (i) $-\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$; (ii) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$.]

Table 1
Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C11–H11B···O2 ⁱ	0.98	2.40	3.324 (3)	156
C6–H6···Cl3 ⁱⁱ	1.00	2.73	3.519 (2)	136
C12–H12A···Cl2 ⁱⁱⁱ	0.98	2.82	3.751 (3)	159
C12–H12B···Cl3 ⁱ	0.98	2.82	3.760 (3)	161

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (iii) $-x - \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$.

3. Supramolecular features

Intermolecular bonding is only very weak: it comprises distal, though relatively directional, C–H···O and C–H···Cl hydrogen-bond interactions between the methine- and methyl-H of the carboxylate and DMSO ligands (Table 1). The shortest bonds found for the chloride acceptors are C6–H6···Cl3ⁱⁱ [C6···Cl3ⁱⁱ = 3.519 (2) Å; symmetry code (ii): $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$], which unite the molecules into chains along the *b* axis (Fig. 2). The hydrogen bonds adopted by two methyl groups of DMSO molecules (referenced by a sulfur atoms S2) assemble these chains into corrugated layers parallel to (101). A very weak bond of this type is found also between adjacent layers: C12···Cl2ⁱⁱⁱ = 3.751 (3) Å; symmetry code (iii): $-\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$] (Table 1). The latter extends the structure into a third direction and provides the formation of a hydrogen-bonded framework.

Table 2
Experimental details.

Crystal data	[Re ₂ (C ₄ H ₇ O ₂) ₂ Cl ₄ (C ₂ H ₆ OS) ₂]
Chemical formula	844.65
<i>M_r</i>	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Crystal system, space group	110
Temperature (K)	10.5581 (4), 14.7406 (5), 15.6088 (6)
<i>a</i> , <i>b</i> , <i>c</i> (Å)	100.794 (2)
β (°)	2386.26 (15)
<i>V</i> (Å ³)	4
<i>Z</i>	Mo <i>K</i> α
Radiation type	10.78
μ (mm ^{−1})	0.22 × 0.18 × 0.09
Crystal size (mm)	
Data collection	Siemens SMART CCD area-detector
Diffractometer	Multi-scan (<i>SADABS</i> ; Bruker, 2008)
Absorption correction	0.133, 0.478
<i>T</i> _{min} , <i>T</i> _{max}	93039, 14497, 11921
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	0.040
<i>R</i> _{int}	0.909
(<i>sin</i> θ / λ) _{max} (Å ^{−1})	
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.025, 0.049, 1.00
No. of reflections	14497
No. of parameters	243
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ^{−3})	1.71, −1.14

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* (Sheldrick 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 1999) and *WinGX* (Farrugia, 2012).

4. Synthesis and crystallization

[NBu₄]₂[Re₂Cl₈] (0.2 g, 0.175 mmol) was added to isobutyric acid (10 ml). The mixture was heated for 3 h in a water bath under an inert atmosphere. DMSO (0.5 ml) was then added to the resulting blue solution at room temperature. A dark-blue crystalline product (0.12 g, yield 81%) was obtained after 12 h, was collected by filtration and dried in air.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H were refined using a riding-model approximation, with C–H = 0.98–1.00 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{C})$ for methyl H atoms. A rotating model was used for the methyl groups. Six outliers (2 6 1, 3 3 3, $\bar{2}$ 4 3, 0 1 1, $\bar{4}$ 3 4, 3 3 7) were omitted in the last cycles of refinement.

Acknowledgements

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References

- Bera, J. K., Vo, T.-T., Walton, R. A. & Dunbar, K. R. (2003). *Polyhedron*, **22**, 3009–3014.
- Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Bruker (2008). *SADABS*, *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Cotton, F. A., Murillo, C. A. & Walton, R. A. (2005). *Multiple Bonds between Metal Atoms*, 3rd ed., pp. 271–376. New York: Springer Science and Business Media Inc.
- Dimitrov, N. V. & Eastland, G. W. (1978). *Current Chemotherapy*, edited by W. Siegenthaler & R. Luthy, Vol. 2, pp. 1319–1321. Washington, DC: American Society for Microbiology Publishing.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Golichenko, A. A., Domasevitch, K. V., Kytova, D. E. & Shtemenko, A. V. (2015). *Acta Cryst.* **E71**, 45–47.
- Golichenko, A. A. & Shtemenko, A. V. (2006). *Russ. J. Coord. Chem.* **32**, 242–249.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Shtemenko, N. I., Chifotides, H. T., Domasevitch, K. V., Golichenko, A. A., Babiy, S. A., Li, Z., Paramonova, K. V., Shtemenko, A. V. & Dunbar, K. R. (2013). *J. Inorg. Biochem.* **129**, 127–134.
- Shtemenko, N., Collery, P. & Shtemenko, A. (2007). *Anticancer Res.* **27**, 2487–2492.
- Shtemenko, A. V., Collery, P., Shtemenko, N. I., Domasevitch, K. V., Zabitskaya, E. D. & Golichenko, A. A. (2009). *Dalton Trans.* pp. 5132–5136.
- Shtemenko, A., Golichenko, A., Tretyak, S., Shtemenko, N. & Randarevich, M. (2008). *Metal Ions in Biology and Medicine*, Vol. 10, pp. 229–234. Paris: John Libbey Eurotext.

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Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINTE* (Bruker, 2008); data reduction: *SAINTE* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Di- μ -isobutyrate- κ^4 O:O'-bis[*cis*-dichlorido(dimethyl sulfoxide- κ S)rhenium(III)]

Crystal data

[Re₂(C₄H₇O₂)₂Cl₄(C₂H₆OS)₂]

$M_r = 844.65$

Monoclinic, $P2_1/n$

$a = 10.5581$ (4) Å

$b = 14.7406$ (5) Å

$c = 15.6088$ (6) Å

$\beta = 100.794$ (2)°

$V = 2386.26$ (15) Å³

$Z = 4$

$F(000) = 1584$

$D_x = 2.351$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9919 reflections

$\theta = 2.4\text{--}39.0^\circ$

$\mu = 10.78$ mm⁻¹

$T = 110$ K

Plate, blue

0.22 × 0.18 × 0.09 mm

Data collection

Siemens SMART CCD area-detector diffractometer

Graphite monochromator

phi and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2008)

$T_{\min} = 0.133$, $T_{\max} = 0.478$

93039 measured reflections

14497 independent reflections

11921 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.040$

$\theta_{\max} = 40.2^\circ$, $\theta_{\min} = 2.2^\circ$

$h = -19 \rightarrow 18$

$k = -25 \rightarrow 26$

$l = -28 \rightarrow 27$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.049$

$S = 1.00$

14497 reflections

243 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0183P)^2 + 1.7981P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 1.71$ e Å⁻³

$\Delta\rho_{\min} = -1.14$ e Å⁻³

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Re1	-0.06723 (2)	0.17363 (2)	0.27880 (2)	0.01130 (2)
Re2	0.10986 (2)	0.16371 (2)	0.21905 (2)	0.01147 (2)
Cl1	-0.01954 (5)	0.08982 (4)	0.40554 (3)	0.02107 (9)
Cl2	-0.19965 (5)	0.05974 (3)	0.21084 (3)	0.01810 (8)
Cl3	0.06421 (5)	0.04494 (3)	0.12210 (3)	0.01726 (8)
Cl4	0.25202 (5)	0.07759 (3)	0.31739 (3)	0.02151 (9)
S1	0.41251 (5)	0.24240 (4)	0.20176 (3)	0.01935 (9)
S2	-0.23871 (5)	0.25929 (3)	0.42297 (3)	0.01756 (9)
O1	-0.14493 (13)	0.26371 (9)	0.18365 (9)	0.0142 (2)
O2	0.02927 (14)	0.25241 (9)	0.12399 (9)	0.0145 (2)
O3	0.18421 (14)	0.27603 (9)	0.28722 (9)	0.0159 (3)
O4	0.01121 (14)	0.28533 (9)	0.34802 (9)	0.0158 (3)
O5	0.28531 (14)	0.20575 (10)	0.14988 (10)	0.0189 (3)
O6	-0.24413 (14)	0.23612 (10)	0.32675 (9)	0.0189 (3)
C1	-0.07803 (18)	0.29012 (12)	0.12848 (12)	0.0133 (3)
C2	-0.1181 (2)	0.37225 (13)	0.07331 (14)	0.0181 (4)
H2	-0.1090	0.3585	0.0120	0.022*
C3	-0.2560 (2)	0.40050 (17)	0.07314 (17)	0.0274 (5)
H3A	-0.2788	0.4516	0.0330	0.041*
H3B	-0.2647	0.4188	0.1321	0.041*
H3C	-0.3138	0.3494	0.0542	0.041*
C4	-0.0227 (3)	0.44808 (16)	0.1087 (2)	0.0354 (6)
H4A	0.0658	0.4260	0.1125	0.053*
H4B	-0.0358	0.4662	0.1668	0.053*
H4C	-0.0371	0.5004	0.0694	0.053*
C5	0.1204 (2)	0.31512 (13)	0.33854 (12)	0.0152 (3)
C6	0.1796 (2)	0.39547 (14)	0.38935 (14)	0.0197 (4)
H6	0.2283	0.4313	0.3518	0.024*
C7	0.0785 (3)	0.4565 (2)	0.4167 (2)	0.0469 (8)
H7A	0.0176	0.4764	0.3649	0.070*
H7B	0.1206	0.5095	0.4476	0.070*
H7C	0.0321	0.4229	0.4554	0.070*
C8	0.2750 (3)	0.36103 (19)	0.46883 (17)	0.0337 (6)
H8A	0.3380	0.3207	0.4495	0.051*
H8B	0.2282	0.3276	0.5074	0.051*
H8C	0.3200	0.4127	0.5004	0.051*
C9	0.4146 (3)	0.36054 (17)	0.1775 (2)	0.0360 (6)
H9A	0.4047	0.3689	0.1143	0.054*
H9B	0.4968	0.3868	0.2065	0.054*

H9C	0.3435	0.3908	0.1984	0.054*
C10	0.5306 (2)	0.20667 (18)	0.14113 (18)	0.0291 (5)
H10A	0.5367	0.1403	0.1425	0.044*
H10B	0.6144	0.2329	0.1669	0.044*
H10C	0.5057	0.2272	0.0806	0.044*
C11	-0.3361 (3)	0.17496 (16)	0.46035 (17)	0.0286 (5)
H11A	-0.4191	0.1709	0.4200	0.043*
H11B	-0.3508	0.1913	0.5186	0.043*
H11C	-0.2922	0.1162	0.4631	0.043*
C12	-0.3441 (3)	0.35344 (17)	0.42132 (18)	0.0338 (6)
H12A	-0.3087	0.4057	0.3950	0.051*
H12B	-0.3529	0.3685	0.4811	0.051*
H12C	-0.4289	0.3381	0.3870	0.051*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Re1	0.01040 (3)	0.01222 (3)	0.01171 (3)	-0.00114 (2)	0.00320 (2)	0.00002 (2)
Re2	0.00953 (3)	0.01154 (3)	0.01360 (3)	0.00081 (2)	0.00288 (2)	0.00041 (2)
Cl1	0.0222 (2)	0.0241 (2)	0.0166 (2)	-0.00111 (18)	0.00305 (17)	0.00674 (16)
Cl2	0.0161 (2)	0.01640 (19)	0.0219 (2)	-0.00426 (15)	0.00380 (17)	-0.00305 (15)
Cl3	0.0169 (2)	0.01521 (19)	0.0201 (2)	0.00138 (15)	0.00460 (16)	-0.00402 (14)
Cl4	0.0167 (2)	0.0215 (2)	0.0244 (2)	0.00463 (17)	-0.00088 (18)	0.00541 (17)
S1	0.0130 (2)	0.0223 (2)	0.0230 (2)	-0.00283 (17)	0.00407 (18)	-0.00136 (17)
S2	0.0194 (2)	0.0189 (2)	0.0162 (2)	-0.00284 (17)	0.00824 (17)	-0.00281 (15)
O1	0.0120 (6)	0.0153 (6)	0.0159 (6)	0.0000 (5)	0.0041 (5)	0.0022 (4)
O2	0.0133 (6)	0.0153 (6)	0.0157 (6)	0.0025 (5)	0.0048 (5)	0.0026 (4)
O3	0.0136 (6)	0.0161 (6)	0.0186 (6)	-0.0023 (5)	0.0044 (5)	-0.0023 (5)
O4	0.0156 (7)	0.0163 (6)	0.0162 (6)	-0.0038 (5)	0.0050 (5)	-0.0034 (5)
O5	0.0108 (6)	0.0225 (7)	0.0238 (7)	-0.0020 (5)	0.0040 (5)	-0.0011 (5)
O6	0.0164 (7)	0.0255 (7)	0.0167 (7)	-0.0009 (5)	0.0076 (5)	-0.0038 (5)
C1	0.0134 (8)	0.0128 (7)	0.0135 (8)	0.0015 (6)	0.0022 (6)	-0.0002 (5)
C2	0.0175 (9)	0.0170 (8)	0.0199 (9)	0.0037 (7)	0.0034 (7)	0.0046 (6)
C3	0.0184 (10)	0.0275 (11)	0.0353 (13)	0.0065 (8)	0.0025 (9)	0.0084 (9)
C4	0.0254 (12)	0.0162 (10)	0.0617 (18)	-0.0007 (8)	0.0004 (12)	0.0048 (10)
C5	0.0161 (9)	0.0132 (8)	0.0155 (8)	-0.0013 (6)	0.0015 (7)	-0.0012 (6)
C6	0.0206 (10)	0.0179 (9)	0.0204 (9)	-0.0062 (7)	0.0028 (7)	-0.0044 (7)
C7	0.0375 (16)	0.0298 (14)	0.072 (2)	-0.0008 (11)	0.0079 (15)	-0.0319 (14)
C8	0.0341 (14)	0.0370 (14)	0.0254 (12)	-0.0122 (11)	-0.0065 (10)	-0.0026 (9)
C9	0.0340 (14)	0.0203 (11)	0.0549 (17)	-0.0051 (10)	0.0113 (13)	-0.0022 (10)
C10	0.0134 (9)	0.0340 (13)	0.0412 (14)	0.0010 (8)	0.0083 (9)	-0.0067 (10)
C11	0.0379 (14)	0.0239 (11)	0.0294 (12)	-0.0072 (9)	0.0206 (11)	-0.0015 (8)
C12	0.0494 (17)	0.0237 (11)	0.0322 (13)	0.0104 (11)	0.0172 (12)	-0.0002 (9)

Geometric parameters (Å, °)

Re1—O1	2.0459 (13)	C3—H3C	0.9800
Re1—O4	2.0565 (13)	C4—H4A	0.9800

Re1—Re2	2.2450 (1)	C4—H4B	0.9800
Re1—C11	2.3065 (5)	C4—H4C	0.9800
Re1—C12	2.3115 (5)	C5—C6	1.495 (3)
Re1—O6	2.3282 (15)	C6—C7	1.517 (4)
Re2—O2	2.0401 (13)	C6—C8	1.531 (3)
Re2—O3	2.0437 (14)	C6—H6	1.0000
Re2—C13	2.3052 (5)	C7—H7A	0.9800
Re2—C14	2.3147 (5)	C7—H7B	0.9800
Re2—O5	2.3938 (15)	C7—H7C	0.9800
S1—O5	1.5310 (15)	C8—H8A	0.9800
S1—C10	1.780 (2)	C8—H8B	0.9800
S1—C9	1.783 (3)	C8—H8C	0.9800
S2—O6	1.5308 (15)	C9—H9A	0.9800
S2—C12	1.776 (3)	C9—H9B	0.9800
S2—C11	1.780 (2)	C9—H9C	0.9800
O1—C1	1.273 (2)	C10—H10A	0.9800
O2—C1	1.276 (2)	C10—H10B	0.9800
O3—C5	1.276 (2)	C10—H10C	0.9800
O4—C5	1.268 (3)	C11—H11A	0.9800
C1—C2	1.500 (3)	C11—H11B	0.9800
C2—C3	1.514 (3)	C11—H11C	0.9800
C2—C4	1.536 (3)	C12—H12A	0.9800
C2—H2	1.0000	C12—H12B	0.9800
C3—H3A	0.9800	C12—H12C	0.9800
C3—H3B	0.9800		
O1—Re1—O4	85.93 (6)	C2—C3—H3C	109.5
O1—Re1—Re2	89.58 (4)	H3A—C3—H3C	109.5
O4—Re1—Re2	89.18 (4)	H3B—C3—H3C	109.5
O1—Re1—C11	164.51 (4)	C2—C4—H4A	109.5
O4—Re1—C11	88.65 (4)	C2—C4—H4B	109.5
Re2—Re1—C11	104.857 (14)	H4A—C4—H4B	109.5
O1—Re1—C12	90.71 (4)	C2—C4—H4C	109.5
O4—Re1—C12	166.43 (4)	H4A—C4—H4C	109.5
Re2—Re1—C12	103.960 (13)	H4B—C4—H4C	109.5
C11—Re1—C12	91.189 (19)	O4—C5—O3	121.00 (17)
O1—Re1—O6	74.92 (5)	O4—C5—C6	120.74 (18)
O4—Re1—O6	77.45 (6)	O3—C5—C6	118.24 (18)
Re2—Re1—O6	160.04 (4)	C5—C6—C7	111.87 (19)
C11—Re1—O6	89.75 (4)	C5—C6—C8	108.26 (18)
C12—Re1—O6	88.98 (4)	C7—C6—C8	111.1 (2)
O2—Re2—O3	85.80 (6)	C5—C6—H6	108.5
O2—Re2—Re1	89.66 (4)	C7—C6—H6	108.5
O3—Re2—Re1	89.97 (4)	C8—C6—H6	108.5
O2—Re2—C13	90.11 (4)	C6—C7—H7A	109.5
O3—Re2—C13	165.87 (4)	C6—C7—H7B	109.5
Re1—Re2—C13	103.544 (13)	H7A—C7—H7B	109.5
O2—Re2—C14	164.60 (4)	C6—C7—H7C	109.5

O3—Re2—C14	87.76 (4)	H7A—C7—H7C	109.5
Re1—Re2—C14	104.318 (15)	H7B—C7—H7C	109.5
C13—Re2—C14	92.789 (18)	C6—C8—H8A	109.5
O2—Re2—O5	76.03 (5)	C6—C8—H8B	109.5
O3—Re2—O5	76.76 (5)	H8A—C8—H8B	109.5
Re1—Re2—O5	161.00 (4)	C6—C8—H8C	109.5
C13—Re2—O5	89.13 (4)	H8A—C8—H8C	109.5
C14—Re2—O5	88.89 (4)	H8B—C8—H8C	109.5
O5—S1—C10	104.28 (10)	S1—C9—H9A	109.5
O5—S1—C9	106.08 (12)	S1—C9—H9B	109.5
C10—S1—C9	97.94 (14)	H9A—C9—H9B	109.5
O6—S2—C12	104.59 (11)	S1—C9—H9C	109.5
O6—S2—C11	104.36 (10)	H9A—C9—H9C	109.5
C12—S2—C11	98.71 (14)	H9B—C9—H9C	109.5
C1—O1—Re1	119.46 (12)	S1—C10—H10A	109.5
C1—O2—Re2	119.54 (12)	S1—C10—H10B	109.5
C5—O3—Re2	119.74 (13)	H10A—C10—H10B	109.5
C5—O4—Re1	120.10 (13)	S1—C10—H10C	109.5
S1—O5—Re2	121.94 (8)	H10A—C10—H10C	109.5
S2—O6—Re1	121.25 (8)	H10B—C10—H10C	109.5
O1—C1—O2	121.00 (17)	S2—C11—H11A	109.5
O1—C1—C2	120.20 (17)	S2—C11—H11B	109.5
O2—C1—C2	118.55 (17)	H11A—C11—H11B	109.5
C1—C2—C3	112.98 (18)	S2—C11—H11C	109.5
C1—C2—C4	106.60 (17)	H11A—C11—H11C	109.5
C3—C2—C4	111.48 (19)	H11B—C11—H11C	109.5
C1—C2—H2	108.6	S2—C12—H12A	109.5
C3—C2—H2	108.6	S2—C12—H12B	109.5
C4—C2—H2	108.6	H12A—C12—H12B	109.5
C2—C3—H3A	109.5	S2—C12—H12C	109.5
C2—C3—H3B	109.5	H12A—C12—H12C	109.5
H3A—C3—H3B	109.5	H12B—C12—H12C	109.5

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C11—H11B...O2 ⁱ	0.98	2.40	3.324 (3)	156
C6—H6...Cl3 ⁱⁱ	1.00	2.73	3.519 (2)	136
C12—H12A...C12 ⁱⁱⁱ	0.98	2.82	3.751 (3)	159
C12—H12B...Cl3 ⁱ	0.98	2.82	3.760 (3)	161

Symmetry codes: (i) $x-1/2, -y+1/2, z+1/2$; (ii) $-x+1/2, y+1/2, -z+1/2$; (iii) $-x-1/2, y+1/2, -z+1/2$.