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Nonacarbonyl(μ_2-methanethiolato)(μ_3-trimethylsilylacetylene)triruthenium

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.025
wR factor = 0.060
Data-to-parameter ratio = 29.1

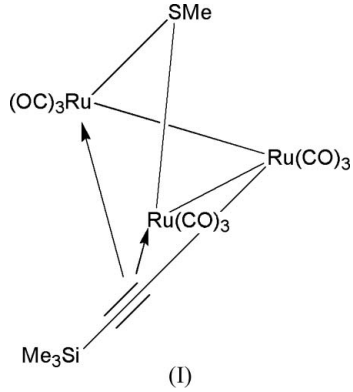
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The structure of the title compound, [$Ru_3(\mu_2CH_3S)\{\mu_3$-$C_2Si(CH_3)_3\}(CO)_9$], contains an open triangle of Ru atoms. The open edge is bridged on one side by a μ_2-$S(CH_3)$ unit, and the other side of the triangle is capped by a [C≡$CSi(CH_3)_3$] group, with the acetylenic bond perpendicular to the open Ru···Ru edge.

Comment

The homogeneous desulfurization of thiophene with transition metal compounds has provided an important model for the catalytic heterogeneous dehydrosulfurization of thiophenic components of crude oil (Rauschfuss, 1991). Increased catalytic activity has been observed, particularly toward thiophenes, when late transition metals (group 8) are employed (Angelici, 1997).

In the context of catalysis, we have been investigating the reactivity of ruthenium carbonyl clusters with thiol derivatives. The reaction of $Ru_3(CO)_{12}$ with the asymmetric acetylene derivative $Me_3SC{\equiv}CSiMe_3$ under reflux in hexane afforded [$Ru_3(CO)_9(\mu_2$-$H_3CS)(\mu_3$-$C_2Si(CH_3)_3$], (I), in which the ruthenium cluster has inserted into a C—S bond. This type of reaction has been observed previously (Arce *et al.*, 1994).



(I)

The cluster consists of an open ruthenium triangle (Fig. 1), with the 'non bonding' edge having an Ru···Ru distance of 3.360 (1) Å. This edge is bridged symmetrically by a μ_2-$S(CH_3)$ group, and the other side of the metal triangle is capped by a ($C{\equiv}CSiMe_3$) group in which one acetylenic C atom σ-bonds to Ru2 while the acetylenic triple bond is π-bound to Ru1 and Ru3, adopting a bonding mode perpendicular to the long Ru1···Ru3 edge. The nine carbonyl ligands are terminal and essentially linear, three being bound to each Ru centre. Overall, the cluster has an electron count of 50, consistent with the observed open triangular metal framework.

Experimental

Powdered $Ru_3(CO)_{12}$ (0.102 g, 0.16 mmol) and $Me_3SC{\equiv}CSiMe_3$ (0.085 g, 0.75 mmol) were dissolved in hexane (20 ml) and the mixture refluxed for 3 h, after which a second portion of $Me_3SC{\equiv}CSiMe_3$ [0.090 g, 0.79 mmol, in hexane (5 ml)] was added. The mixture was further refluxed for 1 h and subsequently cooled. Upon solvent removal, the crude product was purified by preparative thin layer chromatography using hexane as an eluent. The title compound was obtained from the yellow band with the highest R_f value after that of $Ru_3(CO)_{12}$. The product was recrystallized from a 1:1 mixture of CH_2Cl_2/hexane to give yellow block crystals.

Crystal data

$[Ru_3(CH_3S)(C_5H_9Si)(CO)_9]$	V = 1119.81 (10) Å^3
M_r = 699.61	Z = 2
Triclinic, $P\overline{1}$	D_x = 2.075 Mg m^{-3}
a = 9.0510 (1) Å	Mo $K\alpha$ radiation
b = 9.6680 (1) Å	μ = 2.19 mm^{-1}
c = 14.5830 (2) Å	T = 150 (2) K
α = 76.319 (1)°	Block, yellow
β = 88.116 (1)°	0.4 × 0.35 × 0.35 mm
γ = 64.933 (10)°	

Data collection

Bruker–Nonius KappaCCD diffractometer	25218 measured reflections
	7649 independent reflections
ω and φ scans	7024 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)	R_{int} = 0.034
	θ_{max} = 32.0°
T_{min} = 0.393, T_{max} = 0.466	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0244P)^2 + 0.728P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.025	
$wR(F^2)$ = 0.060	
S = 1.06	$(\Delta/\sigma)_{max} < 0.001$
7649 reflections	$\Delta\rho_{max}$ = 1.16 e Å^{-3}
263 parameters	$\Delta\rho_{min}$ = −1.05 e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXL97*
	Extinction coefficient: 0.0125 (5)

The methyl H atoms were constrained as riding atoms with C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C). The highest residual electron-density peak is 1.81 Å from O8 and the deepest hole is 0.69 Å from Ru2.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *DIRDIF99* (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

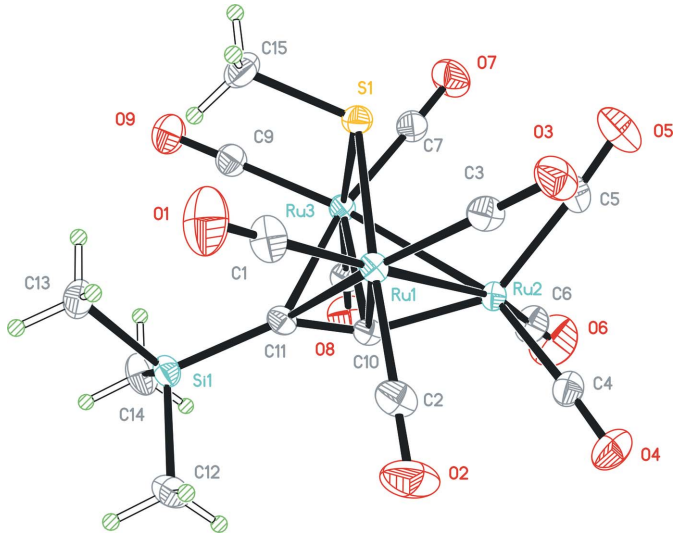


Figure 1
The molecular structure of (I), showing the atom-numbering scheme (50% probability displacement ellipsoids).

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Block, yellow
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25218 measured reflections
7649 independent reflections
7024 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 32.0°$, $\theta_{min} = 3.7°$
$h = -13 \rightarrow 13$
$k = -13 \rightarrow 14$
$l = -18 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.060$
$S = 1.06$
7649 reflections
263 parameters
0 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0244P)^2 + 0.728P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.16$ e Å^{-3}
$\Delta\rho_{min} = -1.05$ e Å^{-3}
Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0125 (5)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ru1	0.141581 (16)	0.205411 (16)	0.227713 (10)	0.01705 (4)
Ru2	0.159195 (16)	0.453982 (16)	0.290179 (10)	0.01715 (4)
Ru3	0.448076 (16)	0.317260 (16)	0.199009 (10)	0.01684 (4)
S1	0.25288 (5)	0.31333 (5)	0.09168 (3)	0.01993 (9)

C1	0.1589 (3)	0.0279 (2)	0.18020 (17)	0.0293 (4)
O1	0.1615 (2)	−0.0723 (2)	0.15244 (17)	0.0508 (5)
C2	0.0595 (2)	0.1353 (3)	0.34375 (15)	0.0276 (4)
O2	0.0129 (2)	0.0942 (3)	0.41279 (13)	0.0482 (5)
C3	−0.0712 (2)	0.3528 (2)	0.17291 (14)	0.0231 (4)
O3	−0.19797 (18)	0.4410 (2)	0.13891 (12)	0.0337 (3)
C4	−0.0089 (2)	0.4664 (2)	0.37529 (14)	0.0242 (4)
O4	−0.1040 (2)	0.4682 (2)	0.42852 (12)	0.0357 (4)
C5	0.0312 (2)	0.6309 (2)	0.18696 (16)	0.0266 (4)
O5	−0.0381 (2)	0.7301 (2)	0.12321 (14)	0.0446 (4)
C6	0.2378 (3)	0.5724 (3)	0.34570 (16)	0.0303 (4)
O6	0.2833 (3)	0.6430 (3)	0.37957 (17)	0.0549 (5)
C7	0.4168 (2)	0.5173 (2)	0.12179 (14)	0.0250 (4)
O7	0.3990 (2)	0.63528 (19)	0.07424 (13)	0.0396 (4)
C8	0.5770 (2)	0.3371 (2)	0.29268 (14)	0.0241 (4)
O8	0.6535 (2)	0.3509 (2)	0.34671 (12)	0.0375 (4)
C9	0.6388 (2)	0.1860 (2)	0.14350 (15)	0.0256 (4)
O9	0.7511 (2)	0.1104 (2)	0.11253 (13)	0.0401 (4)
C10	0.3184 (2)	0.2342 (2)	0.31745 (12)	0.0175 (3)
C11	0.4126 (2)	0.1028 (2)	0.29716 (13)	0.0191 (3)
Si1	0.56728 (6)	−0.10449 (6)	0.34213 (4)	0.02014 (10)
C12	0.4938 (3)	−0.1902 (2)	0.45160 (15)	0.0297 (4)
H12A	0.39	−0.1916	0.4362	0.045*
H12B	0.4776	−0.1261	0.4973	0.045*
H12C	0.5751	−0.298	0.4791	0.045*
C13	0.5906 (3)	−0.2166 (3)	0.25057 (15)	0.0301 (4)
H13A	0.6295	−0.1691	0.1937	0.045*
H13B	0.4846	−0.2133	0.2346	0.045*
H13C	0.6698	−0.3263	0.2753	0.045*
C14	0.7655 (3)	−0.1011 (3)	0.37012 (18)	0.0315 (4)
H14A	0.8032	−0.0555	0.312	0.047*
H14B	0.8473	−0.2088	0.3972	0.047*
H14C	0.75	−0.0372	0.4158	0.047*
C15	0.3635 (3)	0.1569 (3)	0.03268 (15)	0.0291 (4)
H15A	0.4101	0.1976	−0.023	0.044*
H15B	0.2882	0.1186	0.0129	0.044*
H15C	0.4517	0.0701	0.0764	0.044*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ru1	0.01543 (7)	0.01754 (7)	0.01896 (7)	−0.00819 (5)	−0.00003 (5)	−0.00350 (5)
Ru2	0.01528 (7)	0.01648 (7)	0.01918 (7)	−0.00573 (5)	0.00145 (5)	−0.00554 (5)
Ru3	0.01455 (7)	0.01741 (7)	0.01837 (7)	−0.00731 (5)	0.00219 (5)	−0.00329 (5)
S1	0.01897 (19)	0.0221 (2)	0.01693 (19)	−0.00742 (16)	0.00085 (15)	−0.00414 (16)
C1	0.0244 (9)	0.0260 (9)	0.0399 (11)	−0.0116 (8)	−0.0015 (8)	−0.0101 (9)
O1	0.0462 (11)	0.0392 (10)	0.0787 (15)	−0.0200 (9)	−0.0014 (10)	−0.0313 (10)
C2	0.0233 (9)	0.0300 (10)	0.0288 (10)	−0.0148 (8)	−0.0014 (7)	0.0007 (8)

O2	0.0468 (11)	0.0593 (12)	0.0359 (9)	−0.0307 (10)	0.0059 (8)	0.0081 (9)
C3	0.0189 (8)	0.0283 (9)	0.0235 (9)	−0.0128 (7)	0.0019 (6)	−0.0039 (7)
O3	0.0192 (7)	0.0381 (8)	0.0364 (8)	−0.0102 (6)	−0.0032 (6)	0.0009 (7)
C4	0.0207 (8)	0.0258 (9)	0.0255 (9)	−0.0077 (7)	0.0019 (7)	−0.0095 (7)
O4	0.0290 (8)	0.0464 (9)	0.0348 (8)	−0.0164 (7)	0.0126 (6)	−0.0162 (7)
C5	0.0220 (9)	0.0210 (8)	0.0333 (10)	−0.0071 (7)	−0.0009 (7)	−0.0040 (8)
O5	0.0387 (9)	0.0337 (9)	0.0475 (11)	−0.0109 (7)	−0.0130 (8)	0.0083 (8)
C6	0.0296 (10)	0.0312 (10)	0.0357 (11)	−0.0158 (9)	0.0053 (8)	−0.0137 (9)
O6	0.0630 (13)	0.0619 (13)	0.0666 (14)	−0.0417 (11)	0.0061 (11)	−0.0354 (11)
C7	0.0245 (9)	0.0243 (9)	0.0263 (9)	−0.0115 (7)	0.0053 (7)	−0.0049 (7)
O7	0.0458 (10)	0.0270 (8)	0.0415 (9)	−0.0175 (7)	0.0066 (8)	0.0030 (7)
C8	0.0210 (8)	0.0273 (9)	0.0261 (9)	−0.0135 (7)	0.0032 (7)	−0.0046 (7)
O8	0.0346 (8)	0.0512 (10)	0.0356 (9)	−0.0262 (8)	−0.0031 (7)	−0.0110 (8)
C9	0.0205 (8)	0.0265 (9)	0.0275 (9)	−0.0091 (7)	0.0034 (7)	−0.0047 (8)
O9	0.0277 (8)	0.0397 (9)	0.0416 (9)	−0.0041 (7)	0.0112 (7)	−0.0109 (8)
C10	0.0158 (7)	0.0193 (8)	0.0173 (7)	−0.0086 (6)	0.0005 (6)	−0.0023 (6)
C11	0.0182 (7)	0.0191 (8)	0.0196 (8)	−0.0088 (6)	−0.0004 (6)	−0.0021 (6)
Si1	0.0199 (2)	0.0164 (2)	0.0215 (2)	−0.00547 (18)	−0.00286 (18)	−0.00376 (18)
C12	0.0411 (12)	0.0239 (9)	0.0232 (9)	−0.0155 (9)	−0.0030 (8)	−0.0004 (8)
C13	0.0287 (10)	0.0260 (10)	0.0289 (10)	−0.0022 (8)	−0.0029 (8)	−0.0123 (8)
C14	0.0220 (9)	0.0253 (9)	0.0429 (12)	−0.0066 (8)	−0.0088 (8)	−0.0058 (9)
C15	0.0292 (10)	0.0347 (11)	0.0242 (9)	−0.0104 (8)	0.0043 (7)	−0.0154 (8)

Geometric parameters (Å, º)

Ru1—C1	1.944 (2)	C5—O5	1.133 (3)
Ru1—C2	1.917 (2)	C6—O6	1.136 (3)
Ru1—C3	1.9014 (19)	C7—O7	1.134 (2)
Ru1—C10	2.2451 (17)	C8—O8	1.132 (2)
Ru1—C11	2.3775 (18)	C9—O9	1.126 (3)
Ru1—S1	2.4122 (5)	C10—C11	1.293 (2)
Ru1—Ru2	2.8285 (2)	C11—Si1	1.8619 (18)
Ru2—C4	1.914 (2)	Si1—C12	1.857 (2)
Ru2—C5	1.937 (2)	Si1—C13	1.864 (2)
Ru2—C6	1.908 (2)	Si1—C14	1.869 (2)
Ru2—C10	1.9474 (18)	C12—H12A	0.98
Ru2—Ru3	2.8329 (2)	C12—H12B	0.98
Ru3—C7	1.902 (2)	C12—H12C	0.98
Ru3—C8	1.919 (2)	C13—H13A	0.98
Ru3—C9	1.946 (2)	C13—H13B	0.98
Ru3—C10	2.2390 (17)	C13—H13C	0.98
Ru3—C11	2.3628 (18)	C14—H14A	0.98
Ru3—S1	2.4165 (5)	C14—H14B	0.98
S1—C15	1.818 (2)	C14—H14C	0.98
C1—O1	1.126 (3)	C15—H15A	0.98
C2—O2	1.129 (3)	C15—H15B	0.98
C3—O3	1.139 (2)	C15—H15C	0.98
C4—O4	1.137 (2)		

C3—Ru1—C2	92.71 (8)	S1—Ru3—Ru2	80.780 (11)
C3—Ru1—C1	98.86 (9)	C15—S1—Ru1	107.75 (8)
C2—Ru1—C1	92.78 (10)	C15—S1—Ru3	107.46 (7)
C3—Ru1—C10	129.73 (7)	Ru1—S1—Ru3	88.197 (15)
C2—Ru1—C10	86.71 (8)	O1—C1—Ru1	176.9 (2)
C1—Ru1—C10	131.40 (8)	O2—C2—Ru1	179.0 (2)
C3—Ru1—C11	160.31 (7)	O3—C3—Ru1	179.09 (18)
C2—Ru1—C11	93.47 (7)	O4—C4—Ru2	177.03 (19)
C1—Ru1—C11	99.49 (8)	O5—C5—Ru2	176.2 (2)
C10—Ru1—C11	32.34 (6)	O6—C6—Ru2	179.2 (2)
C3—Ru1—S1	88.47 (6)	O7—C7—Ru3	178.62 (19)
C2—Ru1—S1	172.95 (7)	O8—C8—Ru3	178.75 (19)
C1—Ru1—S1	93.91 (7)	O9—C9—Ru3	178.6 (2)
C10—Ru1—S1	87.19 (5)	C11—C10—Ru2	155.62 (15)
C11—Ru1—S1	83.23 (4)	C11—C10—Ru3	79.02 (11)
C3—Ru1—Ru2	86.63 (6)	Ru2—C10—Ru3	84.87 (6)
C2—Ru1—Ru2	92.18 (7)	C11—C10—Ru1	79.47 (11)
C1—Ru1—Ru2	172.42 (6)	Ru2—C10—Ru1	84.54 (6)
C10—Ru1—Ru2	43.26 (4)	Ru3—C10—Ru1	97.07 (7)
C11—Ru1—Ru2	74.48 (4)	C10—C11—Si1	146.86 (15)
S1—Ru1—Ru2	80.943 (12)	C10—C11—Ru3	68.47 (11)
C6—Ru2—C4	94.63 (9)	Si1—C11—Ru3	128.62 (9)
C6—Ru2—C5	94.29 (9)	C10—C11—Ru1	68.19 (11)
C4—Ru2—C5	98.92 (9)	Si1—C11—Ru1	130.61 (9)
C6—Ru2—C10	110.12 (8)	Ru3—C11—Ru1	90.29 (6)
C4—Ru2—C10	106.94 (8)	C12—Si1—C11	107.21 (9)
C5—Ru2—C10	142.30 (8)	C12—Si1—C13	111.17 (10)
C6—Ru2—Ru1	162.17 (7)	C11—Si1—C13	109.82 (9)
C4—Ru2—Ru1	93.48 (6)	C12—Si1—C14	110.06 (11)
C5—Ru2—Ru1	100.11 (6)	C11—Si1—C14	108.08 (9)
C10—Ru2—Ru1	52.20 (5)	C13—Si1—C14	110.40 (11)
C6—Ru2—Ru3	94.61 (7)	Si1—C12—H12A	109.5
C4—Ru2—Ru3	158.83 (6)	Si1—C12—H12B	109.5
C5—Ru2—Ru3	99.34 (6)	H12A—C12—H12B	109.5
C10—Ru2—Ru3	51.92 (5)	Si1—C12—H12C	109.5
Ru1—Ru2—Ru3	72.818 (5)	H12A—C12—H12C	109.5
C7—Ru3—C8	90.71 (9)	H12B—C12—H12C	109.5
C7—Ru3—C9	98.61 (8)	Si1—C13—H13A	109.5
C8—Ru3—C9	93.40 (9)	Si1—C13—H13B	109.5
C7—Ru3—C10	134.79 (7)	H13A—C13—H13B	109.5
C8—Ru3—C10	87.66 (7)	Si1—C13—H13C	109.5
C9—Ru3—C10	126.60 (8)	H13A—C13—H13C	109.5
C7—Ru3—C11	165.05 (7)	H13B—C13—H13C	109.5
C8—Ru3—C11	95.49 (7)	Si1—C14—H14A	109.5
C9—Ru3—C11	94.59 (7)	Si1—C14—H14B	109.5
C10—Ru3—C11	32.51 (6)	H14A—C14—H14B	109.5
C7—Ru3—S1	88.51 (6)	Si1—C14—H14C	109.5

C8—Ru3—S1	171.98 (6)	H14A—C14—H14C	109.5
C9—Ru3—S1	94.61 (6)	H14B—C14—H14C	109.5
C10—Ru3—S1	87.23 (4)	S1—C15—H15A	109.5
C11—Ru3—S1	83.45 (4)	S1—C15—H15B	109.5
C7—Ru3—Ru2	91.72 (6)	H15A—C15—H15B	109.5
C8—Ru3—Ru2	91.27 (6)	S1—C15—H15C	109.5
C9—Ru3—Ru2	168.60 (6)	H15A—C15—H15C	109.5
C10—Ru3—Ru2	43.21 (4)	H15B—C15—H15C	109.5
C11—Ru3—Ru2	74.60 (4)		

C3—Ru1—Ru2—C6	−176.4 (2)	C5—Ru2—C10—Ru1	−50.20 (14)
C2—Ru1—Ru2—C6	91.0 (2)	Ru3—Ru2—C10—Ru1	−97.63 (6)
C10—Ru1—Ru2—C6	8.1 (2)	C7—Ru3—C10—C11	167.28 (12)
C11—Ru1—Ru2—C6	−2.0 (2)	C8—Ru3—C10—C11	−104.04 (12)
S1—Ru1—Ru2—C6	−87.4 (2)	C9—Ru3—C10—C11	−11.53 (15)
C3—Ru1—Ru2—C4	66.65 (8)	S1—Ru3—C10—C11	82.15 (11)
C2—Ru1—Ru2—C4	−25.94 (9)	Ru2—Ru3—C10—C11	161.61 (14)
C10—Ru1—Ru2—C4	−108.80 (9)	C7—Ru3—C10—Ru2	5.67 (13)
C11—Ru1—Ru2—C4	−118.94 (7)	C8—Ru3—C10—Ru2	94.35 (8)
S1—Ru1—Ru2—C4	155.63 (6)	C9—Ru3—C10—Ru2	−173.15 (8)
C3—Ru1—Ru2—C5	−33.06 (8)	C11—Ru3—C10—Ru2	−161.61 (14)
C2—Ru1—Ru2—C5	−125.64 (9)	S1—Ru3—C10—Ru2	−79.47 (5)
C10—Ru1—Ru2—C5	151.49 (9)	C7—Ru3—C10—Ru1	89.50 (11)
C11—Ru1—Ru2—C5	141.36 (8)	C8—Ru3—C10—Ru1	178.18 (8)
S1—Ru1—Ru2—C5	55.92 (6)	C9—Ru3—C10—Ru1	−89.32 (10)
C3—Ru1—Ru2—C10	175.45 (9)	C11—Ru3—C10—Ru1	−77.78 (11)
C2—Ru1—Ru2—C10	82.86 (9)	S1—Ru3—C10—Ru1	4.36 (5)
C11—Ru1—Ru2—C10	−10.14 (8)	Ru2—Ru3—C10—Ru1	83.83 (6)
S1—Ru1—Ru2—C10	−95.57 (6)	C3—Ru1—C10—C11	−167.43 (12)
C3—Ru1—Ru2—Ru3	−129.80 (6)	C2—Ru1—C10—C11	101.79 (13)
C2—Ru1—Ru2—Ru3	137.62 (6)	C1—Ru1—C10—C11	10.98 (16)
C10—Ru1—Ru2—Ru3	54.75 (6)	S1—Ru1—C10—C11	−81.76 (11)
C11—Ru1—Ru2—Ru3	44.61 (4)	Ru2—Ru1—C10—C11	−161.51 (14)
S1—Ru1—Ru2—Ru3	−40.817 (11)	C3—Ru1—C10—Ru2	−5.91 (11)
C6—Ru2—Ru3—C7	−63.94 (10)	C2—Ru1—C10—Ru2	−96.70 (8)
C4—Ru2—Ru3—C7	−179.54 (17)	C1—Ru1—C10—Ru2	172.49 (9)
C5—Ru2—Ru3—C7	31.18 (9)	C11—Ru1—C10—Ru2	161.51 (14)
C10—Ru2—Ru3—C7	−175.98 (9)	S1—Ru1—C10—Ru2	79.75 (5)
Ru1—Ru2—Ru3—C7	128.96 (6)	C3—Ru1—C10—Ru3	−90.04 (10)
C6—Ru2—Ru3—C8	26.81 (9)	C2—Ru1—C10—Ru3	179.18 (8)
C4—Ru2—Ru3—C8	−88.79 (17)	C1—Ru1—C10—Ru3	88.37 (11)
C5—Ru2—Ru3—C8	121.94 (9)	C11—Ru1—C10—Ru3	77.39 (11)
C10—Ru2—Ru3—C8	−85.22 (9)	S1—Ru1—C10—Ru3	−4.37 (5)
Ru1—Ru2—Ru3—C8	−140.28 (6)	Ru2—Ru1—C10—Ru3	−84.12 (7)
C6—Ru2—Ru3—C9	141.0 (3)	Ru2—C10—C11—Si1	178.09 (18)
C4—Ru2—Ru3—C9	25.4 (4)	Ru3—C10—C11—Si1	128.5 (3)
C5—Ru2—Ru3—C9	−123.8 (3)	Ru1—C10—C11—Si1	−132.0 (3)
C10—Ru2—Ru3—C9	29.0 (3)	Ru2—C10—C11—Ru3	49.5 (3)

Ru1—Ru2—Ru3—C9	−26.1 (3)	Ru1—C10—C11—Ru3	99.42 (5)
C6—Ru2—Ru3—C10	112.04 (10)	Ru2—C10—C11—Ru1	−49.9 (3)
C4—Ru2—Ru3—C10	−3.56 (17)	Ru3—C10—C11—Ru1	−99.42 (5)
C5—Ru2—Ru3—C10	−152.84 (9)	C7—Ru3—C11—C10	−37.3 (3)
Ru1—Ru2—Ru3—C10	−55.06 (6)	C8—Ru3—C11—C10	76.86 (12)
C6—Ru2—Ru3—C11	122.16 (8)	C9—Ru3—C11—C10	170.73 (12)
C4—Ru2—Ru3—C11	6.56 (17)	S1—Ru3—C11—C10	−95.15 (11)
C5—Ru2—Ru3—C11	−142.71 (8)	Ru2—Ru3—C11—C10	−12.94 (10)
C10—Ru2—Ru3—C11	10.13 (8)	C7—Ru3—C11—Si1	175.9 (3)
Ru1—Ru2—Ru3—C11	−44.93 (4)	C8—Ru3—C11—Si1	−69.96 (12)
C6—Ru2—Ru3—S1	−152.15 (7)	C9—Ru3—C11—Si1	23.91 (13)
C4—Ru2—Ru3—S1	92.25 (16)	C10—Ru3—C11—Si1	−146.82 (19)
C5—Ru2—Ru3—S1	−57.03 (6)	S1—Ru3—C11—Si1	118.03 (11)
C10—Ru2—Ru3—S1	95.81 (6)	Ru2—Ru3—C11—Si1	−159.77 (12)
Ru1—Ru2—Ru3—S1	40.754 (12)	C7—Ru3—C11—Ru1	29.1 (3)
C3—Ru1—S1—C15	−118.31 (10)	C8—Ru3—C11—Ru1	143.20 (7)
C1—Ru1—S1—C15	−19.54 (10)	C9—Ru3—C11—Ru1	−122.93 (7)
C10—Ru1—S1—C15	111.78 (9)	C10—Ru3—C11—Ru1	66.34 (10)
C11—Ru1—S1—C15	79.57 (9)	S1—Ru3—C11—Ru1	−28.81 (4)
Ru2—Ru1—S1—C15	154.86 (7)	Ru2—Ru3—C11—Ru1	53.39 (4)
C3—Ru1—S1—Ru3	133.92 (6)	C3—Ru1—C11—C10	29.8 (3)
C1—Ru1—S1—Ru3	−127.30 (6)	C2—Ru1—C11—C10	−78.27 (13)
C10—Ru1—S1—Ru3	4.02 (5)	C1—Ru1—C11—C10	−171.67 (12)
C11—Ru1—S1—Ru3	−28.19 (4)	S1—Ru1—C11—C10	95.48 (11)
Ru2—Ru1—S1—Ru3	47.094 (10)	Ru2—Ru1—C11—C10	13.03 (10)
C7—Ru3—S1—C15	112.94 (10)	C3—Ru1—C11—Si1	177.46 (17)
C9—Ru3—S1—C15	14.42 (10)	C2—Ru1—C11—Si1	69.40 (13)
C10—Ru3—S1—C15	−112.08 (9)	C1—Ru1—C11—Si1	−24.01 (14)
C11—Ru3—S1—C15	−79.68 (9)	C10—Ru1—C11—Si1	147.66 (19)
Ru2—Ru3—S1—C15	−155.08 (8)	S1—Ru1—C11—Si1	−116.86 (12)
C7—Ru3—S1—Ru1	−139.01 (6)	Ru2—Ru1—C11—Si1	160.70 (12)
C9—Ru3—S1—Ru1	122.48 (6)	C3—Ru1—C11—Ru3	−36.8 (2)
C10—Ru3—S1—Ru1	−4.03 (5)	C2—Ru1—C11—Ru3	−144.86 (8)
C11—Ru3—S1—Ru1	28.37 (4)	C1—Ru1—C11—Ru3	121.73 (8)
Ru2—Ru3—S1—Ru1	−47.024 (10)	C10—Ru1—C11—Ru3	−66.60 (10)
C6—Ru2—C10—C11	−128.3 (3)	S1—Ru1—C11—Ru3	28.88 (4)
C4—Ru2—C10—C11	130.1 (3)	Ru2—Ru1—C11—Ru3	−53.56 (4)
C5—Ru2—C10—C11	−1.2 (4)	C10—C11—Si1—C12	44.6 (3)
Ru1—Ru2—C10—C11	49.0 (3)	Ru3—C11—Si1—C12	156.01 (11)
Ru3—Ru2—C10—C11	−48.6 (3)	Ru1—C11—Si1—C12	−70.09 (14)
C6—Ru2—C10—Ru3	−79.73 (9)	C10—C11—Si1—C13	165.5 (3)
C4—Ru2—C10—Ru3	178.66 (7)	Ru3—C11—Si1—C13	−83.09 (13)
C5—Ru2—C10—Ru3	47.43 (14)	Ru1—C11—Si1—C13	50.81 (15)
Ru1—Ru2—C10—Ru3	97.63 (6)	C10—C11—Si1—C14	−74.0 (3)
C6—Ru2—C10—Ru1	−177.36 (8)	Ru3—C11—Si1—C14	37.40 (15)
C4—Ru2—C10—Ru1	81.03 (8)	Ru1—C11—Si1—C14	171.30 (12)