

μ -Oxalato- $\kappa^2 O^1, O^2: \kappa^2 O^1', O^2'$ -bis[(η^5 -pentamethylcyclopentadienyl)(trifluoromethanesulfonato- κO)rhodium(III)]

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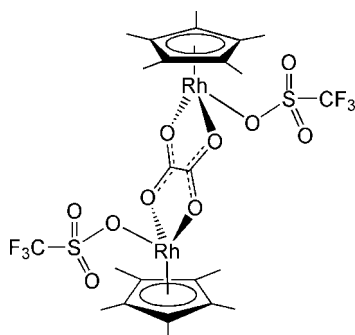
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(C-C) = 0.008$ Å; R factor = 0.051; wR factor = 0.139; data-to-parameter ratio = 13.6.

In the title dinuclear rhodium complex, $[(\mu-C_2O_4)\{(\eta^5-C_5Me_5)Rh(O_3SCF_3)_2\}]_2$ or $[Rh(CF_3O_3S)_2(C_{10}H_{15})_2(C_2O_4)]_2$, the terminal trifluoromethanesulfonate ligands adopt a *trans* configuration with respect to each other and the Rh...Rh distances range from 5.5157 (8) to 5.5389 (6) Å. There are two and a half molecules within the asymmetric unit, one of the molecules lying on an inversion centre. Interestingly, in one molecule, the S—O bond of a coordinated O atom is shorter than the two S—O bonds of the noncoordinated O atoms, and the corresponding Rh—O distance is significantly longer than the other M—O distances.

Related literature

For similar dinuclear oxalate complexes, see: Bottomley *et al.* (1981); Yan *et al.* (1997); Grotjahn *et al.* (2000); Govindaswamy *et al.* (2006); Dale & Elsegood (2006); Govindaswamy *et al.* (2007). For (η^5 -Cp*)Rh(O₃SCF₃) derivatives, see: Herberich & Ganter (2001); Han & Lee (2003).



Experimental

Crystal data

$[Rh(CF_3O_3S)_2(C_{10}H_{15})_2(C_2O_4)]_2$

$M_r = 862.42$

Orthorhombic, *Pbca*

$a = 14.5462$ (5) Å
 $b = 25.5247$ (9) Å
 $c = 41.5719$ (12) Å
 $V = 15435.1$ (9) Å³

$Z = 20$

Mo $K\alpha$ radiation
 $\mu = 1.29$ mm⁻¹
 $T = 173$ (2) K
 $0.14 \times 0.12 \times 0.07$ mm

Data collection

Stoe IPDS diffractometer
 Absorption correction: none
 96861 measured reflections

13761 independent reflections
 9348 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.081$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.139$
 $S = 0.92$
 13761 reflections

1014 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 1.57$ e Å⁻³
 $\Delta\rho_{min} = -1.34$ e Å⁻³

Table 1

Selected bond lengths (Å).

O1—Rh1	2.134 (3)	O13—Rh3	2.229 (4)
O2—Rh1	2.132 (3)	O14—S3	1.435 (4)
O3—S1	1.460 (4)	O15—S3	1.442 (5)
O3—Rh1	2.201 (4)	O16—Rh4	2.133 (3)
O4—S1	1.413 (4)	O17—Rh4	2.133 (3)
O5—S1	1.431 (4)	O18—Rh5	2.142 (3)
O6—Rh2	2.125 (3)	O19—Rh5	2.148 (3)
O7—Rh2	2.144 (3)	O20—S4	1.468 (4)
O8—Rh3	2.118 (4)	O20—Rh4	2.205 (4)
O9—Rh3	2.147 (3)	O21—S4	1.425 (4)
O10—S2	1.463 (4)	O22—S4	1.425 (4)
O10—Rh2	2.193 (4)	O23—S5	1.463 (4)
O11—S2	1.425 (5)	O23—Rh5	2.191 (4)
O12—S2	1.419 (4)	O24—S5	1.423 (5)
O13—S3	1.430 (4)	O25—S5	1.435 (5)

Data collection: *EXPOSE* in *IPDS Software* (Stoe & Cie, 2000); cell refinement: *CELL* in *IPDS Software*; data reduction: *INTEGRATE* in *IPDS Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2210).

References

- Bottomley, F., Lin, I. J. B. & White, P. S. (1981). *J. Organomet. Chem.* **212**, 341–349.
- Dale, S. H. & Elsegood, M. R. J. (2006). *Acta Cryst.* **C62**, m166–m170.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Govindaswamy, P., Linder, D., Lacour, J., Süss-Fink, G. & Therrien, B. (2006). *Chem. Commun.* pp. 4691–4693.
- Govindaswamy, P., Süss-Fink, G. & Therrien, B. (2007). In preparation.
- Grotjahn, D. B., Lo, H. C., Dinoso, J., Adkins, C. D., Li, C., Nolan, S. P. & Hubbard, J. L. (2000). *Inorg. Chem.* **39**, 2493–2499.
- Han, W. S. & Lee, S. W. (2003). *Inorg. Chim. Acta*, **348**, 15–24.
- Herberich, G. E. & Ganter, B. (2001). *Inorg. Chem. Commun.* **4**, 100–103.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Stoe & Cie (2000). *IPDS Software*. Stoe & Cie GmbH, Darmstadt, Germany.
- Yan, H., Süss-Fink, G., Neels, A. & Stoeckli-Evans, H. (1997). *J. Chem. Soc. Dalton Trans.* pp. 4345–4350.

supplementary materials

Acta Cryst. (2007). E63, m2046 [doi:10.1107/S1600536807031790]

μ -Oxalato- $\kappa^2O^1, O^2:\kappa^2O^{1'}, O^{2'}$ -bis[(η^5 -pentamethylcyclopentadienyl)(trifluoromethanesulfonato- κO)rhodium(III)]

P. Govindaswamy, G. Süß-Fink and B. Therrien

Comment

Recently, we synthesized cationic trigonal metalloprisms of the type $[(\eta^5\text{-Cp}^*)_6M_6(\mu\text{-tpt})_2(\mu\text{-C}_2\text{O}_4)_3]^{6+}$ ($M = \text{Rh, Ir}$) containing bridging oxalato ($\text{C}_2\text{O}_4^{2-}$) ligands and 2,4,6-tri(pyridine-4-yl)-1,3,5-triazine (tpt) tritopic subunits (Govindaswamy *et al.*, 2007). The synthesis involves the reaction of the chloro precursor $[(\mu\text{-C}_2\text{O}_4)\{(\eta^5\text{-Cp}^*)\text{MCl}\}_2]$ with AgO_3SCF_3 to give AgCl and an intermediate supposed to be the trifluoromethanesulfonate salt of the coordinatively unsaturated cation $[(\mu\text{-C}_2\text{O}_4)\{(\eta^5\text{-Cp}^*)M\}_2]^{2+}$. We now isolated this compound and found a neutral di-trifluoromethanesulfonato complex. We present here the single X-ray structure analysis of the trifluoromethanesulfonato rhodium complex, $[(\mu\text{-C}_2\text{O}_4)\{(\eta^5\text{-Cp}^*)\text{Rh}(\text{O}_3\text{SCF}_3)_2\}_2]$ (1).

There are two and a half independent molecules in the asymmetric unit, among which, one possesses an inversion center (1 A) whereas the two other (1 B) and (1 C) are located around general positions (Fig. 1). In all cases, the rhodium atoms are in a slightly distorted octahedral geometry and surrounded by a $\eta^5\text{-C}_5\text{Me}_5$ ligand, an oxygen atom of a trifluoromethanesulfonato ligand and two oxygen atoms of an oxalato ligand. The dianionic $\text{C}_2\text{O}_4^{2-}$ bridging ligand connects the two metals through its four oxygen atoms. The metal-metal distances are comparable in 1 A and 1 B, 5.5157 (8) and 5.5183 (6) Å, respectively, but slightly longer in 1 C, 5.5389 (6) Å. These metal-metal separations are comparable to those found in other oxalato bridged dinuclear $M(\text{arene})$ or $M(\text{Cp}^*)$ complexes (range 5.48 – 5.63 Å) (Bottomley *et al.*, 1981), (Yan *et al.*, 1997), (Grotjahn *et al.*, 2000), (Dale & Elsegood, 2006), (Govindaswamy *et al.*, 2006), (Govindaswamy *et al.*, 2007).

In all crystallographically independent dinuclear complexes 1 A, 1 B and 1 C, the trifluoromethanesulfonato ligands are *trans* oriented with respect to each other. The geometrical parameters of the three independent molecules are similar. However, in 1 B, the S—O bond of the coordinated oxygen atom O(13) is not longer [1.430 (4) Å] than the two S—O bonds of the non-coordinated oxygen atoms [1.435 (4) and 1.442 (5) Å] and the corresponding Rh(3)—O(13) distance [2.229 (4) Å] is significantly longer than the other metal-oxygen distances, ranging from 2.191 (4) to 2.205 (4) Å. Nevertheless, these metal-oxygen distances remain longer than the one observed in other $\text{Cp}^*\text{Rh}(\text{O}_3\text{SCF}_3)$ derivatives (Herberich & Ganter, 2001; Han & Lee, 2003).

Experimental

$[(\mu\text{-C}_2\text{O}_4)\{(\eta^5\text{-Cp}^*)\text{RhCl}\}_2]$ is dissolved in chloroform followed by addition of AgO_3SCF_3 , and crystals suitable for X-ray diffraction analysis are obtained by slow evaporation of the chloroform solution.

^1H NMR (200 MHz, CDCl_3): δ (p.p.m.) = 1.69 (s, 30H, C_5Me_5); IR (CDCl_3 , cm^{-1}): 2254(s), 1625(s) (CO).

Refinement

The H atoms were included in calculated positions and refined using a riding model, with C—H = 0.96 Å and with $U_{\text{iso}}(\text{H}) = 1.5$ times $U_{\text{eq}}(\text{C})$. Residual electron density greater than $1 \text{ e } \text{Å}^{-3}$ is located at 1.1 Å from O(13).

Figures

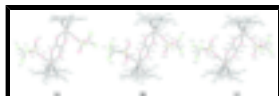


Fig. 1. The molecular structure of 1 A, 1B and 1 C. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

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Crystal data

[Rh(CF₃O₃S)₂(C₁₀H₁₅)₂(C₂O₄)]

$M_r = 862.42$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 14.5462$ (5) Å

$b = 25.5247$ (9) Å

$c = 41.5719$ (12) Å

$V = 15435.1$ (9) Å³

$Z = 20$

$F_{000} = 8600$

$D_x = 1.856 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 54500 reflections

$\theta = 1.4$ – 25.7°

$\mu = 1.29 \text{ mm}^{-1}$

$T = 173$ (2) K

Block, orange

$0.14 \times 0.12 \times 0.07 \text{ mm}$

Data collection

Stoe IPDS
diffractometer

13761 independent reflections

Radiation source: fine-focus sealed tube

9348 reflections with $I > 2\sigma(I)$

Monochromator: graphite

$R_{\text{int}} = 0.081$

Detector resolution: 0.81 pixels mm^{-1}

$\theta_{\text{max}} = 25.2^\circ$

$T = 173$ (2) K

$\theta_{\text{min}} = 1.6^\circ$

ϕ oscillation scans

$h = -17 \rightarrow 17$

Absorption correction: none

$k = -30 \rightarrow 30$

96861 measured reflections

$l = -49 \rightarrow 49$

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

Least-squares matrix: full

Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.051$

H-atom parameters constrained

$wR(F^2) = 0.139$	$w = 1/[\sigma^2(F_o^2) + (0.093P)^2]$
$S = 0.92$	where $P = (F_o^2 + 2F_c^2)/3$
13761 reflections	$(\Delta/\sigma)_{\max} = 0.001$
1014 parameters	$\Delta\rho_{\max} = 1.57 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -1.33 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

Special details

Experimental. A crystal was mounted at 173 K on a Stoe Image Plate Diffraction System (Stoe & Cie, 2000) using Mo *K* α graphite monochromated radiation. Image plate distance 70 mm, ϕ oscillation scans 0 – 200°, step $\Delta\phi = 0.5^\circ$, 10 minutes per frame.

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	1.0315 (3)	0.5081 (2)	-0.01389 (12)	0.0391 (12)
C2	1.1640 (5)	0.3147 (3)	0.01750 (16)	0.0588 (16)
C3	0.9400 (4)	0.3598 (2)	-0.07412 (13)	0.0443 (12)
C4	0.9044 (4)	0.4097 (2)	-0.08409 (12)	0.0406 (12)
C5	0.8267 (4)	0.4226 (2)	-0.06401 (13)	0.0462 (13)
C6	0.8111 (4)	0.3798 (2)	-0.04242 (14)	0.0503 (14)
C7	0.8812 (4)	0.3406 (2)	-0.04792 (13)	0.0500 (14)
C8	1.0206 (4)	0.3325 (2)	-0.08704 (15)	0.0598 (16)
H8A	1.0015	0.3081	-0.1033	0.090*
H8B	1.0511	0.3140	-0.0700	0.090*
H8C	1.0621	0.3576	-0.0963	0.090*
C9	0.9418 (4)	0.4442 (2)	-0.10961 (13)	0.0527 (14)
H9A	1.0058	0.4365	-0.1128	0.079*
H9B	0.9350	0.4801	-0.1033	0.079*
H9C	0.9089	0.4382	-0.1293	0.079*
C10	0.7686 (4)	0.4703 (3)	-0.06778 (15)	0.0611 (17)
H10A	0.7321	0.4672	-0.0869	0.092*
H10B	0.8074	0.5006	-0.0694	0.092*
H10C	0.7290	0.4738	-0.0495	0.092*
C11	0.7383 (5)	0.3760 (3)	-0.01753 (17)	0.074 (2)
H11A	0.7288	0.4098	-0.0080	0.112*
H11B	0.7569	0.3515	-0.0012	0.112*
H11C	0.6822	0.3642	-0.0273	0.112*

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C12	0.8903 (5)	0.2895 (2)	-0.03125 (16)	0.069 (2)
H12A	0.8658	0.2924	-0.0099	0.104*
H12B	0.9541	0.2800	-0.0301	0.104*
H12C	0.8570	0.2632	-0.0429	0.104*
C13	0.9742 (3)	-0.0026 (2)	0.11045 (12)	0.0400 (12)
C14	1.0392 (3)	-0.0125 (2)	0.08192 (12)	0.0379 (11)
C15	1.1633 (4)	0.1778 (2)	0.11841 (15)	0.0551 (15)
C16	0.8385 (5)	-0.1842 (3)	0.0717 (2)	0.0678 (19)
C17	0.8417 (4)	0.0692 (2)	0.02945 (14)	0.0491 (13)
C18	0.9076 (4)	0.1071 (2)	0.01865 (14)	0.0517 (14)
C19	0.9035 (4)	0.1505 (2)	0.04029 (15)	0.0536 (15)
C20	0.8358 (4)	0.1397 (2)	0.06447 (14)	0.0516 (14)
C21	0.7963 (4)	0.0900 (2)	0.05678 (15)	0.0505 (14)
C22	0.8195 (5)	0.0180 (3)	0.01308 (17)	0.074 (2)
H22A	0.8069	-0.0083	0.0290	0.111*
H22B	0.8709	0.0072	0.0002	0.111*
H22C	0.7665	0.0224	-0.0004	0.111*
C23	0.9704 (5)	0.1014 (3)	-0.00974 (15)	0.080 (2)
H23A	0.9405	0.1148	-0.0286	0.120*
H23B	0.9847	0.0650	-0.0129	0.120*
H23C	1.0260	0.1206	-0.0059	0.120*
C24	0.9621 (5)	0.1984 (3)	0.0394 (2)	0.082 (2)
H24A	1.0088	0.1943	0.0233	0.123*
H24B	0.9904	0.2035	0.0600	0.123*
H24C	0.9247	0.2283	0.0343	0.123*
C25	0.8058 (5)	0.1742 (3)	0.09132 (18)	0.079 (2)
H25A	0.7529	0.1939	0.0848	0.118*
H25B	0.8548	0.1978	0.0968	0.118*
H25C	0.7906	0.1531	0.1097	0.118*
C26	0.7238 (4)	0.0620 (3)	0.07539 (17)	0.072 (2)
H26A	0.6657	0.0659	0.0647	0.108*
H26B	0.7201	0.0765	0.0967	0.108*
H26C	0.7391	0.0254	0.0767	0.108*
C27	1.1782 (4)	-0.0841 (2)	0.15982 (14)	0.0487 (13)
C28	1.2095 (4)	-0.1207 (3)	0.13588 (13)	0.0531 (15)
C29	1.1499 (5)	-0.1648 (2)	0.13623 (15)	0.0570 (16)
C30	1.0830 (4)	-0.1569 (2)	0.16148 (15)	0.0514 (14)
C31	1.1017 (4)	-0.1079 (2)	0.17603 (13)	0.0480 (13)
C32	1.2214 (5)	-0.0333 (3)	0.1681 (2)	0.080 (2)
H32A	1.1746	-0.0088	0.1743	0.120*
H32B	1.2538	-0.0200	0.1497	0.120*
H32C	1.2637	-0.0382	0.1856	0.120*
C33	1.2895 (5)	-0.1126 (4)	0.11378 (19)	0.087 (3)
H33A	1.3448	-0.1243	0.1241	0.131*
H33B	1.2948	-0.0761	0.1086	0.131*
H33C	1.2801	-0.1323	0.0944	0.131*
C34	1.1527 (6)	-0.2125 (3)	0.11501 (19)	0.091 (3)
H34A	1.1986	-0.2078	0.0986	0.136*
H34B	1.0937	-0.2174	0.1051	0.136*

H34C	1.1677	-0.2427	0.1277	0.136*
C35	1.0088 (5)	-0.1936 (3)	0.1709 (2)	0.083 (2)
H35A	1.0355	-0.2256	0.1786	0.125*
H35B	0.9706	-0.2008	0.1526	0.125*
H35C	0.9723	-0.1780	0.1876	0.125*
C36	1.0491 (5)	-0.0832 (3)	0.20299 (15)	0.072 (2)
H36A	1.0432	-0.0462	0.1991	0.108*
H36B	1.0812	-0.0887	0.2229	0.108*
H36C	0.9891	-0.0987	0.2043	0.108*
C37	0.4624 (3)	-0.0039 (2)	0.18731 (12)	0.0384 (11)
C38	0.5205 (3)	-0.0195 (2)	0.21695 (12)	0.0390 (11)
C39	0.6553 (4)	0.1804 (2)	0.18413 (16)	0.0553 (15)
C40	0.3237 (4)	-0.1977 (2)	0.21821 (14)	0.0522 (14)
C41	0.3130 (4)	0.0706 (2)	0.25869 (14)	0.0505 (14)
C42	0.3841 (4)	0.0853 (2)	0.28069 (13)	0.0442 (13)
C43	0.4207 (4)	0.1348 (2)	0.27134 (13)	0.0466 (13)
C44	0.3705 (4)	0.1521 (2)	0.24333 (14)	0.0527 (15)
C45	0.3034 (4)	0.1125 (3)	0.23583 (15)	0.0575 (16)
C46	0.2558 (5)	0.0226 (3)	0.26059 (19)	0.076 (2)
H46A	0.2930	-0.0063	0.2675	0.114*
H46B	0.2304	0.0151	0.2398	0.114*
H46C	0.2067	0.0280	0.2757	0.114*
C47	0.4159 (5)	0.0529 (3)	0.30851 (14)	0.0613 (16)
H47A	0.3786	0.0604	0.3270	0.092*
H47B	0.4790	0.0610	0.3132	0.092*
H47C	0.4107	0.0164	0.3032	0.092*
C48	0.4976 (5)	0.1637 (3)	0.28670 (16)	0.0661 (18)
H48A	0.4735	0.1877	0.3023	0.099*
H48B	0.5311	0.1827	0.2706	0.099*
H48C	0.5381	0.1393	0.2971	0.099*
C49	0.3849 (6)	0.2026 (3)	0.22622 (17)	0.077 (2)
H49A	0.3615	0.1999	0.2047	0.115*
H49B	0.4495	0.2104	0.2255	0.115*
H49C	0.3532	0.2301	0.2374	0.115*
C50	0.2391 (5)	0.1144 (4)	0.20802 (18)	0.092 (3)
H50A	0.1901	0.0898	0.2114	0.137*
H50B	0.2716	0.1055	0.1887	0.137*
H50C	0.2142	0.1490	0.2061	0.137*
C51	0.6346 (4)	-0.1675 (2)	0.15977 (13)	0.0457 (13)
C52	0.6937 (4)	-0.1253 (2)	0.16851 (13)	0.0463 (13)
C53	0.6784 (4)	-0.0830 (2)	0.14610 (13)	0.0425 (12)
C54	0.6131 (4)	-0.1008 (2)	0.12232 (12)	0.0414 (12)
C55	0.5847 (4)	-0.1530 (2)	0.13121 (13)	0.0445 (13)
C56	0.6268 (5)	-0.2192 (2)	0.17659 (17)	0.0680 (19)
H56A	0.6533	-0.2165	0.1977	0.102*
H56B	0.6588	-0.2455	0.1645	0.102*
H56C	0.5631	-0.2287	0.1784	0.102*
C57	0.7554 (5)	-0.1237 (3)	0.19704 (15)	0.0683 (19)
H57A	0.7198	-0.1167	0.2160	0.103*

supplementary materials

H57B	0.8004	-0.0965	0.1942	0.103*
H57C	0.7860	-0.1568	0.1993	0.103*
C58	0.7250 (4)	-0.0311 (2)	0.14607 (16)	0.0605 (16)
H58A	0.7470	-0.0233	0.1673	0.091*
H58B	0.6822	-0.0045	0.1395	0.091*
H58C	0.7759	-0.0318	0.1314	0.091*
C59	0.5797 (4)	-0.0702 (3)	0.09428 (13)	0.0555 (15)
H59A	0.6196	-0.0761	0.0762	0.083*
H59B	0.5793	-0.0336	0.0996	0.083*
H59C	0.5184	-0.0812	0.0889	0.083*
C60	0.5175 (5)	-0.1863 (3)	0.11381 (17)	0.0672 (18)
H60A	0.4778	-0.1646	0.1011	0.101*
H60B	0.4816	-0.2058	0.1291	0.101*
H60C	0.5498	-0.2102	0.1000	0.101*
F1	1.2433 (3)	0.33377 (19)	0.00867 (13)	0.0998 (16)
F2	1.1406 (4)	0.27819 (18)	-0.00349 (12)	0.1034 (16)
F3	1.1777 (3)	0.28965 (18)	0.04507 (11)	0.0923 (14)
F4	1.2423 (3)	0.15588 (18)	0.11105 (12)	0.0933 (15)
F5	1.1459 (4)	0.21358 (18)	0.09601 (11)	0.1016 (16)
F6	1.1757 (3)	0.20284 (16)	0.14552 (9)	0.0769 (12)
F7	0.8728 (4)	-0.1847 (2)	0.04186 (12)	0.1076 (16)
F8	0.7493 (3)	-0.18487 (19)	0.06909 (15)	0.117 (2)
F9	0.8641 (3)	-0.22826 (15)	0.08649 (13)	0.0993 (15)
F10	0.6248 (3)	0.21529 (16)	0.20516 (11)	0.0833 (12)
F11	0.7369 (3)	0.16407 (16)	0.19459 (12)	0.0856 (13)
F12	0.6701 (3)	0.20600 (16)	0.15684 (10)	0.0796 (12)
F13	0.2999 (3)	-0.21629 (17)	0.24682 (9)	0.0864 (13)
F14	0.2497 (3)	-0.18010 (18)	0.20462 (13)	0.0995 (16)
F15	0.3526 (3)	-0.23866 (17)	0.20171 (12)	0.0953 (14)
O1	0.9168 (2)	0.45321 (14)	0.00960 (8)	0.0426 (8)
O2	1.0281 (2)	0.48145 (14)	-0.03915 (8)	0.0418 (8)
O3	1.0688 (3)	0.38275 (16)	-0.01157 (9)	0.0536 (10)
O4	1.1133 (3)	0.40073 (18)	0.04321 (11)	0.0729 (13)
O5	0.9966 (3)	0.33538 (18)	0.03216 (10)	0.0639 (11)
O6	0.9211 (2)	0.03618 (13)	0.10880 (8)	0.0406 (8)
O7	1.0301 (2)	0.01639 (13)	0.05752 (9)	0.0433 (8)
O8	0.9768 (2)	-0.03439 (14)	0.13328 (8)	0.0434 (9)
O9	1.0971 (2)	-0.04852 (14)	0.08478 (8)	0.0429 (8)
O10	1.0642 (3)	0.11235 (15)	0.08813 (9)	0.0493 (9)
O11	0.9938 (3)	0.1610 (2)	0.13151 (10)	0.0700 (13)
O12	1.1044 (3)	0.09258 (18)	0.14326 (11)	0.0703 (13)
O13	0.9753 (3)	-0.13389 (16)	0.09193 (10)	0.0590 (11)
O14	0.8431 (4)	-0.08431 (18)	0.07567 (14)	0.0912 (17)
O15	0.8410 (3)	-0.1370 (2)	0.12555 (11)	0.0784 (14)
O16	0.4153 (2)	0.03706 (13)	0.18933 (8)	0.0398 (8)
O17	0.5169 (2)	0.01011 (13)	0.24097 (8)	0.0398 (8)
O18	0.4663 (2)	-0.03336 (14)	0.16307 (8)	0.0411 (8)
O19	0.5681 (2)	-0.05989 (13)	0.21494 (8)	0.0408 (8)
O20	0.5658 (2)	0.10736 (15)	0.21151 (9)	0.0487 (9)

O21	0.6233 (3)	0.09249 (17)	0.15768 (11)	0.0636 (12)
O22	0.4952 (3)	0.15229 (16)	0.16617 (9)	0.0522 (10)
O23	0.4296 (3)	-0.13721 (16)	0.18787 (9)	0.0541 (10)
O24	0.3692 (4)	-0.10613 (18)	0.23837 (13)	0.0821 (16)
O25	0.4860 (3)	-0.1749 (2)	0.23794 (11)	0.0737 (13)
S1	1.07561 (10)	0.36392 (6)	0.02152 (3)	0.0478 (3)
S2	1.07084 (10)	0.13074 (6)	0.12138 (3)	0.0462 (3)
S3	0.87774 (11)	-0.12787 (6)	0.09381 (4)	0.0569 (4)
S4	0.57534 (9)	0.12732 (5)	0.17856 (3)	0.0438 (3)
S5	0.41220 (11)	-0.14837 (6)	0.22184 (4)	0.0503 (3)
Rh1	0.94376 (3)	0.413555 (15)	-0.034591 (9)	0.03828 (12)
Rh2	0.93884 (3)	0.080836 (16)	0.066107 (10)	0.03821 (12)
Rh3	1.07209 (3)	-0.096142 (16)	0.126428 (10)	0.03894 (12)
Rh4	0.43670 (3)	0.078921 (16)	0.233111 (10)	0.03799 (12)
Rh5	0.55463 (3)	-0.099646 (16)	0.169641 (9)	0.03729 (12)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.037 (3)	0.051 (3)	0.030 (3)	0.004 (2)	0.000 (2)	0.004 (2)
C2	0.059 (4)	0.064 (4)	0.054 (4)	0.001 (3)	0.002 (3)	0.009 (3)
C3	0.049 (3)	0.047 (3)	0.037 (3)	0.001 (2)	-0.005 (2)	-0.005 (2)
C4	0.042 (3)	0.046 (3)	0.033 (3)	-0.006 (2)	-0.006 (2)	-0.002 (2)
C5	0.047 (3)	0.053 (3)	0.038 (3)	-0.004 (3)	-0.007 (2)	-0.007 (2)
C6	0.048 (3)	0.057 (3)	0.046 (3)	-0.012 (3)	0.000 (3)	-0.004 (3)
C7	0.062 (4)	0.049 (3)	0.039 (3)	-0.013 (3)	-0.011 (3)	0.003 (3)
C8	0.065 (4)	0.062 (4)	0.053 (4)	0.015 (3)	-0.004 (3)	-0.014 (3)
C9	0.066 (4)	0.056 (3)	0.037 (3)	-0.006 (3)	0.000 (3)	0.008 (3)
C10	0.051 (4)	0.068 (4)	0.064 (4)	0.016 (3)	-0.009 (3)	-0.003 (3)
C11	0.056 (4)	0.100 (5)	0.067 (4)	-0.026 (4)	0.014 (3)	-0.003 (4)
C12	0.103 (6)	0.040 (3)	0.064 (4)	-0.017 (3)	-0.015 (4)	0.008 (3)
C13	0.040 (3)	0.045 (3)	0.035 (3)	-0.004 (2)	-0.001 (2)	-0.004 (2)
C14	0.035 (3)	0.044 (3)	0.035 (3)	-0.005 (2)	-0.001 (2)	-0.006 (2)
C15	0.060 (4)	0.056 (4)	0.049 (4)	-0.004 (3)	0.001 (3)	-0.008 (3)
C16	0.052 (4)	0.057 (4)	0.094 (6)	0.009 (3)	-0.007 (4)	0.002 (4)
C17	0.052 (3)	0.048 (3)	0.047 (3)	0.002 (3)	-0.012 (3)	-0.002 (3)
C18	0.047 (3)	0.067 (4)	0.042 (3)	0.006 (3)	-0.010 (3)	0.009 (3)
C19	0.053 (4)	0.049 (3)	0.058 (4)	0.001 (3)	-0.015 (3)	0.016 (3)
C20	0.049 (3)	0.055 (3)	0.051 (3)	0.014 (3)	-0.010 (3)	0.002 (3)
C21	0.041 (3)	0.058 (3)	0.052 (3)	-0.003 (3)	-0.010 (3)	0.009 (3)
C22	0.078 (5)	0.069 (4)	0.074 (5)	-0.009 (4)	-0.023 (4)	-0.023 (4)
C23	0.075 (5)	0.122 (6)	0.042 (4)	-0.003 (5)	0.002 (3)	0.014 (4)
C24	0.091 (5)	0.054 (4)	0.102 (6)	-0.020 (4)	-0.028 (5)	0.030 (4)
C25	0.078 (5)	0.079 (5)	0.079 (5)	0.033 (4)	-0.015 (4)	-0.026 (4)
C26	0.049 (4)	0.096 (5)	0.072 (5)	-0.014 (4)	-0.001 (3)	0.013 (4)
C27	0.044 (3)	0.055 (3)	0.046 (3)	0.001 (3)	-0.009 (3)	0.003 (3)
C28	0.046 (3)	0.075 (4)	0.038 (3)	0.014 (3)	0.002 (3)	0.007 (3)
C29	0.066 (4)	0.053 (3)	0.052 (4)	0.019 (3)	-0.019 (3)	-0.005 (3)

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C30	0.046 (3)	0.052 (3)	0.057 (4)	0.006 (3)	-0.007 (3)	0.015 (3)
C31	0.046 (3)	0.059 (3)	0.039 (3)	0.014 (3)	-0.003 (2)	0.007 (3)
C32	0.069 (5)	0.066 (4)	0.104 (6)	-0.018 (4)	-0.033 (4)	-0.007 (4)
C33	0.052 (4)	0.133 (7)	0.077 (5)	0.021 (4)	0.015 (4)	0.025 (5)
C34	0.115 (7)	0.067 (5)	0.090 (6)	0.041 (5)	-0.022 (5)	-0.024 (4)
C35	0.075 (5)	0.073 (5)	0.101 (6)	-0.012 (4)	-0.012 (4)	0.040 (4)
C36	0.079 (5)	0.099 (5)	0.038 (3)	0.029 (4)	0.005 (3)	0.004 (3)
C37	0.034 (3)	0.051 (3)	0.031 (3)	-0.003 (2)	0.003 (2)	0.006 (2)
C38	0.036 (3)	0.045 (3)	0.037 (3)	-0.004 (2)	0.002 (2)	0.005 (2)
C39	0.047 (3)	0.061 (4)	0.057 (4)	-0.005 (3)	-0.004 (3)	0.009 (3)
C40	0.061 (4)	0.053 (3)	0.043 (3)	-0.004 (3)	-0.003 (3)	0.007 (3)
C41	0.041 (3)	0.061 (4)	0.049 (3)	0.005 (3)	0.004 (3)	-0.008 (3)
C42	0.043 (3)	0.048 (3)	0.042 (3)	0.009 (2)	0.007 (2)	-0.003 (2)
C43	0.050 (3)	0.047 (3)	0.042 (3)	0.008 (3)	0.006 (3)	-0.007 (2)
C44	0.057 (4)	0.052 (3)	0.048 (3)	0.018 (3)	0.005 (3)	-0.003 (3)
C45	0.041 (3)	0.079 (4)	0.053 (4)	0.021 (3)	-0.002 (3)	-0.012 (3)
C46	0.061 (4)	0.085 (5)	0.083 (5)	-0.020 (4)	0.014 (4)	-0.020 (4)
C47	0.079 (4)	0.069 (4)	0.035 (3)	0.007 (3)	0.005 (3)	0.005 (3)
C48	0.068 (4)	0.060 (4)	0.070 (4)	-0.003 (3)	-0.003 (3)	-0.026 (3)
C49	0.108 (6)	0.049 (4)	0.073 (5)	0.033 (4)	0.021 (4)	0.010 (3)
C50	0.066 (5)	0.137 (7)	0.072 (5)	0.047 (5)	-0.027 (4)	-0.010 (5)
C51	0.048 (3)	0.045 (3)	0.044 (3)	0.008 (2)	0.008 (3)	0.004 (2)
C52	0.044 (3)	0.052 (3)	0.042 (3)	0.007 (3)	0.000 (3)	0.000 (2)
C53	0.041 (3)	0.046 (3)	0.040 (3)	0.003 (2)	0.004 (2)	-0.001 (2)
C54	0.040 (3)	0.050 (3)	0.034 (3)	0.006 (2)	0.009 (2)	-0.001 (2)
C55	0.044 (3)	0.047 (3)	0.043 (3)	0.000 (2)	0.008 (2)	-0.009 (2)
C56	0.088 (5)	0.043 (3)	0.073 (4)	0.017 (3)	0.021 (4)	0.015 (3)
C57	0.058 (4)	0.095 (5)	0.052 (4)	0.020 (4)	-0.013 (3)	-0.001 (4)
C58	0.051 (4)	0.057 (4)	0.073 (4)	-0.013 (3)	0.011 (3)	0.000 (3)
C59	0.062 (4)	0.068 (4)	0.036 (3)	0.009 (3)	0.002 (3)	0.010 (3)
C60	0.066 (4)	0.066 (4)	0.069 (4)	-0.004 (3)	-0.004 (4)	-0.028 (3)
F1	0.059 (3)	0.109 (4)	0.132 (4)	0.015 (2)	0.024 (3)	0.047 (3)
F2	0.125 (4)	0.081 (3)	0.103 (4)	0.034 (3)	-0.012 (3)	-0.030 (3)
F3	0.094 (3)	0.099 (3)	0.084 (3)	0.028 (3)	0.002 (3)	0.042 (3)
F4	0.052 (2)	0.110 (3)	0.117 (4)	-0.019 (2)	0.024 (2)	-0.050 (3)
F5	0.129 (4)	0.087 (3)	0.089 (3)	-0.050 (3)	-0.031 (3)	0.033 (3)
F6	0.078 (3)	0.086 (3)	0.067 (2)	-0.022 (2)	0.002 (2)	-0.033 (2)
F7	0.128 (4)	0.114 (4)	0.080 (3)	-0.018 (3)	-0.013 (3)	-0.032 (3)
F8	0.058 (3)	0.097 (3)	0.195 (6)	-0.019 (2)	-0.036 (3)	0.000 (4)
F9	0.101 (3)	0.049 (2)	0.148 (4)	-0.001 (2)	-0.023 (3)	0.005 (2)
F10	0.100 (3)	0.063 (2)	0.086 (3)	-0.015 (2)	-0.010 (2)	-0.020 (2)
F11	0.055 (2)	0.078 (3)	0.123 (4)	-0.013 (2)	-0.030 (2)	0.035 (3)
F12	0.073 (3)	0.081 (3)	0.084 (3)	-0.019 (2)	-0.007 (2)	0.034 (2)
F13	0.104 (3)	0.098 (3)	0.057 (2)	-0.035 (3)	0.003 (2)	0.024 (2)
F14	0.056 (2)	0.107 (3)	0.135 (4)	-0.017 (2)	-0.029 (3)	0.061 (3)
F15	0.107 (3)	0.068 (3)	0.111 (4)	-0.018 (2)	0.014 (3)	-0.027 (3)
O1	0.044 (2)	0.047 (2)	0.0361 (19)	-0.0099 (17)	0.0040 (16)	-0.0039 (16)
O2	0.046 (2)	0.049 (2)	0.0304 (18)	-0.0051 (16)	0.0016 (16)	-0.0026 (16)
O3	0.053 (2)	0.067 (3)	0.040 (2)	0.0027 (19)	-0.0037 (18)	0.0090 (19)

O4	0.084 (3)	0.070 (3)	0.065 (3)	0.004 (2)	-0.027 (3)	-0.019 (2)
O5	0.057 (3)	0.074 (3)	0.061 (3)	-0.004 (2)	0.009 (2)	0.010 (2)
O6	0.0412 (19)	0.0410 (19)	0.0395 (19)	0.0063 (16)	0.0029 (16)	0.0024 (15)
O7	0.048 (2)	0.043 (2)	0.039 (2)	0.0052 (16)	0.0018 (17)	0.0021 (17)
O8	0.047 (2)	0.044 (2)	0.039 (2)	0.0018 (16)	0.0043 (16)	0.0098 (16)
O9	0.043 (2)	0.047 (2)	0.038 (2)	0.0066 (16)	0.0024 (16)	0.0035 (16)
O10	0.049 (2)	0.055 (2)	0.043 (2)	-0.0056 (18)	-0.0051 (17)	-0.0059 (18)
O11	0.050 (3)	0.096 (4)	0.064 (3)	0.006 (2)	0.003 (2)	-0.018 (3)
O12	0.080 (3)	0.069 (3)	0.062 (3)	-0.014 (2)	-0.026 (2)	0.020 (2)
O13	0.050 (2)	0.064 (3)	0.063 (3)	0.000 (2)	0.008 (2)	-0.001 (2)
O14	0.104 (4)	0.056 (3)	0.114 (4)	0.006 (3)	-0.045 (3)	0.025 (3)
O15	0.075 (3)	0.096 (4)	0.064 (3)	0.003 (3)	0.026 (3)	-0.002 (3)
O16	0.0405 (19)	0.0422 (19)	0.0366 (19)	0.0063 (16)	-0.0022 (16)	-0.0025 (15)
O17	0.044 (2)	0.0414 (19)	0.0335 (19)	0.0042 (15)	-0.0037 (16)	-0.0047 (15)
O18	0.045 (2)	0.045 (2)	0.0334 (19)	0.0063 (16)	-0.0030 (15)	-0.0023 (15)
O19	0.045 (2)	0.044 (2)	0.0337 (18)	0.0094 (16)	-0.0009 (16)	-0.0012 (15)
O20	0.046 (2)	0.056 (2)	0.044 (2)	-0.0012 (17)	0.0009 (17)	0.0097 (18)
O21	0.069 (3)	0.064 (3)	0.057 (3)	0.009 (2)	0.015 (2)	-0.013 (2)
O22	0.047 (2)	0.061 (2)	0.048 (2)	0.0042 (19)	-0.0104 (18)	0.0047 (19)
O23	0.052 (2)	0.067 (3)	0.044 (2)	-0.0061 (19)	0.0072 (19)	0.0038 (19)
O24	0.094 (4)	0.064 (3)	0.088 (4)	-0.011 (3)	0.045 (3)	-0.026 (3)
O25	0.062 (3)	0.090 (3)	0.068 (3)	-0.002 (3)	-0.022 (2)	0.015 (3)
S1	0.0519 (8)	0.0532 (8)	0.0384 (7)	0.0020 (6)	-0.0049 (6)	0.0015 (6)
S2	0.0460 (8)	0.0532 (8)	0.0396 (7)	-0.0048 (6)	-0.0030 (6)	0.0005 (6)
S3	0.0508 (9)	0.0528 (9)	0.0669 (10)	0.0003 (7)	-0.0049 (8)	0.0014 (7)
S4	0.0440 (7)	0.0475 (7)	0.0401 (7)	-0.0012 (6)	0.0009 (6)	-0.0011 (6)
S5	0.0552 (9)	0.0530 (8)	0.0428 (8)	-0.0056 (7)	0.0078 (7)	-0.0008 (6)
Rh1	0.0412 (2)	0.0414 (2)	0.0322 (2)	-0.00294 (17)	-0.00206 (17)	-0.00092 (17)
Rh2	0.0402 (2)	0.0388 (2)	0.0356 (2)	0.00016 (17)	-0.00354 (17)	0.00255 (16)
Rh3	0.0387 (2)	0.0404 (2)	0.0377 (2)	0.00261 (17)	-0.00280 (18)	0.00238 (17)
Rh4	0.0390 (2)	0.0415 (2)	0.0335 (2)	0.00419 (17)	0.00072 (17)	-0.00178 (16)
Rh5	0.0390 (2)	0.0404 (2)	0.0325 (2)	0.00235 (17)	0.00206 (17)	-0.00098 (16)

Geometric parameters (Å, °)

C1—O2	1.252 (6)	C36—H36A	0.9600
C1—O1 ⁱ	1.253 (6)	C36—H36B	0.9600
C1—C1 ⁱ	1.532 (10)	C36—H36C	0.9600
C2—F1	1.305 (7)	C37—O16	1.253 (6)
C2—F2	1.321 (8)	C37—O18	1.259 (6)
C2—F3	1.328 (7)	C37—C38	1.546 (7)
C2—S1	1.805 (7)	C38—O19	1.246 (6)
C3—C4	1.437 (7)	C38—O17	1.253 (6)
C3—C8	1.466 (8)	C39—F10	1.325 (7)
C3—C7	1.468 (8)	C39—F12	1.327 (7)
C3—Rh1	2.142 (5)	C39—F11	1.331 (7)
C4—C5	1.443 (8)	C39—S4	1.800 (6)
C4—C9	1.481 (7)	C40—F14	1.296 (7)
C4—Rh1	2.138 (5)	C40—F15	1.318 (7)

supplementary materials

C5—C6	1.432 (8)	C40—F13	1.326 (7)
C5—C10	1.491 (8)	C40—S5	1.808 (6)
C5—Rh1	2.109 (5)	C41—C42	1.430 (8)
C6—C7	1.446 (8)	C41—C45	1.436 (9)
C6—C11	1.484 (8)	C41—C46	1.484 (8)
C6—Rh1	2.138 (5)	C41—Rh4	2.100 (6)
C7—C12	1.483 (8)	C42—C43	1.425 (8)
C7—Rh1	2.145 (5)	C42—C47	1.496 (8)
C8—H8A	0.9600	C42—Rh4	2.127 (5)
C8—H8B	0.9600	C43—C44	1.444 (8)
C8—H8C	0.9600	C43—C48	1.484 (8)
C9—H9A	0.9600	C43—Rh4	2.148 (5)
C9—H9B	0.9600	C44—C45	1.439 (9)
C9—H9C	0.9600	C44—C49	1.487 (9)
C10—H10A	0.9600	C44—Rh4	2.144 (5)
C10—H10B	0.9600	C45—C50	1.488 (9)
C10—H10C	0.9600	C45—Rh4	2.122 (6)
C11—H11A	0.9600	C46—H46A	0.9600
C11—H11B	0.9600	C46—H46B	0.9600
C11—H11C	0.9600	C46—H46C	0.9600
C12—H12A	0.9600	C47—H47A	0.9600
C12—H12B	0.9600	C47—H47B	0.9600
C12—H12C	0.9600	C47—H47C	0.9600
C13—O8	1.250 (6)	C48—H48A	0.9600
C13—O6	1.257 (6)	C48—H48B	0.9600
C13—C14	1.538 (7)	C48—H48C	0.9600
C14—O9	1.253 (6)	C49—H49A	0.9600
C14—O7	1.260 (6)	C49—H49B	0.9600
C15—F6	1.308 (7)	C49—H49C	0.9600
C15—F4	1.315 (7)	C50—H50A	0.9600
C15—F5	1.328 (7)	C50—H50B	0.9600
C15—S2	1.807 (6)	C50—H50C	0.9600
C16—F8	1.302 (8)	C51—C52	1.426 (8)
C16—F9	1.335 (8)	C51—C55	1.440 (8)
C16—F7	1.338 (9)	C51—C56	1.497 (8)
C16—S3	1.799 (7)	C51—Rh5	2.127 (5)
C17—C21	1.418 (8)	C52—C53	1.444 (8)
C17—C18	1.435 (8)	C52—C57	1.488 (8)
C17—C22	1.508 (8)	C52—Rh5	2.127 (5)
C17—Rh2	2.099 (5)	C53—C54	1.445 (8)
C18—C19	1.429 (9)	C53—C58	1.488 (8)
C18—C23	1.499 (9)	C53—Rh5	2.093 (5)
C18—Rh2	2.133 (5)	C54—C55	1.443 (8)
C19—C20	1.434 (8)	C54—C59	1.485 (7)
C19—C24	1.489 (8)	C54—Rh5	2.144 (5)
C19—Rh2	2.140 (5)	C55—C60	1.484 (8)
C20—C21	1.429 (8)	C55—Rh5	2.145 (5)
C20—C25	1.487 (8)	C56—H56A	0.9600
C20—Rh2	2.124 (6)	C56—H56B	0.9600

C21—C26	1.490 (8)	C56—H56C	0.9600
C21—Rh2	2.123 (5)	C57—H57A	0.9600
C22—H22A	0.9600	C57—H57B	0.9600
C22—H22B	0.9600	C57—H57C	0.9600
C22—H22C	0.9600	C58—H58A	0.9600
C23—H23A	0.9600	C58—H58B	0.9600
C23—H23B	0.9600	C58—H58C	0.9600
C23—H23C	0.9600	C59—H59A	0.9600
C24—H24A	0.9600	C59—H59B	0.9600
C24—H24B	0.9600	C59—H59C	0.9600
C24—H24C	0.9600	C60—H60A	0.9600
C25—H25A	0.9600	C60—H60B	0.9600
C25—H25B	0.9600	C60—H60C	0.9600
C25—H25C	0.9600	O1—C1 ⁱ	1.253 (6)
C26—H26A	0.9600	O1—Rh1	2.134 (3)
C26—H26B	0.9600	O2—Rh1	2.132 (3)
C26—H26C	0.9600	O3—S1	1.460 (4)
C27—C31	1.436 (8)	O3—Rh1	2.201 (4)
C27—C28	1.439 (8)	O4—S1	1.413 (4)
C27—C32	1.482 (8)	O5—S1	1.431 (4)
C27—Rh3	2.099 (5)	O6—Rh2	2.125 (3)
C28—C29	1.422 (9)	O7—Rh2	2.144 (3)
C28—C33	1.496 (8)	O8—Rh3	2.118 (4)
C28—Rh3	2.132 (6)	O9—Rh3	2.147 (3)
C29—C30	1.445 (9)	O10—S2	1.463 (4)
C29—C34	1.504 (9)	O10—Rh2	2.193 (4)
C29—Rh3	2.125 (6)	O11—S2	1.425 (5)
C30—C31	1.415 (9)	O12—S2	1.419 (4)
C30—C35	1.482 (9)	O13—S3	1.430 (4)
C30—Rh3	2.133 (6)	O13—Rh3	2.229 (4)
C31—C36	1.496 (8)	O14—S3	1.435 (4)
C31—Rh3	2.128 (5)	O15—S3	1.442 (5)
C32—H32A	0.9600	O16—Rh4	2.133 (3)
C32—H32B	0.9600	O17—Rh4	2.133 (3)
C32—H32C	0.9600	O18—Rh5	2.142 (3)
C33—H33A	0.9600	O19—Rh5	2.148 (3)
C33—H33B	0.9600	O20—S4	1.468 (4)
C33—H33C	0.9600	O20—Rh4	2.205 (4)
C34—H34A	0.9600	O21—S4	1.425 (4)
C34—H34B	0.9600	O22—S4	1.425 (4)
C34—H34C	0.9600	O23—S5	1.463 (4)
C35—H35A	0.9600	O23—Rh5	2.191 (4)
C35—H35B	0.9600	O24—S5	1.423 (5)
C35—H35C	0.9600	O25—S5	1.435 (5)
O2—C1—O1 ⁱ	124.8 (5)	H47A—C47—H47C	109.5
O2—C1—C1 ⁱ	117.5 (6)	H47B—C47—H47C	109.5
O1 ⁱ —C1—C1 ⁱ	117.7 (6)	C43—C48—H48A	109.5
F1—C2—F2	107.7 (6)	C43—C48—H48B	109.5

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F1—C2—F3	106.8 (6)	H48A—C48—H48B	109.5
F2—C2—F3	105.7 (6)	C43—C48—H48C	109.5
F1—C2—S1	113.3 (5)	H48A—C48—H48C	109.5
F2—C2—S1	111.7 (5)	H48B—C48—H48C	109.5
F3—C2—S1	111.3 (5)	C44—C49—H49A	109.5
C4—C3—C8	127.1 (5)	C44—C49—H49B	109.5
C4—C3—C7	107.5 (5)	H49A—C49—H49B	109.5
C8—C3—C7	125.4 (5)	C44—C49—H49C	109.5
C4—C3—Rh1	70.2 (3)	H49A—C49—H49C	109.5
C8—C3—Rh1	124.4 (4)	H49B—C49—H49C	109.5
C7—C3—Rh1	70.1 (3)	C45—C50—H50A	109.5
C3—C4—C5	108.5 (5)	C45—C50—H50B	109.5
C3—C4—C9	126.9 (5)	H50A—C50—H50B	109.5
C5—C4—C9	124.6 (5)	C45—C50—H50C	109.5
C3—C4—Rh1	70.5 (3)	H50A—C50—H50C	109.5
C5—C4—Rh1	69.1 (3)	H50B—C50—H50C	109.5
C9—C4—Rh1	124.3 (4)	C52—C51—C55	108.6 (5)
C6—C5—C4	108.3 (5)	C52—C51—C56	126.4 (6)
C6—C5—C10	126.9 (5)	C55—C51—C56	125.0 (6)
C4—C5—C10	124.6 (5)	C52—C51—Rh5	70.4 (3)
C6—C5—Rh1	71.4 (3)	C55—C51—Rh5	71.0 (3)
C4—C5—Rh1	71.2 (3)	C56—C51—Rh5	125.8 (4)
C10—C5—Rh1	127.4 (4)	C51—C52—C53	108.0 (5)
C5—C6—C7	108.4 (5)	C51—C52—C57	126.0 (6)
C5—C6—C11	126.8 (6)	C53—C52—C57	125.9 (6)
C7—C6—C11	124.7 (6)	C51—C52—Rh5	70.4 (3)
C5—C6—Rh1	69.2 (3)	C53—C52—Rh5	68.8 (3)
C7—C6—Rh1	70.5 (3)	C57—C52—Rh5	123.2 (4)
C11—C6—Rh1	124.3 (4)	C52—C53—C54	107.8 (5)
C6—C7—C3	107.3 (5)	C52—C53—C58	126.6 (5)
C6—C7—C12	126.7 (6)	C54—C53—C58	125.5 (5)
C3—C7—C12	126.0 (6)	C52—C53—Rh5	71.2 (3)
C6—C7—Rh1	70.0 (3)	C54—C53—Rh5	72.0 (3)
C3—C7—Rh1	69.9 (3)	C58—C53—Rh5	125.0 (4)
C12—C7—Rh1	127.2 (4)	C55—C54—C53	107.7 (5)
C3—C8—H8A	109.5	C55—C54—C59	126.3 (5)
C3—C8—H8B	109.5	C53—C54—C59	125.9 (5)
H8A—C8—H8B	109.5	C55—C54—Rh5	70.4 (3)
C3—C8—H8C	109.5	C53—C54—Rh5	68.2 (3)
H8A—C8—H8C	109.5	C59—C54—Rh5	125.6 (4)
H8B—C8—H8C	109.5	C51—C55—C54	107.7 (5)
C4—C9—H9A	109.5	C51—C55—C60	125.9 (5)
C4—C9—H9B	109.5	C54—C55—C60	126.4 (5)
H9A—C9—H9B	109.5	C51—C55—Rh5	69.6 (3)
C4—C9—H9C	109.5	C54—C55—Rh5	70.3 (3)
H9A—C9—H9C	109.5	C60—C55—Rh5	126.3 (4)
H9B—C9—H9C	109.5	C51—C56—H56A	109.5
C5—C10—H10A	109.5	C51—C56—H56B	109.5
C5—C10—H10B	109.5	H56A—C56—H56B	109.5

H10A—C10—H10B	109.5	C51—C56—H56C	109.5
C5—C10—H10C	109.5	H56A—C56—H56C	109.5
H10A—C10—H10C	109.5	H56B—C56—H56C	109.5
H10B—C10—H10C	109.5	C52—C57—H57A	109.5
C6—C11—H11A	109.5	C52—C57—H57B	109.5
C6—C11—H11B	109.5	H57A—C57—H57B	109.5
H11A—C11—H11B	109.5	C52—C57—H57C	109.5
C6—C11—H11C	109.5	H57A—C57—H57C	109.5
H11A—C11—H11C	109.5	H57B—C57—H57C	109.5
H11B—C11—H11C	109.5	C53—C58—H58A	109.5
C7—C12—H12A	109.5	C53—C58—H58B	109.5
C7—C12—H12B	109.5	H58A—C58—H58B	109.5
H12A—C12—H12B	109.5	C53—C58—H58C	109.5
C7—C12—H12C	109.5	H58A—C58—H58C	109.5
H12A—C12—H12C	109.5	H58B—C58—H58C	109.5
H12B—C12—H12C	109.5	C54—C59—H59A	109.5
O8—C13—O6	124.8 (5)	C54—C59—H59B	109.5
O8—C13—C14	117.4 (5)	H59A—C59—H59B	109.5
O6—C13—C14	117.7 (5)	C54—C59—H59C	109.5
O9—C14—O7	125.2 (5)	H59A—C59—H59C	109.5
O9—C14—C13	117.4 (5)	H59B—C59—H59C	109.5
O7—C14—C13	117.4 (5)	C55—C60—H60A	109.5
F6—C15—F4	106.7 (5)	C55—C60—H60B	109.5
F6—C15—F5	107.1 (5)	H60A—C60—H60B	109.5
F4—C15—F5	107.2 (6)	C55—C60—H60C	109.5
F6—C15—S2	111.7 (4)	H60A—C60—H60C	109.5
F4—C15—S2	112.5 (4)	H60B—C60—H60C	109.5
F5—C15—S2	111.3 (4)	C1 ⁱ —O1—Rh1	112.7 (3)
F8—C16—F9	107.8 (6)	C1—O2—Rh1	112.9 (3)
F8—C16—F7	107.1 (7)	S1—O3—Rh1	125.7 (2)
F9—C16—F7	108.3 (6)	C13—O6—Rh2	113.1 (3)
F8—C16—S3	111.7 (5)	C14—O7—Rh2	112.3 (3)
F9—C16—S3	110.5 (5)	C13—O8—Rh3	113.6 (3)
F7—C16—S3	111.3 (5)	C14—O9—Rh3	112.2 (3)
C21—C17—C18	108.0 (5)	S2—O10—Rh2	124.6 (2)
C21—C17—C22	125.9 (6)	S3—O13—Rh3	123.1 (3)
C18—C17—C22	125.9 (6)	C37—O16—Rh4	113.3 (3)
C21—C17—Rh2	71.3 (3)	C38—O17—Rh4	113.4 (3)
C18—C17—Rh2	71.4 (3)	C37—O18—Rh5	113.4 (3)
C22—C17—Rh2	126.5 (4)	C38—O19—Rh5	113.5 (3)
C19—C18—C17	107.4 (5)	S4—O20—Rh4	125.1 (2)
C19—C18—C23	126.7 (6)	S5—O23—Rh5	124.3 (2)
C17—C18—C23	126.0 (6)	O4—S1—O5	116.9 (3)
C19—C18—Rh2	70.8 (3)	O4—S1—O3	114.1 (3)
C17—C18—Rh2	68.9 (3)	O5—S1—O3	113.9 (3)
C23—C18—Rh2	124.6 (4)	O4—S1—C2	104.3 (3)
C18—C19—C20	108.7 (5)	O5—S1—C2	104.2 (3)
C18—C19—C24	126.6 (6)	O3—S1—C2	101.0 (3)
C20—C19—C24	124.7 (6)	O12—S2—O11	117.0 (3)

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C18—C19—Rh2	70.2 (3)	O12—S2—O10	114.1 (3)
C20—C19—Rh2	69.7 (3)	O11—S2—O10	113.7 (2)
C24—C19—Rh2	123.9 (4)	O12—S2—C15	104.1 (3)
C21—C20—C19	106.9 (5)	O11—S2—C15	104.1 (3)
C21—C20—C25	125.1 (6)	O10—S2—C15	101.4 (3)
C19—C20—C25	127.8 (6)	O13—S3—O14	113.8 (3)
C21—C20—Rh2	70.3 (3)	O13—S3—O15	113.6 (3)
C19—C20—Rh2	71.0 (3)	O14—S3—O15	118.4 (4)
C25—C20—Rh2	127.0 (4)	O13—S3—C16	101.6 (3)
C17—C21—C20	109.0 (5)	O14—S3—C16	103.9 (3)
C17—C21—C26	124.4 (6)	O15—S3—C16	102.7 (3)
C20—C21—C26	126.5 (6)	O21—S4—O22	117.4 (3)
C17—C21—Rh2	69.5 (3)	O21—S4—O20	113.5 (3)
C20—C21—Rh2	70.4 (3)	O22—S4—O20	114.5 (2)
C26—C21—Rh2	122.9 (4)	O21—S4—C39	103.4 (3)
C17—C22—H22A	109.5	O22—S4—C39	103.8 (3)
C17—C22—H22B	109.5	O20—S4—C39	101.7 (3)
H22A—C22—H22B	109.5	O24—S5—O25	117.4 (3)
C17—C22—H22C	109.5	O24—S5—O23	113.3 (3)
H22A—C22—H22C	109.5	O25—S5—O23	114.4 (3)
H22B—C22—H22C	109.5	O24—S5—C40	104.8 (3)
C18—C23—H23A	109.5	O25—S5—C40	104.1 (3)
C18—C23—H23B	109.5	O23—S5—C40	100.3 (3)
H23A—C23—H23B	109.5	C5—Rh1—O2	108.95 (18)
C18—C23—H23C	109.5	C5—Rh1—O1	107.42 (18)
H23A—C23—H23C	109.5	O2—Rh1—O1	78.27 (13)
H23B—C23—H23C	109.5	C5—Rh1—C6	39.4 (2)
C19—C24—H24A	109.5	O2—Rh1—C6	146.48 (19)
C19—C24—H24B	109.5	O1—Rh1—C6	99.01 (18)
H24A—C24—H24B	109.5	C5—Rh1—C4	39.7 (2)
C19—C24—H24C	109.5	O2—Rh1—C4	96.07 (16)
H24A—C24—H24C	109.5	O1—Rh1—C4	143.24 (18)
H24B—C24—H24C	109.5	C6—Rh1—C4	66.0 (2)
C20—C25—H25A	109.5	C5—Rh1—C3	66.7 (2)
C20—C25—H25B	109.5	O2—Rh1—C3	117.87 (18)
H25A—C25—H25B	109.5	O1—Rh1—C3	163.71 (17)
C20—C25—H25C	109.5	C6—Rh1—C3	66.5 (2)
H25A—C25—H25C	109.5	C4—Rh1—C3	39.2 (2)
H25B—C25—H25C	109.5	C5—Rh1—C7	66.6 (2)
C21—C26—H26A	109.5	O2—Rh1—C7	157.93 (18)
C21—C26—H26B	109.5	O1—Rh1—C7	123.80 (18)
H26A—C26—H26B	109.5	C6—Rh1—C7	39.5 (2)
C21—C26—H26C	109.5	C4—Rh1—C7	66.3 (2)
H26A—C26—H26C	109.5	C3—Rh1—C7	40.1 (2)
H26B—C26—H26C	109.5	C5—Rh1—O3	163.43 (19)
C31—C27—C28	107.2 (5)	O2—Rh1—O3	81.56 (15)
C31—C27—C32	126.1 (6)	O1—Rh1—O3	86.96 (14)
C28—C27—C32	126.5 (6)	C6—Rh1—O3	131.9 (2)
C31—C27—Rh3	71.2 (3)	C4—Rh1—O3	128.56 (18)

C28—C27—Rh3	71.3 (3)	C3—Rh1—O3	97.24 (18)
C32—C27—Rh3	126.4 (4)	C7—Rh1—O3	98.80 (19)
C29—C28—C27	108.3 (5)	C17—Rh2—C21	39.3 (2)
C29—C28—C33	126.1 (6)	C17—Rh2—C20	66.6 (2)
C27—C28—C33	125.6 (7)	C21—Rh2—C20	39.3 (2)
C29—C28—Rh3	70.2 (3)	C17—Rh2—O6	116.64 (19)
C27—C28—Rh3	68.9 (3)	C21—Rh2—O6	95.33 (18)
C33—C28—Rh3	125.1 (4)	C20—Rh2—O6	108.69 (19)
C28—C29—C30	107.9 (5)	C17—Rh2—C18	39.6 (2)
C28—C29—C34	128.2 (7)	C21—Rh2—C18	65.7 (2)
C30—C29—C34	123.9 (7)	C20—Rh2—C18	66.3 (2)
C28—C29—Rh3	70.7 (3)	O6—Rh2—C18	156.26 (19)
C30—C29—Rh3	70.5 (3)	C17—Rh2—C19	65.9 (2)
C34—C29—Rh3	124.7 (4)	C21—Rh2—C19	65.3 (2)
C31—C30—C29	107.7 (5)	C20—Rh2—C19	39.3 (2)
C31—C30—C35	125.8 (6)	O6—Rh2—C19	146.7 (2)
C29—C30—C35	126.4 (6)	C18—Rh2—C19	39.1 (2)
C31—C30—Rh3	70.4 (3)	C17—Rh2—O7	100.79 (18)
C29—C30—Rh3	69.9 (3)	C21—Rh2—O7	131.27 (19)
C35—C30—Rh3	125.9 (4)	C20—Rh2—O7	167.11 (19)
C30—C31—C27	108.8 (5)	O6—Rh2—O7	78.63 (13)
C30—C31—C36	126.5 (6)	C18—Rh2—O7	102.65 (19)
C27—C31—C36	124.7 (6)	C19—Rh2—O7	134.7 (2)
C30—C31—Rh3	70.8 (3)	C17—Rh2—O10	156.14 (19)
C27—C31—Rh3	69.1 (3)	C21—Rh2—O10	148.0 (2)
C36—C31—Rh3	124.3 (4)	C20—Rh2—O10	109.91 (19)
C27—C32—H32A	109.5	O6—Rh2—O10	87.09 (14)
C27—C32—H32B	109.5	C18—Rh2—O10	116.6 (2)
H32A—C32—H32B	109.5	C19—Rh2—O10	95.96 (19)
C27—C32—H32C	109.5	O7—Rh2—O10	80.55 (14)
H32A—C32—H32C	109.5	C27—Rh3—O8	106.46 (19)
H32B—C32—H32C	109.5	C27—Rh3—C29	66.6 (2)
C28—C33—H33A	109.5	O8—Rh3—C29	159.4 (2)
C28—C33—H33B	109.5	C27—Rh3—C31	39.7 (2)
H33A—C33—H33B	109.5	O8—Rh3—C31	96.12 (18)
C28—C33—H33C	109.5	C29—Rh3—C31	65.8 (2)
H33A—C33—H33C	109.5	C27—Rh3—C28	39.8 (2)
H33B—C33—H33C	109.5	O8—Rh3—C28	143.9 (2)
C29—C34—H34A	109.5	C29—Rh3—C28	39.0 (2)
C29—C34—H34B	109.5	C31—Rh3—C28	65.8 (2)
H34A—C34—H34B	109.5	C27—Rh3—C30	66.4 (2)
C29—C34—H34C	109.5	O8—Rh3—C30	119.82 (19)
H34A—C34—H34C	109.5	C29—Rh3—C30	39.7 (2)
H34B—C34—H34C	109.5	C31—Rh3—C30	38.8 (2)
C30—C35—H35A	109.5	C28—Rh3—C30	65.9 (2)
C30—C35—H35B	109.5	C27—Rh3—O9	109.00 (19)
H35A—C35—H35B	109.5	O8—Rh3—O9	78.37 (13)
C30—C35—H35C	109.5	C29—Rh3—O9	122.1 (2)
H35A—C35—H35C	109.5	C31—Rh3—O9	145.8 (2)

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H35B—C35—H35C	109.5	C28—Rh3—O9	98.96 (18)
C31—C36—H36A	109.5	C30—Rh3—O9	161.76 (19)
C31—C36—H36B	109.5	C27—Rh3—O13	162.48 (19)
H36A—C36—H36B	109.5	O8—Rh3—O13	89.70 (14)
C31—C36—H36C	109.5	C29—Rh3—O13	95.9 (2)
H36A—C36—H36C	109.5	C31—Rh3—O13	133.7 (2)
H36B—C36—H36C	109.5	C28—Rh3—O13	125.7 (2)
O16—C37—O18	125.2 (5)	C30—Rh3—O13	99.9 (2)
O16—C37—C38	117.4 (5)	O9—Rh3—O13	80.39 (15)
O18—C37—C38	117.3 (5)	C41—Rh4—C45	39.8 (2)
O19—C38—O17	125.2 (5)	C41—Rh4—C42	39.5 (2)
O19—C38—C37	117.6 (5)	C45—Rh4—C42	65.8 (2)
O17—C38—C37	117.2 (5)	C41—Rh4—O16	104.84 (19)
F10—C39—F12	106.7 (5)	C45—Rh4—O16	96.54 (19)
F10—C39—F11	107.1 (5)	C42—Rh4—O16	141.17 (18)
F12—C39—F11	106.7 (5)	C41—Rh4—O17	107.91 (19)
F10—C39—S4	112.0 (4)	C45—Rh4—O17	145.4 (2)
F12—C39—S4	111.5 (4)	C42—Rh4—O17	96.74 (17)
F11—C39—S4	112.6 (4)	O16—Rh4—O17	78.36 (13)
F14—C40—F15	108.3 (6)	C41—Rh4—C44	66.6 (2)
F14—C40—F13	107.4 (5)	C45—Rh4—C44	39.4 (2)
F15—C40—F13	105.5 (5)	C42—Rh4—C44	65.6 (2)
F14—C40—S5	112.7 (4)	O16—Rh4—C44	122.66 (19)
F15—C40—S5	111.6 (4)	O17—Rh4—C44	158.81 (18)
F13—C40—S5	111.1 (4)	C41—Rh4—C43	66.4 (2)
C42—C41—C45	107.4 (5)	C45—Rh4—C43	66.0 (2)
C42—C41—C46	126.0 (6)	C42—Rh4—C43	38.9 (2)
C45—C41—C46	126.5 (6)	O16—Rh4—C43	161.43 (18)
C42—C41—Rh4	71.2 (3)	O17—Rh4—C43	119.49 (18)
C45—C41—Rh4	70.9 (3)	C44—Rh4—C43	39.3 (2)
C46—C41—Rh4	126.2 (4)	C41—Rh4—O20	165.70 (19)
C43—C42—C41	109.2 (5)	C45—Rh4—O20	131.8 (2)
C43—C42—C47	125.8 (5)	C42—Rh4—O20	131.31 (19)
C41—C42—C47	125.0 (5)	O16—Rh4—O20	86.67 (14)
C43—C42—Rh4	71.3 (3)	O17—Rh4—O20	82.41 (14)
C41—C42—Rh4	69.2 (3)	C44—Rh4—O20	100.2 (2)
C47—C42—Rh4	124.4 (4)	C43—Rh4—O20	100.08 (19)
C42—C43—C44	107.6 (5)	C53—Rh5—C52	40.0 (2)
C42—C43—C48	127.2 (5)	C53—Rh5—C51	66.7 (2)
C44—C43—C48	125.2 (6)	C52—Rh5—C51	39.2 (2)
C42—C43—Rh4	69.8 (3)	C53—Rh5—O18	107.19 (17)
C44—C43—Rh4	70.2 (3)	C52—Rh5—O18	144.16 (18)
C48—C43—Rh4	124.5 (4)	C51—Rh5—O18	161.25 (18)
C45—C44—C43	107.6 (5)	C53—Rh5—C54	39.9 (2)
C45—C44—C49	127.0 (6)	C52—Rh5—C54	66.3 (2)
C43—C44—C49	125.4 (6)	C51—Rh5—C54	66.1 (2)
C45—C44—Rh4	69.5 (3)	O18—Rh5—C54	97.60 (17)
C43—C44—Rh4	70.5 (3)	C53—Rh5—C55	66.8 (2)
C49—C44—Rh4	126.6 (4)	C52—Rh5—C55	66.0 (2)

C41—C45—C44	108.3 (5)	C51—Rh5—C55	39.4 (2)
C41—C45—C50	126.8 (7)	O18—Rh5—C55	121.94 (18)
C44—C45—C50	124.8 (7)	C54—Rh5—C55	39.3 (2)
C41—C45—Rh4	69.3 (3)	C53—Rh5—O19	103.60 (17)
C44—C45—Rh4	71.1 (3)	C52—Rh5—O19	94.46 (17)
C50—C45—Rh4	123.1 (5)	C51—Rh5—O19	120.26 (18)
C41—C46—H46A	109.5	O18—Rh5—O19	78.08 (13)
C41—C46—H46B	109.5	C54—Rh5—O19	140.80 (18)
H46A—C46—H46B	109.5	C55—Rh5—O19	159.13 (18)
C41—C46—H46C	109.5	C53—Rh5—O23	164.74 (18)
H46A—C46—H46C	109.5	C52—Rh5—O23	131.50 (19)
H46B—C46—H46C	109.5	C51—Rh5—O23	99.46 (19)
C42—C47—H47A	109.5	O18—Rh5—O23	83.80 (15)
C42—C47—H47B	109.5	C54—Rh5—O23	129.85 (18)
H47A—C47—H47B	109.5	C55—Rh5—O23	98.58 (18)
C42—C47—H47C	109.5	O19—Rh5—O23	88.81 (14)
C8—C3—C4—C5	-177.5 (5)	C26—C21—Rh2—C19	-160.0 (6)
C7—C3—C4—C5	1.7 (6)	C17—C21—Rh2—O7	-47.1 (4)
Rh1—C3—C4—C5	-58.8 (4)	C20—C21—Rh2—O7	-167.3 (3)
C8—C3—C4—C9	0.1 (9)	C26—C21—Rh2—O7	71.3 (6)
C7—C3—C4—C9	179.3 (5)	C17—C21—Rh2—O10	140.3 (4)
Rh1—C3—C4—C9	118.8 (5)	C20—C21—Rh2—O10	20.2 (6)
C8—C3—C4—Rh1	-118.7 (6)	C26—C21—Rh2—O10	-101.3 (6)
C7—C3—C4—Rh1	60.5 (4)	C21—C20—Rh2—C17	36.6 (3)
C3—C4—C5—C6	-2.4 (6)	C19—C20—Rh2—C17	-80.1 (4)
C9—C4—C5—C6	179.8 (5)	C25—C20—Rh2—C17	156.3 (7)
Rh1—C4—C5—C6	-62.2 (4)	C19—C20—Rh2—C21	-116.8 (5)
C3—C4—C5—C10	-177.3 (5)	C25—C20—Rh2—C21	119.7 (8)
C9—C4—C5—C10	5.0 (8)	C21—C20—Rh2—O6	-75.0 (4)
Rh1—C4—C5—C10	123.0 (5)	C19—C20—Rh2—O6	168.2 (3)
C3—C4—C5—Rh1	59.7 (4)	C25—C20—Rh2—O6	44.7 (6)
C9—C4—C5—Rh1	-118.0 (5)	C21—C20—Rh2—C18	80.0 (4)
C4—C5—C6—C7	2.2 (6)	C19—C20—Rh2—C18	-36.7 (3)
C10—C5—C6—C7	176.9 (5)	C25—C20—Rh2—C18	-160.2 (7)
Rh1—C5—C6—C7	-59.8 (4)	C21—C20—Rh2—C19	116.8 (5)
C4—C5—C6—C11	-179.9 (5)	C25—C20—Rh2—C19	-123.5 (8)
C10—C5—C6—C11	-5.2 (10)	C21—C20—Rh2—O7	48.0 (10)
Rh1—C5—C6—C11	118.0 (6)	C19—C20—Rh2—O7	-68.7 (10)
C4—C5—C6—Rh1	62.1 (4)	C25—C20—Rh2—O7	167.7 (7)
C10—C5—C6—Rh1	-123.3 (6)	C21—C20—Rh2—O10	-168.8 (3)
C5—C6—C7—C3	-1.2 (6)	C19—C20—Rh2—O10	74.4 (4)
C11—C6—C7—C3	-179.1 (5)	C25—C20—Rh2—O10	-49.1 (6)
Rh1—C6—C7—C3	-60.2 (4)	C13—O6—Rh2—C17	101.6 (4)
C5—C6—C7—C12	-178.9 (5)	C13—O6—Rh2—C21	136.2 (4)
C11—C6—C7—C12	3.2 (9)	C13—O6—Rh2—C20	174.1 (4)
Rh1—C6—C7—C12	122.1 (6)	C13—O6—Rh2—C18	100.8 (5)
C5—C6—C7—Rh1	59.0 (4)	C13—O6—Rh2—C19	-172.2 (4)
C11—C6—C7—Rh1	-118.9 (6)	C13—O6—Rh2—O7	5.1 (3)
C4—C3—C7—C6	-0.3 (6)	C13—O6—Rh2—O10	-75.8 (3)

supplementary materials

C8—C3—C7—C6	178.9 (5)	C19—C18—Rh2—C17	118.3 (5)
Rh1—C3—C7—C6	60.3 (4)	C23—C18—Rh2—C17	-119.9 (7)
C4—C3—C7—C12	177.4 (5)	C19—C18—Rh2—C21	80.2 (4)
C8—C3—C7—C12	-3.4 (9)	C17—C18—Rh2—C21	-38.1 (3)
Rh1—C3—C7—C12	-122.0 (6)	C23—C18—Rh2—C21	-158.0 (7)
C4—C3—C7—Rh1	-60.6 (4)	C19—C18—Rh2—C20	36.9 (3)
C8—C3—C7—Rh1	118.6 (5)	C17—C18—Rh2—C20	-81.3 (4)
O8—C13—C14—O9	-7.2 (7)	C23—C18—Rh2—C20	158.8 (7)
O6—C13—C14—O9	174.3 (4)	C19—C18—Rh2—O6	119.5 (5)
O8—C13—C14—O7	173.0 (4)	C17—C18—Rh2—O6	1.2 (7)
O6—C13—C14—O7	-5.5 (7)	C23—C18—Rh2—O6	-118.7 (6)
C21—C17—C18—C19	1.7 (6)	C17—C18—Rh2—C19	-118.3 (5)
C22—C17—C18—C19	177.3 (6)	C23—C18—Rh2—C19	121.8 (7)
Rh2—C17—C18—C19	-60.6 (4)	C19—C18—Rh2—O7	-150.0 (3)
C21—C17—C18—C23	-179.5 (6)	C17—C18—Rh2—O7	91.7 (3)
C22—C17—C18—C23	-3.9 (10)	C23—C18—Rh2—O7	-28.2 (6)
Rh2—C17—C18—C23	118.2 (6)	C19—C18—Rh2—O10	-64.4 (4)
C21—C17—C18—Rh2	62.3 (4)	C17—C18—Rh2—O10	177.4 (3)
C22—C17—C18—Rh2	-122.1 (6)	C23—C18—Rh2—O10	57.5 (6)
C17—C18—C19—C20	0.2 (6)	C18—C19—Rh2—C17	-38.0 (3)
C23—C18—C19—C20	-178.6 (6)	C20—C19—Rh2—C17	81.8 (4)
Rh2—C18—C19—C20	-59.3 (4)	C24—C19—Rh2—C17	-159.4 (7)
C17—C18—C19—C24	177.5 (6)	C18—C19—Rh2—C21	-81.2 (4)
C23—C18—C19—C24	-1.3 (10)	C20—C19—Rh2—C21	38.5 (3)
Rh2—C18—C19—C24	118.0 (6)	C24—C19—Rh2—C21	157.4 (7)
C17—C18—C19—Rh2	59.5 (4)	C18—C19—Rh2—C20	-119.8 (5)
C23—C18—C19—Rh2	-119.3 (6)	C24—C19—Rh2—C20	118.8 (8)
C18—C19—C20—C21	-1.9 (6)	C18—C19—Rh2—O6	-140.4 (4)
C24—C19—C20—C21	-179.3 (5)	C20—C19—Rh2—O6	-20.6 (5)
Rh2—C19—C20—C21	-61.5 (4)	C24—C19—Rh2—O6	98.2 (7)
C18—C19—C20—C25	-177.9 (6)	C20—C19—Rh2—C18	119.8 (5)
C24—C19—C20—C25	4.7 (10)	C24—C19—Rh2—C18	-121.4 (8)
Rh2—C19—C20—C25	122.5 (6)	C18—C19—Rh2—O7	43.3 (4)
C18—C19—C20—Rh2	59.5 (4)	C20—C19—Rh2—O7	163.0 (3)
C24—C19—C20—Rh2	-117.8 (6)	C24—C19—Rh2—O7	-78.2 (7)
C18—C17—C21—C20	-2.9 (6)	C18—C19—Rh2—O10	125.9 (3)
C22—C17—C21—C20	-178.5 (5)	C20—C19—Rh2—O10	-114.4 (3)
Rh2—C17—C21—C20	59.5 (4)	C24—C19—Rh2—O10	4.4 (6)
C18—C17—C21—C26	-178.9 (5)	C14—O7—Rh2—C17	-123.4 (4)
C22—C17—C21—C26	5.5 (9)	C14—O7—Rh2—C21	-95.2 (4)
Rh2—C17—C21—C26	-116.5 (6)	C14—O7—Rh2—C20	-134.1 (9)
C18—C17—C21—Rh2	-62.4 (4)	C14—O7—Rh2—O6	-8.1 (3)
C22—C17—C21—Rh2	122.0 (6)	C14—O7—Rh2—C18	-163.9 (4)
C19—C20—C21—C17	3.0 (6)	C14—O7—Rh2—C19	169.8 (3)
C25—C20—C21—C17	179.1 (5)	C14—O7—Rh2—O10	80.8 (3)
Rh2—C20—C21—C17	-58.9 (4)	S2—O10—Rh2—C17	140.6 (4)
C19—C20—C21—C26	178.9 (6)	S2—O10—Rh2—C21	50.3 (5)
C25—C20—C21—C26	-5.0 (9)	S2—O10—Rh2—C20	63.7 (3)
Rh2—C20—C21—C26	116.9 (6)	S2—O10—Rh2—O6	-45.1 (3)

C19—C20—C21—Rh2	61.9 (4)	S2—O10—Rh2—C18	136.4 (3)
C25—C20—C21—Rh2	-122.0 (6)	S2—O10—Rh2—C19	101.5 (3)
C31—C27—C28—C29	3.2 (6)	S2—O10—Rh2—O7	-124.1 (3)
C32—C27—C28—C29	178.6 (6)	C31—C27—Rh3—O8	79.5 (3)
Rh3—C27—C28—C29	-59.4 (4)	C28—C27—Rh3—O8	-164.1 (3)
C31—C27—C28—C33	-178.6 (6)	C32—C27—Rh3—O8	-42.0 (6)
C32—C27—C28—C33	-3.2 (10)	C31—C27—Rh3—C29	-79.8 (4)
Rh3—C27—C28—C33	118.8 (6)	C28—C27—Rh3—C29	36.6 (4)
C31—C27—C28—Rh3	62.6 (4)	C32—C27—Rh3—C29	158.6 (7)
C32—C27—C28—Rh3	-122.0 (6)	C28—C27—Rh3—C31	116.4 (5)
C27—C28—C29—C30	-2.4 (6)	C32—C27—Rh3—C31	-121.5 (7)
C33—C28—C29—C30	179.4 (6)	C31—C27—Rh3—C28	-116.4 (5)
Rh3—C28—C29—C30	-61.0 (4)	C32—C27—Rh3—C28	122.1 (8)
C27—C28—C29—C34	178.1 (6)	C31—C27—Rh3—C30	-36.4 (3)
C33—C28—C29—C34	-0.1 (10)	C28—C27—Rh3—C30	80.0 (4)
Rh3—C28—C29—C34	119.5 (6)	C32—C27—Rh3—C30	-157.9 (7)
C27—C28—C29—Rh3	58.6 (4)	C31—C27—Rh3—O9	162.6 (3)
C33—C28—C29—Rh3	-119.6 (6)	C28—C27—Rh3—O9	-81.0 (4)
C28—C29—C30—C31	0.7 (6)	C32—C27—Rh3—O9	41.1 (6)
C34—C29—C30—C31	-179.8 (6)	C31—C27—Rh3—O13	-77.1 (7)
Rh3—C29—C30—C31	-60.5 (4)	C28—C27—Rh3—O13	39.3 (8)
C28—C29—C30—C35	-178.5 (6)	C32—C27—Rh3—O13	161.3 (6)
C34—C29—C30—C35	1.1 (9)	C13—O8—Rh3—C27	111.1 (4)
Rh3—C29—C30—C35	120.4 (6)	C13—O8—Rh3—C29	178.0 (6)
C28—C29—C30—Rh3	61.1 (4)	C13—O8—Rh3—C31	150.3 (4)
C34—C29—C30—Rh3	-119.3 (6)	C13—O8—Rh3—C28	93.7 (4)
C29—C30—C31—C27	1.4 (6)	C13—O8—Rh3—C30	-177.1 (4)
C35—C30—C31—C27	-179.5 (6)	C13—O8—Rh3—O9	4.4 (3)
Rh3—C30—C31—C27	-58.8 (4)	C13—O8—Rh3—O13	-75.8 (4)
C29—C30—C31—C36	179.1 (5)	C28—C29—Rh3—C27	-37.2 (3)
C35—C30—C31—C36	-1.8 (9)	C30—C29—Rh3—C27	80.8 (4)
Rh3—C30—C31—C36	119.0 (6)	C34—C29—Rh3—C27	-160.9 (7)
C29—C30—C31—Rh3	60.1 (4)	C28—C29—Rh3—O8	-111.3 (6)
C35—C30—C31—Rh3	-120.7 (6)	C30—C29—Rh3—O8	6.7 (8)
C28—C27—C31—C30	-2.8 (6)	C34—C29—Rh3—O8	125.0 (7)
C32—C27—C31—C30	-178.3 (6)	C28—C29—Rh3—C31	-80.8 (4)
Rh3—C27—C31—C30	59.9 (4)	C30—C29—Rh3—C31	37.2 (3)
C28—C27—C31—C36	179.4 (5)	C34—C29—Rh3—C31	155.5 (7)
C32—C27—C31—C36	3.9 (9)	C30—C29—Rh3—C28	118.0 (5)
Rh3—C27—C31—C36	-117.9 (5)	C34—C29—Rh3—C28	-123.7 (8)
C28—C27—C31—Rh3	-62.7 (4)	C28—C29—Rh3—C30	-118.0 (5)
C32—C27—C31—Rh3	121.9 (6)	C34—C29—Rh3—C30	118.3 (8)
O16—C37—C38—O19	-179.4 (4)	C28—C29—Rh3—O9	61.2 (4)
O18—C37—C38—O19	0.6 (7)	C30—C29—Rh3—O9	179.2 (3)
O16—C37—C38—O17	-0.4 (7)	C34—C29—Rh3—O9	-62.5 (7)
O18—C37—C38—O17	179.7 (4)	C28—C29—Rh3—O13	143.6 (3)
C45—C41—C42—C43	-1.8 (6)	C30—C29—Rh3—O13	-98.4 (3)
C46—C41—C42—C43	-178.0 (6)	C34—C29—Rh3—O13	19.9 (7)
Rh4—C41—C42—C43	60.4 (4)	C30—C31—Rh3—C27	-119.9 (5)

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C45—C41—C42—C47	179.7 (5)	C36—C31—Rh3—C27	118.5 (7)
C46—C41—C42—C47	3.5 (9)	C30—C31—Rh3—O8	131.7 (3)
Rh4—C41—C42—C47	-118.2 (5)	C27—C31—Rh3—O8	-108.5 (3)
C45—C41—C42—Rh4	-62.1 (4)	C36—C31—Rh3—O8	10.1 (6)
C46—C41—C42—Rh4	121.7 (6)	C30—C31—Rh3—C29	-38.0 (4)
C41—C42—C43—C44	1.2 (6)	C27—C31—Rh3—C29	81.9 (4)
C47—C42—C43—C44	179.7 (5)	C36—C31—Rh3—C29	-159.6 (7)
Rh4—C42—C43—C44	60.3 (4)	C30—C31—Rh3—C28	-81.0 (4)
C41—C42—C43—C48	-177.6 (5)	C27—C31—Rh3—C28	38.9 (3)
C47—C42—C43—C48	0.9 (9)	C36—C31—Rh3—C28	157.4 (7)
Rh4—C42—C43—C48	-118.6 (6)	C27—C31—Rh3—C30	119.9 (5)
C41—C42—C43—Rh4	-59.1 (4)	C36—C31—Rh3—C30	-121.6 (7)
C47—C42—C43—Rh4	119.4 (6)	C30—C31—Rh3—O9	-150.1 (3)
C42—C43—C44—C45	-0.2 (6)	C27—C31—Rh3—O9	-30.2 (5)
C48—C43—C44—C45	178.7 (5)	C36—C31—Rh3—O9	88.3 (6)
Rh4—C43—C44—C45	59.8 (4)	C30—C31—Rh3—O13	36.2 (4)
C42—C43—C44—C49	178.3 (5)	C27—C31—Rh3—O13	156.1 (3)
C48—C43—C44—C49	-2.8 (9)	C36—C31—Rh3—O13	-85.4 (6)
Rh4—C43—C44—C49	-121.6 (6)	C29—C28—Rh3—C27	119.7 (5)
C42—C43—C44—Rh4	-60.0 (4)	C33—C28—Rh3—C27	-119.4 (8)
C48—C43—C44—Rh4	118.9 (6)	C29—C28—Rh3—O8	146.2 (3)
C42—C41—C45—C44	1.6 (6)	C27—C28—Rh3—O8	26.5 (5)
C46—C41—C45—C44	177.8 (6)	C33—C28—Rh3—O8	-92.9 (7)
Rh4—C41—C45—C44	-60.7 (4)	C27—C28—Rh3—C29	-119.7 (5)
C42—C41—C45—C50	178.8 (6)	C33—C28—Rh3—C29	120.9 (8)
C46—C41—C45—C50	-5.0 (10)	C29—C28—Rh3—C31	80.9 (4)
Rh4—C41—C45—C50	116.5 (6)	C27—C28—Rh3—C31	-38.9 (3)
C42—C41—C45—Rh4	62.3 (4)	C33—C28—Rh3—C31	-158.3 (7)
C46—C41—C45—Rh4	-121.5 (6)	C29—C28—Rh3—C30	38.2 (4)
C43—C44—C45—C41	-0.8 (6)	C27—C28—Rh3—C30	-81.6 (4)
C49—C44—C45—C41	-179.4 (6)	C33—C28—Rh3—C30	159.0 (7)
Rh4—C44—C45—C41	59.6 (4)	C29—C28—Rh3—O9	-131.3 (3)
C43—C44—C45—C50	-178.1 (6)	C27—C28—Rh3—O9	109.0 (3)
C49—C44—C45—C50	3.3 (10)	C33—C28—Rh3—O9	-10.4 (7)
Rh4—C44—C45—C50	-117.7 (6)	C29—C28—Rh3—O13	-46.7 (4)
C43—C44—C45—Rh4	-60.4 (4)	C27—C28—Rh3—O13	-166.4 (3)
C49—C44—C45—Rh4	121.0 (6)	C33—C28—Rh3—O13	74.2 (7)
C55—C51—C52—C53	2.3 (6)	C31—C30—Rh3—C27	37.2 (3)
C56—C51—C52—C53	-179.3 (5)	C29—C30—Rh3—C27	-81.2 (4)
Rh5—C51—C52—C53	-58.7 (4)	C35—C30—Rh3—C27	157.8 (7)
C55—C51—C52—C57	178.4 (5)	C31—C30—Rh3—O8	-58.9 (4)
C56—C51—C52—C57	-3.2 (9)	C29—C30—Rh3—O8	-177.3 (3)
Rh5—C51—C52—C57	117.4 (6)	C35—C30—Rh3—O8	61.7 (7)
C55—C51—C52—Rh5	61.0 (4)	C31—C30—Rh3—C29	118.4 (5)
C56—C51—C52—Rh5	-120.6 (6)	C35—C30—Rh3—C29	-121.0 (8)
C51—C52—C53—C54	-3.3 (6)	C29—C30—Rh3—C31	-118.4 (5)
C57—C52—C53—C54	-179.5 (5)	C35—C30—Rh3—C31	120.6 (8)
Rh5—C52—C53—C54	-63.1 (3)	C31—C30—Rh3—C28	80.9 (4)
C51—C52—C53—C58	179.9 (5)	C29—C30—Rh3—C28	-37.5 (3)

C57—C52—C53—C58	3.8 (9)	C35—C30—Rh3—C28	-158.6 (7)
Rh5—C52—C53—C58	120.2 (6)	C31—C30—Rh3—O9	116.3 (6)
C51—C52—C53—Rh5	59.7 (4)	C29—C30—Rh3—O9	-2.1 (8)
C57—C52—C53—Rh5	-116.4 (6)	C35—C30—Rh3—O9	-123.1 (7)
C52—C53—C54—C55	3.1 (6)	C31—C30—Rh3—O13	-154.3 (3)
C58—C53—C54—C55	179.9 (5)	C29—C30—Rh3—O13	87.3 (4)
Rh5—C53—C54—C55	-59.5 (4)	C35—C30—Rh3—O13	-33.7 (7)
C52—C53—C54—C59	-178.4 (5)	C14—O9—Rh3—C27	-111.9 (4)
C58—C53—C54—C59	-1.6 (9)	C14—O9—Rh3—O8	-8.3 (3)
Rh5—C53—C54—C59	119.0 (5)	C14—O9—Rh3—C29	174.4 (3)
C52—C53—C54—Rh5	62.6 (4)	C14—O9—Rh3—C31	-92.0 (4)
C58—C53—C54—Rh5	-120.6 (5)	C14—O9—Rh3—C28	-151.7 (4)
C52—C51—C55—C54	-0.3 (6)	C14—O9—Rh3—C30	175.9 (6)
C56—C51—C55—C54	-178.8 (5)	C14—O9—Rh3—O13	83.4 (3)
Rh5—C51—C55—C54	60.3 (4)	S3—O13—Rh3—C27	128.8 (6)
C52—C51—C55—C60	178.6 (5)	S3—O13—Rh3—O8	-28.8 (3)
C56—C51—C55—C60	0.2 (9)	S3—O13—Rh3—C29	131.3 (3)
Rh5—C51—C55—C60	-120.8 (6)	S3—O13—Rh3—C31	69.4 (4)
C52—C51—C55—Rh5	-60.6 (4)	S3—O13—Rh3—C28	158.7 (3)
C56—C51—C55—Rh5	121.0 (6)	S3—O13—Rh3—C30	91.4 (3)
C53—C54—C55—C51	-1.7 (6)	S3—O13—Rh3—O9	-107.1 (3)
C59—C54—C55—C51	179.8 (5)	C42—C41—Rh4—C45	-116.8 (5)
Rh5—C54—C55—C51	-59.8 (4)	C46—C41—Rh4—C45	121.8 (7)
C53—C54—C55—C60	179.3 (5)	C45—C41—Rh4—C42	116.8 (5)
C59—C54—C55—C60	0.8 (9)	C46—C41—Rh4—C42	-121.4 (7)
Rh5—C54—C55—C60	121.2 (6)	C42—C41—Rh4—O16	160.9 (3)
C53—C54—C55—Rh5	58.1 (3)	C45—C41—Rh4—O16	-82.3 (4)
C59—C54—C55—Rh5	-120.4 (5)	C46—C41—Rh4—O16	39.5 (6)
O1 ⁱ —C1—O2—Rh1	172.8 (4)	C42—C41—Rh4—O17	78.6 (3)
C1 ⁱ —C1—O2—Rh1	-6.6 (7)	C45—C41—Rh4—O17	-164.6 (3)
O8—C13—O6—Rh2	179.7 (4)	C46—C41—Rh4—O17	-42.8 (6)
C14—C13—O6—Rh2	-1.9 (5)	C42—C41—Rh4—C44	-79.5 (4)
O9—C14—O7—Rh2	-170.2 (4)	C45—C41—Rh4—C44	37.3 (3)
C13—C14—O7—Rh2	9.6 (5)	C46—C41—Rh4—C44	159.1 (6)
O6—C13—O8—Rh3	177.8 (4)	C42—C41—Rh4—C43	-36.5 (3)
C14—C13—O8—Rh3	-0.6 (6)	C45—C41—Rh4—C43	80.3 (4)
O7—C14—O9—Rh3	-169.6 (4)	C46—C41—Rh4—C43	-157.9 (6)
C13—C14—O9—Rh3	10.5 (5)	C42—C41—Rh4—O20	-56.3 (9)
O18—C37—O16—Rh4	-175.2 (4)	C45—C41—Rh4—O20	60.5 (9)
C38—C37—O16—Rh4	4.8 (5)	C46—C41—Rh4—O20	-177.7 (6)
O19—C38—O17—Rh4	174.7 (4)	C44—C45—Rh4—C41	118.9 (5)
C37—C38—O17—Rh4	-4.3 (5)	C50—C45—Rh4—C41	-121.2 (8)
O16—C37—O18—Rh5	-179.6 (4)	C41—C45—Rh4—C42	-38.5 (3)
C38—C37—O18—Rh5	0.3 (5)	C44—C45—Rh4—C42	80.4 (4)
O17—C38—O19—Rh5	179.8 (4)	C50—C45—Rh4—C42	-159.8 (7)
C37—C38—O19—Rh5	-1.2 (5)	C41—C45—Rh4—O16	105.4 (3)
Rh1—O3—S1—O4	-99.5 (3)	C44—C45—Rh4—O16	-135.7 (3)
Rh1—O3—S1—O5	38.2 (4)	C50—C45—Rh4—O16	-15.9 (7)

supplementary materials

Rh1—O3—S1—C2	149.3 (3)	C41—C45—Rh4—O17	26.4 (5)
F1—C2—S1—O4	-55.1 (6)	C44—C45—Rh4—O17	145.3 (3)
F2—C2—S1—O4	-177.0 (5)	C50—C45—Rh4—O17	-94.8 (7)
F3—C2—S1—O4	65.2 (5)	C41—C45—Rh4—C44	-118.9 (5)
F1—C2—S1—O5	-178.3 (5)	C50—C45—Rh4—C44	119.9 (8)
F2—C2—S1—O5	59.9 (5)	C41—C45—Rh4—C43	-81.3 (4)
F3—C2—S1—O5	-57.9 (5)	C44—C45—Rh4—C43	37.6 (3)
F1—C2—S1—O3	63.4 (5)	C50—C45—Rh4—C43	157.4 (7)
F2—C2—S1—O3	-58.4 (5)	C41—C45—Rh4—O20	-163.2 (3)
F3—C2—S1—O3	-176.2 (5)	C44—C45—Rh4—O20	-44.3 (4)
Rh2—O10—S2—O12	95.4 (3)	C50—C45—Rh4—O20	75.5 (7)
Rh2—O10—S2—O11	-42.2 (4)	C43—C42—Rh4—C41	-119.9 (5)
Rh2—O10—S2—C15	-153.3 (3)	C47—C42—Rh4—C41	118.9 (6)
F6—C15—S2—O12	-66.8 (5)	C43—C42—Rh4—C45	-81.2 (4)
F4—C15—S2—O12	53.1 (5)	C41—C42—Rh4—C45	38.7 (4)
F5—C15—S2—O12	173.5 (5)	C47—C42—Rh4—C45	157.7 (6)
F6—C15—S2—O11	56.2 (5)	C43—C42—Rh4—O16	-150.2 (3)
F4—C15—S2—O11	176.2 (5)	C41—C42—Rh4—O16	-30.3 (5)
F5—C15—S2—O11	-63.4 (5)	C47—C42—Rh4—O16	88.6 (6)
F6—C15—S2—O10	174.5 (4)	C43—C42—Rh4—O17	130.0 (3)
F4—C15—S2—O10	-65.6 (5)	C41—C42—Rh4—O17	-110.1 (3)
F5—C15—S2—O10	54.8 (5)	C47—C42—Rh4—O17	8.8 (5)
Rh3—O13—S3—O14	90.4 (4)	C43—C42—Rh4—C44	-37.8 (3)
Rh3—O13—S3—O15	-49.1 (4)	C41—C42—Rh4—C44	82.2 (4)
Rh3—O13—S3—C16	-158.7 (3)	C47—C42—Rh4—C44	-158.9 (6)
F8—C16—S3—O13	-176.8 (6)	C41—C42—Rh4—C43	119.9 (5)
F9—C16—S3—O13	63.2 (6)	C47—C42—Rh4—C43	-121.2 (6)
F7—C16—S3—O13	-57.1 (5)	C43—C42—Rh4—O20	44.2 (4)
F8—C16—S3—O14	-58.4 (7)	C41—C42—Rh4—O20	164.1 (3)
F9—C16—S3—O14	-178.5 (5)	C47—C42—Rh4—O20	-77.0 (5)
F7—C16—S3—O14	61.2 (6)	C37—O16—Rh4—C41	-111.0 (4)
F8—C16—S3—O15	65.5 (6)	C37—O16—Rh4—C45	-150.6 (4)
F9—C16—S3—O15	-54.5 (6)	C37—O16—Rh4—C42	-91.6 (4)
F7—C16—S3—O15	-174.9 (5)	C37—O16—Rh4—O17	-5.3 (3)
Rh4—O20—S4—O21	-107.9 (3)	C37—O16—Rh4—C44	177.6 (3)
Rh4—O20—S4—O22	30.5 (4)	C37—O16—Rh4—C43	-170.2 (6)
Rh4—O20—S4—C39	141.8 (3)	C37—O16—Rh4—O20	77.6 (3)
F10—C39—S4—O21	-175.2 (4)	C38—O17—Rh4—C41	107.1 (4)
F12—C39—S4—O21	65.4 (5)	C38—O17—Rh4—C45	89.7 (5)
F11—C39—S4—O21	-54.5 (5)	C38—O17—Rh4—C42	146.1 (4)
F10—C39—S4—O22	61.8 (5)	C38—O17—Rh4—O16	5.1 (3)
F12—C39—S4—O22	-57.6 (5)	C38—O17—Rh4—C44	178.4 (5)
F11—C39—S4—O22	-177.5 (5)	C38—O17—Rh4—C43	179.6 (3)
F10—C39—S4—O20	-57.4 (5)	C38—O17—Rh4—O20	-83.0 (3)
F12—C39—S4—O20	-176.8 (4)	C45—C44—Rh4—C41	-37.6 (4)
F11—C39—S4—O20	63.3 (5)	C43—C44—Rh4—C41	80.8 (4)
Rh5—O23—S5—O24	88.3 (4)	C49—C44—Rh4—C41	-159.0 (7)
Rh5—O23—S5—O25	-49.8 (4)	C43—C44—Rh4—C45	118.4 (5)
Rh5—O23—S5—C40	-160.5 (3)	C49—C44—Rh4—C45	-121.4 (8)

F14—C40—S5—O24	54.7 (6)	C45—C44—Rh4—C42	-81.0 (4)
F15—C40—S5—O24	176.7 (5)	C43—C44—Rh4—C42	37.4 (3)
F13—C40—S5—O24	-65.8 (5)	C49—C44—Rh4—C42	157.6 (7)
F14—C40—S5—O25	178.6 (5)	C45—C44—Rh4—O16	55.5 (4)
F15—C40—S5—O25	-59.4 (5)	C43—C44—Rh4—O16	173.9 (3)
F13—C40—S5—O25	58.1 (5)	C49—C44—Rh4—O16	-65.9 (7)
F14—C40—S5—O23	-62.9 (5)	C45—C44—Rh4—O17	-116.7 (6)
F15—C40—S5—O23	59.1 (5)	C43—C44—Rh4—O17	1.7 (7)
F13—C40—S5—O23	176.6 (4)	C49—C44—Rh4—O17	121.9 (6)
C6—C5—Rh1—O2	-166.2 (3)	C45—C44—Rh4—C43	-118.4 (5)
C4—C5—Rh1—O2	76.2 (3)	C49—C44—Rh4—C43	120.2 (8)
C10—C5—Rh1—O2	-43.5 (6)	C45—C44—Rh4—O20	148.1 (3)
C6—C5—Rh1—O1	-82.9 (3)	C43—C44—Rh4—O20	-93.5 (3)
C4—C5—Rh1—O1	159.5 (3)	C49—C44—Rh4—O20	26.6 (6)
C10—C5—Rh1—O1	39.7 (6)	C42—C43—Rh4—C41	37.0 (3)
C4—C5—Rh1—C6	-117.6 (5)	C44—C43—Rh4—C41	-81.3 (4)
C10—C5—Rh1—C6	122.6 (7)	C48—C43—Rh4—C41	159.0 (6)
C6—C5—Rh1—C4	117.6 (5)	C42—C43—Rh4—C45	80.7 (4)
C10—C5—Rh1—C4	-119.7 (7)	C44—C43—Rh4—C45	-37.7 (4)
C6—C5—Rh1—C3	80.9 (4)	C48—C43—Rh4—C45	-157.4 (6)
C4—C5—Rh1—C3	-36.8 (3)	C44—C43—Rh4—C42	-118.3 (5)
C10—C5—Rh1—C3	-156.5 (6)	C48—C43—Rh4—C42	121.9 (7)
C6—C5—Rh1—C7	37.0 (3)	C42—C43—Rh4—O16	102.0 (6)
C4—C5—Rh1—C7	-80.6 (3)	C44—C43—Rh4—O16	-16.3 (8)
C10—C5—Rh1—C7	159.7 (6)	C48—C43—Rh4—O16	-136.1 (6)
C6—C5—Rh1—O3	66.3 (8)	C42—C43—Rh4—O17	-60.9 (4)
C4—C5—Rh1—O3	-51.3 (8)	C44—C43—Rh4—O17	-179.3 (3)
C10—C5—Rh1—O3	-171.0 (5)	C48—C43—Rh4—O17	61.0 (6)
C1—O2—Rh1—C5	112.4 (4)	C42—C43—Rh4—C44	118.3 (5)
C1—O2—Rh1—O1	7.8 (3)	C48—C43—Rh4—C44	-119.7 (7)
C1—O2—Rh1—C6	96.5 (4)	C42—C43—Rh4—O20	-147.9 (3)
C1—O2—Rh1—C4	151.1 (4)	C44—C43—Rh4—O20	93.8 (3)
C1—O2—Rh1—C3	-174.5 (3)	C48—C43—Rh4—O20	-25.9 (5)
C1—O2—Rh1—C7	-173.4 (5)	S4—O20—Rh4—C41	-98.9 (8)
C1—O2—Rh1—O3	-80.8 (3)	S4—O20—Rh4—C45	-50.5 (4)
C1 ⁱ —O1—Rh1—C5	-114.5 (4)	S4—O20—Rh4—C42	-143.7 (3)
C1 ⁱ —O1—Rh1—O2	-8.1 (3)	S4—O20—Rh4—O16	45.3 (3)
C1 ⁱ —O1—Rh1—C6	-154.1 (4)	S4—O20—Rh4—O17	124.0 (3)
C1 ⁱ —O1—Rh1—C4	-92.5 (4)	S4—O20—Rh4—C44	-77.3 (3)
C1 ⁱ —O1—Rh1—C3	179.5 (6)	S4—O20—Rh4—C43	-117.3 (3)
C1 ⁱ —O1—Rh1—C7	172.5 (4)	C54—C53—Rh5—C52	116.8 (4)
C1 ⁱ —O1—Rh1—O3	73.9 (4)	C58—C53—Rh5—C52	-122.1 (6)
C7—C6—Rh1—C5	119.6 (5)	C52—C53—Rh5—C51	-36.8 (3)
C11—C6—Rh1—C5	-121.2 (7)	C54—C53—Rh5—C51	80.0 (3)
C5—C6—Rh1—O2	24.2 (5)	C58—C53—Rh5—C51	-158.9 (6)
C7—C6—Rh1—O2	143.8 (3)	C52—C53—Rh5—O18	162.1 (3)
C11—C6—Rh1—O2	-97.0 (6)	C54—C53—Rh5—O18	-81.1 (3)

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C5—C6—Rh1—O1	106.5 (3)	C58—C53—Rh5—O18	40.0 (5)
C7—C6—Rh1—O1	-133.9 (3)	C52—C53—Rh5—C54	-116.8 (4)
C11—C6—Rh1—O1	-14.6 (6)	C58—C53—Rh5—C54	121.1 (6)
C5—C6—Rh1—C4	-38.3 (3)	C52—C53—Rh5—C55	-79.9 (3)
C7—C6—Rh1—C4	81.3 (3)	C54—C53—Rh5—C55	36.9 (3)
C11—C6—Rh1—C4	-159.5 (6)	C58—C53—Rh5—C55	158.0 (6)
C5—C6—Rh1—C3	-81.3 (3)	C52—C53—Rh5—O19	80.6 (3)
C7—C6—Rh1—C3	38.3 (3)	C54—C53—Rh5—O19	-162.6 (3)
C11—C6—Rh1—C3	157.5 (6)	C58—C53—Rh5—O19	-41.5 (5)
C5—C6—Rh1—C7	-119.6 (5)	C52—C53—Rh5—O23	-63.1 (8)
C11—C6—Rh1—C7	119.3 (7)	C54—C53—Rh5—O23	53.7 (8)
C5—C6—Rh1—O3	-159.5 (3)	C58—C53—Rh5—O23	174.8 (6)
C7—C6—Rh1—O3	-39.9 (4)	C51—C52—Rh5—C53	-119.3 (4)
C11—C6—Rh1—O3	79.4 (6)	C57—C52—Rh5—C53	119.9 (7)
C3—C4—Rh1—C5	-119.7 (4)	C53—C52—Rh5—C51	119.3 (4)
C9—C4—Rh1—C5	118.3 (6)	C57—C52—Rh5—C51	-120.8 (7)
C3—C4—Rh1—O2	127.8 (3)	C51—C52—Rh5—O18	-149.4 (3)
C5—C4—Rh1—O2	-112.5 (3)	C53—C52—Rh5—O18	-30.1 (5)
C9—C4—Rh1—O2	5.8 (5)	C57—C52—Rh5—O18	89.7 (6)
C3—C4—Rh1—O1	-153.7 (3)	C51—C52—Rh5—C54	-80.7 (3)
C5—C4—Rh1—O1	-34.0 (4)	C53—C52—Rh5—C54	38.7 (3)
C9—C4—Rh1—O1	84.3 (5)	C57—C52—Rh5—C54	158.5 (6)
C3—C4—Rh1—C6	-81.7 (3)	C51—C52—Rh5—C55	-37.5 (3)
C5—C4—Rh1—C6	38.0 (3)	C53—C52—Rh5—C55	81.8 (3)
C9—C4—Rh1—C6	156.3 (5)	C57—C52—Rh5—C55	-158.3 (6)
C5—C4—Rh1—C3	119.7 (4)	C51—C52—Rh5—O19	134.8 (3)
C9—C4—Rh1—C3	-122.0 (6)	C53—C52—Rh5—O19	-105.9 (3)
C3—C4—Rh1—C7	-38.4 (3)	C57—C52—Rh5—O19	14.0 (5)
C5—C4—Rh1—C7	81.3 (3)	C51—C52—Rh5—O23	42.4 (4)
C9—C4—Rh1—C7	-160.4 (5)	C53—C52—Rh5—O23	161.7 (3)
C3—C4—Rh1—O3	43.8 (4)	C57—C52—Rh5—O23	-78.4 (6)
C5—C4—Rh1—O3	163.5 (3)	C52—C51—Rh5—C53	37.6 (3)
C9—C4—Rh1—O3	-78.2 (5)	C55—C51—Rh5—C53	-81.2 (3)
C4—C3—Rh1—C5	37.2 (3)	C56—C51—Rh5—C53	158.9 (6)
C8—C3—Rh1—C5	159.3 (6)	C55—C51—Rh5—C52	-118.8 (5)
C7—C3—Rh1—C5	-80.8 (3)	C56—C51—Rh5—C52	121.3 (7)
C4—C3—Rh1—O2	-62.7 (3)	C52—C51—Rh5—O18	112.1 (6)
C8—C3—Rh1—O2	59.4 (5)	C55—C51—Rh5—O18	-6.6 (7)
C7—C3—Rh1—O2	179.3 (3)	C56—C51—Rh5—O18	-126.5 (6)
C4—C3—Rh1—O1	108.9 (6)	C52—C51—Rh5—C54	81.3 (3)
C8—C3—Rh1—O1	-129.0 (6)	C55—C51—Rh5—C54	-37.5 (3)
C7—C3—Rh1—O1	-9.0 (8)	C56—C51—Rh5—C54	-157.4 (6)
C4—C3—Rh1—C6	80.3 (3)	C52—C51—Rh5—C55	118.8 (5)
C8—C3—Rh1—C6	-157.6 (6)	C56—C51—Rh5—C55	-119.9 (7)
C7—C3—Rh1—C6	-37.7 (3)	C52—C51—Rh5—O19	-55.0 (4)
C8—C3—Rh1—C4	122.1 (6)	C55—C51—Rh5—O19	-173.8 (3)
C7—C3—Rh1—C4	-118.0 (5)	C56—C51—Rh5—O19	66.3 (6)
C4—C3—Rh1—C7	118.0 (5)	C52—C51—Rh5—O23	-149.2 (3)
C8—C3—Rh1—C7	-119.9 (6)	C55—C51—Rh5—O23	92.0 (3)

C4—C3—Rh1—O3	-146.9 (3)	C56—C51—Rh5—O23	-27.9 (6)
C8—C3—Rh1—O3	-24.8 (5)	C37—O18—Rh5—C53	-101.4 (4)
C7—C3—Rh1—O3	95.1 (3)	C37—O18—Rh5—C52	-81.7 (4)
C6—C7—Rh1—C5	-37.0 (3)	C37—O18—Rh5—C51	-169.4 (5)
C3—C7—Rh1—C5	81.1 (3)	C37—O18—Rh5—C54	-141.1 (4)
C12—C7—Rh1—C5	-158.4 (7)	C37—O18—Rh5—C55	-174.3 (3)
C6—C7—Rh1—O2	-119.7 (5)	C37—O18—Rh5—O19	-0.7 (3)
C3—C7—Rh1—O2	-1.6 (7)	C37—O18—Rh5—O23	89.4 (3)
C12—C7—Rh1—O2	118.9 (6)	C55—C54—Rh5—C53	119.4 (4)
C6—C7—Rh1—O1	58.9 (4)	C59—C54—Rh5—C53	-119.4 (6)
C3—C7—Rh1—O1	177.0 (3)	C55—C54—Rh5—C52	80.6 (3)
C12—C7—Rh1—O1	-62.6 (7)	C53—C54—Rh5—C52	-38.8 (3)
C3—C7—Rh1—C6	118.1 (5)	C59—C54—Rh5—C52	-158.2 (6)
C12—C7—Rh1—C6	-121.4 (7)	C55—C54—Rh5—C51	37.6 (3)
C6—C7—Rh1—C4	-80.5 (3)	C53—C54—Rh5—C51	-81.8 (3)
C3—C7—Rh1—C4	37.6 (3)	C59—C54—Rh5—C51	158.8 (6)
C12—C7—Rh1—C4	158.1 (7)	C55—C54—Rh5—O18	-132.8 (3)
C6—C7—Rh1—C3	-118.1 (5)	C53—C54—Rh5—O18	107.8 (3)
C12—C7—Rh1—C3	120.5 (7)	C59—C54—Rh5—O18	-11.6 (5)
C6—C7—Rh1—O3	151.1 (3)	C53—C54—Rh5—C55	-119.4 (4)
C3—C7—Rh1—O3	-90.8 (3)	C59—C54—Rh5—C55	121.2 (6)
C12—C7—Rh1—O3	29.7 (6)	C55—C54—Rh5—O19	146.7 (3)
S1—O3—Rh1—C5	-109.6 (7)	C53—C54—Rh5—O19	27.3 (4)
S1—O3—Rh1—O2	119.7 (3)	C59—C54—Rh5—O19	-92.0 (5)
S1—O3—Rh1—O1	41.1 (3)	C55—C54—Rh5—O23	-44.6 (4)
S1—O3—Rh1—C6	-58.3 (4)	C53—C54—Rh5—O23	-164.0 (3)
S1—O3—Rh1—C4	-149.3 (3)	C59—C54—Rh5—O23	76.7 (5)
S1—O3—Rh1—C3	-123.1 (3)	C51—C55—Rh5—C53	81.1 (3)
S1—O3—Rh1—C7	-82.6 (3)	C54—C55—Rh5—C53	-37.4 (3)
C18—C17—Rh2—C21	117.3 (5)	C60—C55—Rh5—C53	-158.7 (6)
C22—C17—Rh2—C21	-121.3 (7)	C51—C55—Rh5—C52	37.3 (3)
C21—C17—Rh2—C20	-36.7 (3)	C54—C55—Rh5—C52	-81.2 (3)
C18—C17—Rh2—C20	80.6 (4)	C60—C55—Rh5—C52	157.5 (6)
C22—C17—Rh2—C20	-158.0 (6)	C54—C55—Rh5—C51	-118.5 (5)
C21—C17—Rh2—O6	63.3 (4)	C60—C55—Rh5—C51	120.2 (7)
C18—C17—Rh2—O6	-179.5 (3)	C51—C55—Rh5—O18	177.5 (3)
C22—C17—Rh2—O6	-58.0 (6)	C54—C55—Rh5—O18	59.0 (4)
C21—C17—Rh2—C18	-117.3 (5)	C60—C55—Rh5—O18	-62.3 (6)
C22—C17—Rh2—C18	121.4 (7)	C51—C55—Rh5—C54	118.5 (5)
C21—C17—Rh2—C19	-79.8 (4)	C60—C55—Rh5—C54	-121.2 (7)
C18—C17—Rh2—C19	37.5 (3)	C51—C55—Rh5—O19	15.2 (7)
C22—C17—Rh2—C19	158.9 (7)	C54—C55—Rh5—O19	-103.3 (5)
C21—C17—Rh2—O7	145.9 (3)	C60—C55—Rh5—O19	135.4 (5)
C18—C17—Rh2—O7	-96.9 (3)	C51—C55—Rh5—O23	-94.5 (3)
C22—C17—Rh2—O7	24.6 (6)	C54—C55—Rh5—O23	147.0 (3)
C21—C17—Rh2—O10	-123.1 (5)	C60—C55—Rh5—O23	25.7 (6)
C18—C17—Rh2—O10	-5.8 (7)	C38—O19—Rh5—C53	106.1 (4)
C22—C17—Rh2—O10	115.6 (6)	C38—O19—Rh5—C52	145.6 (4)
C20—C21—Rh2—C17	-120.1 (5)	C38—O19—Rh5—C51	176.8 (3)

supplementary materials

C26—C21—Rh2—C17	118.5 (7)	C38—O19—Rh5—O18	1.0 (3)
C17—C21—Rh2—C20	120.1 (5)	C38—O19—Rh5—C54	88.5 (4)
C26—C21—Rh2—C20	-121.4 (7)	C38—O19—Rh5—C55	165.7 (5)
C17—C21—Rh2—O6	-126.7 (3)	C38—O19—Rh5—O23	-82.9 (3)
C20—C21—Rh2—O6	113.2 (3)	S5—O23—Rh5—C53	116.5 (7)
C26—C21—Rh2—O6	-8.2 (6)	S5—O23—Rh5—C52	66.5 (4)
C17—C21—Rh2—C18	38.5 (3)	S5—O23—Rh5—C51	92.1 (3)
C20—C21—Rh2—C18	-81.6 (4)	S5—O23—Rh5—O18	-106.5 (3)
C26—C21—Rh2—C18	156.9 (6)	S5—O23—Rh5—C54	158.7 (3)
C17—C21—Rh2—C19	81.6 (4)	S5—O23—Rh5—C55	132.0 (3)
C20—C21—Rh2—C19	-38.5 (3)	S5—O23—Rh5—O19	-28.4 (3)

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

Fig. 1

