

{2-[Bis(2,4-di-*tert*-butylphenoxy)phosphanyloxy- κ P]-3,5-di-*tert*-butylphenyl- κ C¹]{3,3'-di-*tert*-butyl-5,5'-dimethoxy-2,2'-bis[(1,1,2,2-tetraphenylethane-1,2-dioxy)phosphanyloxy- κ P]biphenyl}rhodium(I) toluene-*d*₈ 2.7-solvate

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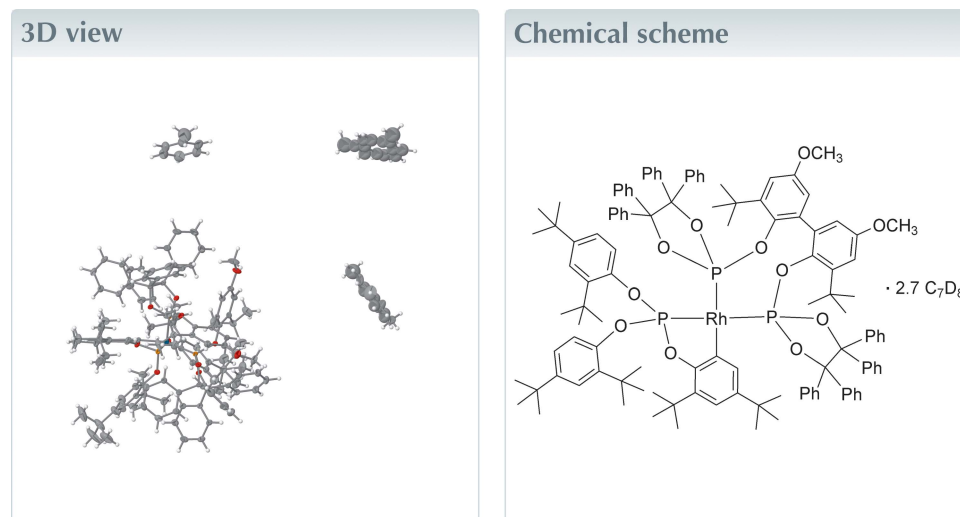
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Structural data: full structural data are available from iucrdata.iucr.org

The molecule of the title compound, [Rh(C₄₂H₆₂O₃P)(C₇₄H₆₈O₄P₂)·2.7C₇D₈], consists of two phospharhodacyclic substructures sharing the Rh atom, which are formed by coordination/*ortho*-metallation of a triaryl phosphite, and by the coordination of a rigid bisphosphite, respectively. The metal displays a tetrahedrally distorted square-planar coordination geometry. A *tert*-butyl group shows rotational disorder over two positions with refined site occupancy of 0.561 (3):0.439 (3). Two partial-occupancy toluene solvent molecules are disordered over two orientations with site occupancies of 0.5:0.3 and 0.5:0.4, respectively. Intramolecular C—H···O hydrogen bonds are observed. In the crystal, complex molecules and toluene solvent molecules pack as alternating layers parallel to the *ac* plane.



Structure description

The title compound was formed as a product of cyclooctadiene-1.5 substitution by the reaction of {2-[bis(2,4-di-*tert*-butylphenoxy)phosphinoxy- κ P]-3,5-di-*tert*-butylphenyl- κ C¹}(1,2,5,6- η)-cycloocta-1,5-diene}rhodium(I) with the bisphosphite 2,2'-[(3,3'-di-*tert*-butyl-5,5'-dimethoxy-[1,1'-biphenyl]-2,2'-diyl)bis(oxy)]bis(4,4,5,5-tetraphenyl-1,3,2-dioxaphospholane).

The coordination geometry around the rhodium atom (Fig. 1) can be described as square planar with a pronounced tetrahedral distortion, resulting in angles P1—Rh1—P2 = 102.172 (18)°, P1—Rh1—P3 = 143.592 (18)°, P1—Rh1—C2 = 77.71 (5)°, P2—Rh1—P3 = 100.696 (18)°, P2—Rh1—C2 = 159.49 (6)° and P3—Rh1—C2 = 90.23 (5)°. This should be induced by steric congestion of the molecule. In the title compound, an Rh1—C2 distance

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>
C30—H30···O4	0.95	2.35	3.234 (2)	155
C46—H46···O2	0.95	2.52	3.405 (2)	155
C56—H56···O5	0.95	2.56	3.136 (3)	120

of 2.070 (2) Å and an angle P1—Rh1—C2 of 77.71 (5)° are observed [for comparison, values of 2.0771 (14) Å and 79.14 (4)°, respectively, were determined for the starting rhodium complex (Selent *et al.*, 2012*a*)]. The coordination of the bisphosphite is characterized by an angle P2—Rh1—P3 of 100.696 (18)°, which is significantly smaller compared to the values determined for complexes containing the same ligand [104.49 (2)° in the π-allyl rhodium(I) bisphosphite complex (Selent *et al.*, 2011); 109.662 (19)° in the hydrido rhodium bisphosphite dicarbonyl complex (Selent *et al.*, 2012*b*); 117.18 (2) and 117.99 (2)° in the hydrido rhodium bisphosphite triphenylphosphine monocarbonyl complex (Selent *et al.*, 2013)]. No exceptional values were found for Rh—P distances. Weak intramolecular C—H···O hydrogen bonds are observed (Table 1).

The crystal is built up by layers oriented parallel to the *ac* plane with the solvent molecules arranged between the layers.

Synthesis and crystallization

A mixture of {2-[bis(2,4-di-*tert*-butylphenoxy)phosphinoxy-*κ*P]-3,5-di-*tert*-butylphenyl-*κ*C¹][(1,2,5,6-*η*)-cycloocta-1,5-di-

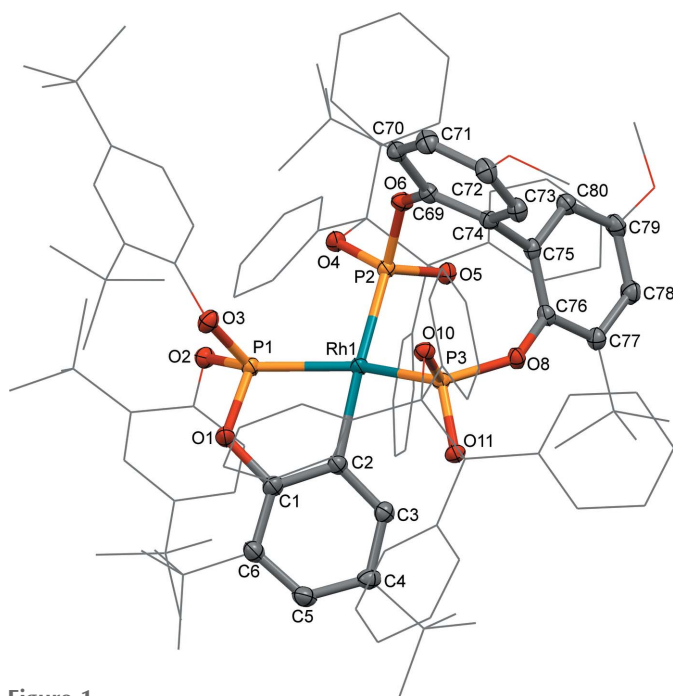


Figure 1
The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level for the central motif. All other parts of the molecule are shown as wireframe. H atoms and solvent molecules have been omitted for clarity.

Table 2
Experimental details.

Crystal data	
Chemical formula	[Rh(C ₄₂ H ₆₂ O ₃ P)(C ₇₄ H ₆₈ O ₄ P ₂)]·2.7C ₇ D ₈
<i>M_r</i>	2144.77
Crystal system, space group	Monoclinic, <i>P</i> ₂ / <i>n</i>
Temperature (K)	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	15.4222 (5), 27.9355 (9), 26.9314 (9)
β (°)	93.4633 (13)
<i>V</i> (Å ³)	11581.6 (7)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.25
Crystal size (mm)	0.32 × 0.21 × 0.15
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2014)
<i>T_{min}</i> , <i>T_{max}</i>	0.93, 0.96
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	272267, 27950, 23070
<i>R_{int}</i> (sin θ/λ) _{max} (Å ⁻¹)	0.049, 0.661
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.043, 0.120, 1.03
No. of reflections	27950
No. of parameters	1372
No. of restraints	63
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	1.35, -0.63

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2006), *pubCIF* (Westrip, 2010) and *PLATON* (Spek, 2009).

ene]rhodium(I) (0.2373 g, 0.25 mmol) and 2,2'-(3,3'-di-*tert*-butyl-5,5'-dimethoxy-[1,1'-biphenyl]-2,2'-diyl)bis(oxy)]bis(4,4-, 5,5-tetraphenyl-1,3,2-dioxaphospholane) (0.2868 g, 0.25 mmol) was reacted in toluene (15 ml) under an atmosphere of carbon monoxide at 373 K for 7 h. The pure title compound was obtained by column chromatography (dichloromethane/hexane). Orange crystals were grown by slowly evaporating a solution of the title compound in deuterated toluene at room temperature.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystals of the title compound contain deuterated toluene molecules, some of them are disordered over two sites with occupancies 0.5(C117–C123):0.3(C217–C223) and 0.5(C131–C137):0.4(C231–C237). The C atoms of the toluene rings were constrained to resemble an ideal hexagon, with C–C distances of 1.39 Å. Additionally, DFIX, DANG and FLAT instructions were used to improve the geometry of the disordered solvent (concerning the CH₃ group). Furthermore, the isotropic displacement parameters of C131–C136, C231–C236 and C217–C222 were restrained to be equal (EADP). One *tert*-butyl group is disordered over two orientations, with

occupancies 0.561 (3):0.439 (3). SADI and SIMU instructions were also applied to this group.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161914 [https://doi.org/10.1107/S2414314616019143]

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Crystal data

[Rh(C₄₂H₆₂O₃P)(C₇₄H₆₈O₄P₂)]·2.7C₇D₈

M_r = 2144.77

Monoclinic, *P*2₁/*n*

a = 15.4222 (5) Å

b = 27.9355 (9) Å

c = 26.9314 (9) Å

β = 93.4633 (13)°

V = 11581.6 (7) Å³

Z = 4

F(000) = 4556

D_x = 1.230 Mg m⁻³

Mo *K* α radiation, λ = 0.71073 Å

Cell parameters from 9302 reflections

θ = 2.6–29.9°

μ = 0.25 mm⁻¹

T = 150 K

Prism, yellow

0.32 × 0.21 × 0.15 mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Detector resolution: 8.3333 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2014)

T_{min} = 0.93, *T_{max}* = 0.96

272267 measured reflections

27950 independent reflections

23070 reflections with *I* > 2 σ (*I*)

R_{int} = 0.049

θ_{\max} = 28.0°, θ_{\min} = 1.5°

h = -20→20

k = -36→36

l = -27→35

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2 σ (*F*²)] = 0.043

wR(*F*²) = 0.120

S = 1.03

27950 reflections

1372 parameters

63 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

w = 1/[$\sigma^2(F_o^2) + (0.0583P)^2 + 12.212P$]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ / σ)_{max} = 0.002

$\Delta\rho_{\max}$ = 1.35 e Å⁻³

$\Delta\rho_{\min}$ = -0.63 e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.13209 (12)	0.81224 (7)	0.15459 (7)	0.0207 (4)	
C2	0.14570 (12)	0.81273 (7)	0.20656 (7)	0.0185 (4)	
C3	0.20134 (12)	0.84792 (7)	0.22661 (7)	0.0198 (4)	
H3	0.2095	0.8505	0.2618	0.024*	
C4	0.24563 (13)	0.87957 (7)	0.19701 (8)	0.0222 (4)	
C5	0.23218 (13)	0.87541 (8)	0.14565 (8)	0.0243 (4)	
H5	0.2637	0.8960	0.1252	0.029*	
C6	0.17466 (13)	0.84241 (8)	0.12244 (7)	0.0226 (4)	
C7	0.30804 (14)	0.91634 (8)	0.22223 (9)	0.0271 (4)	
C8	0.38010 (15)	0.89088 (9)	0.25401 (10)	0.0339 (5)	
H8A	0.4165	0.8724	0.2324	0.051*	
H8B	0.3539	0.8693	0.2776	0.051*	
H8C	0.4159	0.9147	0.2724	0.051*	
C9	0.35108 (18)	0.94789 (9)	0.18443 (10)	0.0411 (6)	
H9A	0.3863	0.9279	0.1635	0.062*	
H9B	0.3884	0.9716	0.2020	0.062*	
H9C	0.3062	0.9644	0.1635	0.062*	
C10	0.25640 (16)	0.94817 (8)	0.25620 (10)	0.0347 (5)	
H10A	0.2940	0.9738	0.2700	0.052*	
H10B	0.2353	0.9288	0.2834	0.052*	
H10C	0.2068	0.9622	0.2369	0.052*	
C11	0.16044 (14)	0.84100 (9)	0.06530 (8)	0.0278 (5)	
C12	0.22049 (18)	0.87644 (10)	0.04039 (9)	0.0401 (6)	
H12A	0.2812	0.8685	0.0497	0.060*	
H12B	0.2081	0.9090	0.0514	0.060*	
H12C	0.2104	0.8744	0.0042	0.060*	
C13	0.06675 (17)	0.85474 (13)	0.04954 (9)	0.0466 (7)	
H13A	0.0594	0.8555	0.0131	0.070*	
H13B	0.0539	0.8864	0.0629	0.070*	
H13C	0.0270	0.8311	0.0625	0.070*	
C14	0.17988 (18)	0.79117 (10)	0.04541 (9)	0.0385 (6)	
H14A	0.1392	0.7680	0.0583	0.058*	
H14B	0.2395	0.7821	0.0562	0.058*	
H14C	0.1735	0.7915	0.0090	0.058*	
C15	-0.09591 (12)	0.83515 (7)	0.13700 (7)	0.0202 (4)	
C16	-0.05154 (14)	0.87073 (8)	0.16336 (8)	0.0256 (4)	
H16	-0.0152	0.8628	0.1919	0.031*	
C17	-0.05978 (16)	0.91773 (9)	0.14840 (9)	0.0327 (5)	
H17	-0.0287	0.9419	0.1668	0.039*	

C18	-0.11262 (17)	0.93035 (8)	0.10710 (9)	0.0343 (5)	
C19	-0.15664 (15)	0.89345 (8)	0.08139 (8)	0.0287 (5)	
H19	-0.1932	0.9017	0.0530	0.034*	
C20	-0.15036 (13)	0.84519 (7)	0.09465 (7)	0.0212 (4)	
C21	-0.1208 (2)	0.98314 (10)	0.09158 (11)	0.0537 (8)	
C22	-0.0308 (3)	1.00205 (13)	0.07983 (14)	0.0778 (13)	
H22A	-0.0350	1.0361	0.0715	0.117*	
H22B	-0.0097	0.9843	0.0516	0.117*	
H22C	0.0097	0.9977	0.1089	0.117*	
C23	-0.1823 (3)	0.98995 (11)	0.04556 (15)	0.0896 (16)	
H23A	-0.2391	0.9760	0.0516	0.134*	
H23B	-0.1583	0.9740	0.0170	0.134*	
H23C	-0.1892	1.0242	0.0385	0.134*	
C24	-0.1545 (3)	1.01198 (11)	0.13430 (14)	0.0715 (11)	
H24A	-0.1576	1.0459	0.1250	0.107*	
H24B	-0.1150	1.0081	0.1639	0.107*	
H24C	-0.2125	1.0006	0.1414	0.107*	
C25	-0.20221 (13)	0.80670 (7)	0.06477 (8)	0.0226 (4)	
C26	-0.24855 (15)	0.82725 (9)	0.01742 (8)	0.0311 (5)	
H26A	-0.2795	0.8015	-0.0010	0.047*	
H26B	-0.2056	0.8416	-0.0035	0.047*	
H26C	-0.2901	0.8518	0.0265	0.047*	
C27	-0.27135 (15)	0.78561 (9)	0.09689 (9)	0.0319 (5)	
H27A	-0.3113	0.8110	0.1060	0.048*	
H27B	-0.2432	0.7716	0.1271	0.048*	
H27C	-0.3039	0.7607	0.0781	0.048*	
C28	-0.14259 (15)	0.76688 (8)	0.04752 (8)	0.0291 (5)	
H28A	-0.1772	0.7432	0.0281	0.044*	
H28B	-0.1136	0.7513	0.0766	0.044*	
H28C	-0.0988	0.7807	0.0268	0.044*	
C29	-0.09706 (12)	0.68532 (7)	0.14892 (7)	0.0195 (4)	
C30	-0.16350 (13)	0.69719 (7)	0.17888 (7)	0.0222 (4)	
H30	-0.1558	0.7227	0.2020	0.027*	
C31	-0.24102 (13)	0.67232 (8)	0.17552 (8)	0.0245 (4)	
H31	-0.2858	0.6808	0.1966	0.029*	
C32	-0.25446 (13)	0.63507 (8)	0.14173 (8)	0.0248 (4)	
C33	-0.18576 (14)	0.62370 (8)	0.11243 (8)	0.0255 (4)	
H33	-0.1941	0.5983	0.0892	0.031*	
C34	-0.10546 (13)	0.64717 (7)	0.11501 (7)	0.0227 (4)	
C35	-0.34061 (14)	0.60756 (8)	0.13736 (8)	0.0313 (5)	
C36A	-0.4131 (3)	0.64150 (17)	0.1194 (3)	0.0549 (11)	0.561 (3)
H36A	-0.4202	0.6664	0.1445	0.082*	0.561 (3)
H36B	-0.4674	0.6236	0.1140	0.082*	0.561 (3)
H36C	-0.3982	0.6564	0.0881	0.082*	0.561 (3)
C37A	-0.3394 (3)	0.56697 (17)	0.0995 (2)	0.0506 (11)	0.561 (3)
H37A	-0.3319	0.5803	0.0663	0.076*	0.561 (3)
H37B	-0.3943	0.5493	0.0992	0.076*	0.561 (3)
H37C	-0.2911	0.5452	0.1085	0.076*	0.561 (3)

C38A	-0.3565 (4)	0.5852 (2)	0.18760 (15)	0.0560 (12)	0.561 (3)
H38A	-0.3069	0.5650	0.1983	0.084*	0.561 (3)
H38B	-0.4093	0.5657	0.1847	0.084*	0.561 (3)
H38C	-0.3633	0.6106	0.2122	0.084*	0.561 (3)
C36B	-0.3897 (4)	0.6185 (3)	0.08788 (18)	0.0514 (12)	0.439 (3)
H36D	-0.4029	0.6528	0.0860	0.077*	0.439 (3)
H36E	-0.4440	0.6002	0.0853	0.077*	0.439 (3)
H36F	-0.3538	0.6096	0.0605	0.077*	0.439 (3)
C37B	-0.3241 (4)	0.55414 (12)	0.1440 (3)	0.0521 (12)	0.439 (3)
H37D	-0.2882	0.5427	0.1177	0.078*	0.439 (3)
H37E	-0.3796	0.5370	0.1422	0.078*	0.439 (3)
H37F	-0.2938	0.5484	0.1765	0.078*	0.439 (3)
C38B	-0.4009 (4)	0.6210 (3)	0.1781 (2)	0.0536 (13)	0.439 (3)
H38D	-0.3690	0.6190	0.2106	0.080*	0.439 (3)
H38E	-0.4503	0.5989	0.1772	0.080*	0.439 (3)
H38F	-0.4221	0.6538	0.1726	0.080*	0.439 (3)
C39	-0.03100 (14)	0.62922 (8)	0.08426 (8)	0.0274 (4)	
C40	-0.05872 (17)	0.58643 (10)	0.05103 (10)	0.0411 (6)	
H40A	-0.1062	0.5962	0.0273	0.062*	
H40B	-0.0784	0.5602	0.0718	0.062*	
H40C	-0.0092	0.5756	0.0328	0.062*	
C41	0.04341 (15)	0.61123 (9)	0.12008 (9)	0.0318 (5)	
H41A	0.0932	0.6024	0.1011	0.048*	
H41B	0.0239	0.5832	0.1382	0.048*	
H41C	0.0605	0.6366	0.1438	0.048*	
C42	0.00035 (15)	0.66891 (9)	0.05016 (8)	0.0319 (5)	
H42A	0.0168	0.6972	0.0701	0.048*	
H42B	-0.0465	0.6774	0.0255	0.048*	
H42C	0.0508	0.6575	0.0331	0.048*	
C43	-0.18179 (12)	0.78146 (7)	0.31591 (7)	0.0178 (4)	
C44	-0.11196 (12)	0.81414 (7)	0.34558 (7)	0.0173 (4)	
C45	-0.24753 (12)	0.81130 (7)	0.28460 (7)	0.0203 (4)	
C46	-0.22812 (13)	0.82773 (8)	0.23800 (7)	0.0236 (4)	
H46	-0.1769	0.8169	0.2236	0.028*	
C47	-0.28259 (15)	0.85991 (8)	0.21199 (8)	0.0297 (5)	
H47	-0.2685	0.8708	0.1801	0.036*	
C48	-0.35749 (15)	0.87609 (9)	0.23255 (9)	0.0323 (5)	
H48	-0.3941	0.8987	0.2152	0.039*	
C49	-0.37853 (14)	0.85919 (8)	0.27844 (9)	0.0298 (5)	
H49	-0.4301	0.8699	0.2925	0.036*	
C50	-0.32460 (13)	0.82661 (8)	0.30414 (8)	0.0246 (4)	
H50	-0.3403	0.8146	0.3354	0.030*	
C51	-0.22363 (12)	0.74161 (7)	0.34552 (7)	0.0199 (4)	
C52	-0.29807 (13)	0.71914 (8)	0.32489 (8)	0.0250 (4)	
H52	-0.3229	0.7297	0.2937	0.030*	
C53	-0.33657 (15)	0.68162 (9)	0.34914 (9)	0.0321 (5)	
H53	-0.3879	0.6671	0.3348	0.039*	
C54	-0.30029 (15)	0.66537 (9)	0.39415 (9)	0.0322 (5)	

H54	-0.3271	0.6401	0.4112	0.039*
C55	-0.22463 (15)	0.68605 (8)	0.41429 (8)	0.0294 (5)
H55	-0.1986	0.6744	0.4448	0.035*
C56	-0.18659 (13)	0.72381 (8)	0.39018 (8)	0.0238 (4)
H56	-0.1346	0.7377	0.4043	0.029*
C57	-0.12879 (13)	0.82990 (7)	0.39879 (7)	0.0212 (4)
C58	-0.20896 (15)	0.82925 (9)	0.41961 (8)	0.0295 (5)
H58	-0.2578	0.8156	0.4017	0.035*
C59	-0.21794 (17)	0.84858 (10)	0.46663 (9)	0.0366 (5)
H59	-0.2729	0.8476	0.4808	0.044*
C60	-0.14830 (18)	0.86909 (9)	0.49284 (8)	0.0359 (5)
H60	-0.1552	0.8828	0.5247	0.043*
C61	-0.06828 (17)	0.86969 (9)	0.47259 (9)	0.0345 (5)
H61	-0.0196	0.8832	0.4908	0.041*
C62	-0.05876 (14)	0.85066 (8)	0.42592 (8)	0.0274 (4)
H62	-0.0036	0.8517	0.4121	0.033*
C63	-0.09027 (13)	0.86083 (7)	0.31835 (7)	0.0197 (4)
C64	-0.14851 (14)	0.89906 (8)	0.31738 (8)	0.0275 (4)
H64	-0.2031	0.8953	0.3315	0.033*
C65	-0.12798 (16)	0.94228 (8)	0.29614 (9)	0.0336 (5)
H65	-0.1693	0.9675	0.2946	0.040*
C66	-0.04730 (17)	0.94904 (8)	0.27699 (9)	0.0330 (5)
H66	-0.0328	0.9790	0.2630	0.040*
C67	0.01146 (15)	0.91189 (8)	0.27849 (8)	0.0296 (5)
H67	0.0668	0.9162	0.2655	0.035*
C68	-0.00995 (13)	0.86789 (7)	0.29900 (7)	0.0223 (4)
H68	0.0310	0.8425	0.2997	0.027*
C69	0.02209 (12)	0.66095 (7)	0.34234 (7)	0.0170 (3)
C70	0.00858 (13)	0.61288 (7)	0.32705 (7)	0.0200 (4)
C71	0.07042 (14)	0.57992 (7)	0.34429 (8)	0.0237 (4)
H71	0.0635	0.5474	0.3344	0.028*
C72	0.14206 (14)	0.59230 (7)	0.37534 (7)	0.0228 (4)
C73	0.15302 (13)	0.63893 (7)	0.39094 (7)	0.0218 (4)
H73	0.2019	0.6477	0.4122	0.026*
C74	0.09146 (12)	0.67334 (7)	0.37516 (7)	0.0177 (4)
C75	0.09614 (12)	0.71992 (7)	0.40254 (7)	0.0173 (4)
C76	0.15525 (12)	0.75561 (7)	0.39372 (7)	0.0170 (4)
C77	0.16652 (12)	0.79537 (7)	0.42644 (7)	0.0193 (4)
C78	0.11671 (13)	0.79543 (7)	0.46761 (7)	0.0228 (4)
H78	0.1246	0.8207	0.4910	0.027*
C79	0.05580 (13)	0.76029 (8)	0.47631 (7)	0.0226 (4)
C80	0.04415 (13)	0.72271 (7)	0.44359 (7)	0.0199 (4)
H80	0.0015	0.6989	0.4487	0.024*
C81	-0.06753 (14)	0.59607 (8)	0.29194 (8)	0.0260 (4)
C82	-0.0776 (2)	0.54137 (9)	0.29271 (12)	0.0497 (8)
H82A	-0.0856	0.5307	0.3268	0.075*
H82B	-0.0253	0.5264	0.2807	0.075*
H82C	-0.1282	0.5321	0.2711	0.075*

C83	-0.0463 (2)	0.61056 (11)	0.23950 (9)	0.0458 (7)
H83A	-0.0948	0.6020	0.2160	0.069*
H83B	0.0063	0.5938	0.2304	0.069*
H83C	-0.0366	0.6452	0.2383	0.069*
C84	-0.15460 (16)	0.61671 (11)	0.30490 (13)	0.0511 (8)
H84A	-0.1543	0.6515	0.3000	0.077*
H84B	-0.1645	0.6096	0.3397	0.077*
H84C	-0.2011	0.6024	0.2833	0.077*
C85	0.27063 (18)	0.56593 (10)	0.42055 (10)	0.0444 (7)
H85A	0.3049	0.5907	0.4049	0.067*
H85B	0.3061	0.5371	0.4260	0.067*
H85C	0.2523	0.5777	0.4526	0.067*
C86	0.22906 (13)	0.83702 (7)	0.41866 (8)	0.0224 (4)
C87	0.22615 (16)	0.87468 (9)	0.45990 (9)	0.0347 (5)
H87A	0.2656	0.9011	0.4530	0.052*
H87B	0.2442	0.8601	0.4920	0.052*
H87C	0.1668	0.8870	0.4611	0.052*
C88	0.32258 (15)	0.81881 (9)	0.41863 (10)	0.0360 (5)
H88A	0.3274	0.7956	0.3916	0.054*
H88B	0.3386	0.8034	0.4506	0.054*
H88C	0.3618	0.8458	0.4137	0.054*
C89	0.20326 (19)	0.86219 (9)	0.36967 (9)	0.0386 (6)
H89A	0.2065	0.8395	0.3421	0.058*
H89B	0.2430	0.8890	0.3649	0.058*
H89C	0.1437	0.8743	0.3706	0.058*
C90	-0.06208 (17)	0.73753 (10)	0.52445 (9)	0.0362 (5)
H90A	-0.1033	0.7420	0.4957	0.054*
H90B	-0.0896	0.7469	0.5549	0.054*
H90C	-0.0448	0.7038	0.5267	0.054*
C91	0.30923 (12)	0.68722 (7)	0.26210 (7)	0.0173 (4)
C92	0.35959 (12)	0.73530 (7)	0.27841 (7)	0.0171 (4)
C93	0.29475 (12)	0.68329 (7)	0.20526 (7)	0.0188 (4)
C94	0.21491 (13)	0.69361 (8)	0.18139 (8)	0.0237 (4)
H94	0.1665	0.7006	0.2004	0.028*
C95	0.20529 (14)	0.69374 (9)	0.12979 (8)	0.0296 (5)
H95	0.1506	0.7015	0.1137	0.036*
C96	0.27423 (16)	0.68271 (9)	0.10172 (8)	0.0319 (5)
H96	0.2675	0.6837	0.0664	0.038*
C97	0.35325 (15)	0.67021 (9)	0.12506 (8)	0.0292 (5)
H97	0.4006	0.6618	0.1059	0.035*
C98	0.36316 (13)	0.67003 (8)	0.17631 (8)	0.0237 (4)
H98	0.4172	0.6608	0.1922	0.028*
C99	0.34810 (13)	0.63937 (7)	0.27935 (7)	0.0209 (4)
C100	0.29183 (15)	0.60206 (8)	0.28879 (8)	0.0268 (4)
H100	0.2310	0.6077	0.2876	0.032*
C101	0.32381 (18)	0.55671 (8)	0.30002 (10)	0.0367 (5)
H101	0.2849	0.5316	0.3070	0.044*
C102	0.41222 (19)	0.54791 (9)	0.30107 (10)	0.0395 (6)

H102	0.4339	0.5166	0.3081	0.047*	
C103	0.46896 (16)	0.58479 (9)	0.29185 (9)	0.0353 (5)	
H103	0.5297	0.5789	0.2928	0.042*	
C104	0.43700 (14)	0.63031 (8)	0.28123 (8)	0.0273 (4)	
H104	0.4762	0.6556	0.2752	0.033*	
C105	0.40857 (12)	0.73438 (7)	0.32980 (7)	0.0198 (4)	
C106	0.46826 (13)	0.77064 (8)	0.34204 (8)	0.0256 (4)	
H106	0.4795	0.7944	0.3180	0.031*	
C107	0.51172 (14)	0.77260 (10)	0.38891 (9)	0.0340 (5)	
H107	0.5520	0.7976	0.3966	0.041*	
C108	0.49621 (15)	0.73829 (10)	0.42400 (9)	0.0361 (6)	
H108	0.5273	0.7388	0.4555	0.043*	
C109	0.43520 (15)	0.70312 (9)	0.41304 (8)	0.0321 (5)	
H109	0.4235	0.6798	0.4374	0.039*	
C110	0.39087 (14)	0.70152 (8)	0.36678 (8)	0.0248 (4)	
H110	0.3478	0.6777	0.3602	0.030*	
C111	0.41517 (12)	0.75411 (7)	0.23738 (7)	0.0188 (4)	
C112	0.37606 (13)	0.77948 (7)	0.19749 (7)	0.0212 (4)	
H112	0.3159	0.7868	0.1971	0.025*	
C113	0.42409 (14)	0.79415 (8)	0.15835 (8)	0.0277 (4)	
H113	0.3965	0.8114	0.1314	0.033*	
C114	0.51184 (15)	0.78386 (9)	0.15811 (9)	0.0315 (5)	
H114	0.5442	0.7934	0.1309	0.038*	
C115	0.55185 (14)	0.75951 (9)	0.19792 (9)	0.0290 (5)	
H115	0.6124	0.7530	0.1985	0.035*	
C116	0.50396 (13)	0.74458 (8)	0.23708 (8)	0.0231 (4)	
H116	0.5320	0.7276	0.2641	0.028*	
C117	-0.00729 (17)	0.53742 (13)	0.88007 (12)	0.0274 (9)	0.5
C118	0.0454 (2)	0.52018 (13)	0.84397 (11)	0.0361 (12)	0.5
D118	0.0202	0.5043	0.8154	0.043*	0.5
C119	0.1349 (2)	0.52619 (16)	0.84963 (16)	0.060 (2)	0.5
D119	0.1709	0.5144	0.8250	0.072*	0.5
C120	0.17175 (19)	0.54945 (19)	0.89137 (19)	0.073 (3)	0.5
D120	0.2329	0.5536	0.8952	0.088*	0.5
C121	0.1191 (3)	0.5667 (2)	0.92747 (16)	0.087 (3)	0.5
D121	0.1443	0.5826	0.9560	0.104*	0.5
C122	0.0296 (3)	0.56068 (17)	0.92182 (13)	0.065 (2)	0.5
D122	-0.0064	0.5725	0.9465	0.078*	0.5
C123	-0.1039 (2)	0.5291 (3)	0.8756 (3)	0.0602 (18)	0.5
D12D	-0.1306	0.5436	0.9041	0.090*	0.5
D12E	-0.1284	0.5437	0.8447	0.090*	0.5
D12F	-0.1156	0.4946	0.8750	0.090*	0.5
C217	0.0969 (5)	0.5322 (4)	0.8571 (3)	0.0760 (17)*	0.3
C218	0.0102 (6)	0.5197 (4)	0.8478 (3)	0.0760 (17)*	0.3
D218	-0.0064	0.4996	0.8203	0.091*	0.3
C219	-0.0523 (5)	0.5366 (4)	0.8785 (4)	0.0760 (17)*	0.3
D219	-0.1115	0.5280	0.8721	0.091*	0.3
C220	-0.0281 (6)	0.5659 (4)	0.9186 (3)	0.0760 (17)*	0.3

D220	-0.0708	0.5775	0.9396	0.091*	0.3
C221	0.0586 (7)	0.5785 (4)	0.9280 (3)	0.0760 (17)*	0.3
D221	0.0752	0.5985	0.9554	0.091*	0.3
C222	0.1211 (5)	0.5616 (4)	0.8973 (4)	0.0760 (17)*	0.3
D222	0.1803	0.5701	0.9037	0.091*	0.3
C223	0.1642 (7)	0.5149 (7)	0.8231 (6)	0.130 (7)*	0.3
D22D	0.2215	0.5269	0.8350	0.195*	0.3
D22E	0.1649	0.4798	0.8229	0.195*	0.3
D22F	0.1501	0.5267	0.7894	0.195*	0.3
C124	1.00991 (13)	0.57207 (8)	0.55228 (7)	0.0565 (8)	
C125	1.01794 (12)	0.59866 (7)	0.50917 (8)	0.0525 (7)	
D125	1.0625	0.6220	0.5078	0.063*	
C126	0.96084 (15)	0.59102 (7)	0.46801 (7)	0.0596 (8)	
D126	0.9663	0.6092	0.4385	0.072*	
C127	0.89571 (13)	0.55679 (8)	0.46996 (7)	0.0624 (9)	
D127	0.8567	0.5516	0.4418	0.075*	
C128	0.88768 (13)	0.53021 (7)	0.51307 (8)	0.0592 (8)	
D128	0.8432	0.5068	0.5144	0.071*	
C129	0.94478 (14)	0.53785 (7)	0.55423 (7)	0.0558 (8)	
D129	0.9393	0.5197	0.5837	0.067*	
C130	1.0696 (3)	0.58083 (19)	0.59608 (18)	0.0937 (14)	
D13D	1.1274	0.5888	0.5852	0.141*	
D13E	1.0735	0.5520	0.6168	0.141*	
D13F	1.0478	0.6075	0.6154	0.141*	
O1	0.06808 (9)	0.78011 (5)	0.13485 (5)	0.0212 (3)	
O2	-0.08844 (8)	0.78780 (5)	0.15396 (5)	0.0196 (3)	
O3	-0.01747 (9)	0.70997 (5)	0.15397 (5)	0.0213 (3)	
O4	-0.12721 (8)	0.75686 (5)	0.28093 (5)	0.0174 (3)	
O5	-0.03502 (8)	0.78390 (5)	0.34882 (5)	0.0173 (3)	
O6	-0.04051 (8)	0.69540 (5)	0.32844 (5)	0.0183 (3)	
O7	0.19615 (11)	0.55487 (6)	0.38896 (6)	0.0315 (4)	
O8	0.21162 (8)	0.74996 (5)	0.35543 (5)	0.0181 (3)	
O9	0.01243 (11)	0.76631 (6)	0.51876 (6)	0.0303 (3)	
O10	0.22556 (8)	0.69210 (5)	0.28404 (5)	0.0175 (3)	
O11	0.28788 (8)	0.76952 (5)	0.28100 (5)	0.0162 (3)	
P1	0.00158 (3)	0.76292 (2)	0.17579 (2)	0.01697 (10)	
P2	-0.02830 (3)	0.74707 (2)	0.30229 (2)	0.01517 (9)	
P3	0.19648 (3)	0.74666 (2)	0.29532 (2)	0.01483 (9)	
Rh1	0.07333 (2)	0.76915 (2)	0.25048 (2)	0.01516 (4)	
C131	0.1679 (4)	0.0270 (3)	0.3884 (2)	0.0875 (9)*	0.5
C132	0.2083 (3)	0.0280 (3)	0.4359 (2)	0.0875 (9)*	0.5
D132	0.2633	0.0431	0.4414	0.105*	0.5
C133	0.1684 (4)	0.0070 (3)	0.47535 (18)	0.0875 (9)*	0.5
D133	0.1961	0.0077	0.5078	0.105*	0.5
C134	0.0881 (4)	-0.0151 (2)	0.4673 (2)	0.0875 (9)*	0.5
D134	0.0608	-0.0295	0.4942	0.105*	0.5
C135	0.0476 (3)	-0.0162 (2)	0.4197 (2)	0.0875 (9)*	0.5
D135	-0.0073	-0.0313	0.4142	0.105*	0.5

C136	0.0875 (4)	0.0049 (3)	0.38029 (18)	0.0875 (9)*	0.5
D136	0.0599	0.0041	0.3478	0.105*	0.5
C137	0.2058 (8)	0.0504 (5)	0.3442 (3)	0.128 (4)*	0.5
D13G	0.1669	0.0453	0.3145	0.193*	0.5
D13H	0.2124	0.0848	0.3504	0.193*	0.5
D13I	0.2627	0.0363	0.3389	0.193*	0.5
C231	0.1759 (4)	0.0110 (3)	0.4516 (2)	0.0875 (9)*	0.4
C232	0.0969 (4)	-0.0101 (3)	0.4369 (3)	0.0875 (9)*	0.4
D232	0.0657	-0.0275	0.4603	0.105*	0.4
C233	0.0636 (4)	-0.0058 (3)	0.3880 (3)	0.0875 (9)*	0.4
D233	0.0096	-0.0202	0.3780	0.105*	0.4
C234	0.1093 (5)	0.0197 (3)	0.3538 (2)	0.0875 (9)*	0.4
D234	0.0865	0.0227	0.3203	0.105*	0.4
C235	0.1883 (5)	0.0409 (3)	0.3684 (2)	0.0875 (9)*	0.4
D235	0.2195	0.0583	0.3451	0.105*	0.4
C236	0.2216 (4)	0.0365 (3)	0.4174 (3)	0.0875 (9)*	0.4
D236	0.2756	0.0510	0.4274	0.105*	0.4
C237	0.2121 (7)	0.0063 (4)	0.5046 (2)	0.134 (6)*	0.4
D23D	0.2678	0.0232	0.5085	0.201*	0.4
D23E	0.1712	0.0203	0.5270	0.201*	0.4
D23F	0.2208	-0.0276	0.5127	0.201*	0.4

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0144 (8)	0.0265 (10)	0.0213 (9)	-0.0008 (7)	0.0005 (7)	0.0016 (8)
C2	0.0141 (8)	0.0241 (9)	0.0172 (9)	0.0012 (7)	0.0014 (7)	0.0030 (7)
C3	0.0168 (9)	0.0226 (9)	0.0199 (9)	0.0016 (7)	0.0000 (7)	0.0020 (7)
C4	0.0179 (9)	0.0221 (9)	0.0265 (10)	-0.0005 (7)	0.0004 (8)	0.0044 (8)
C5	0.0196 (9)	0.0288 (11)	0.0249 (10)	-0.0017 (8)	0.0033 (8)	0.0083 (8)
C6	0.0185 (9)	0.0306 (11)	0.0188 (9)	0.0017 (8)	0.0020 (7)	0.0054 (8)
C7	0.0247 (10)	0.0236 (10)	0.0329 (11)	-0.0054 (8)	0.0010 (9)	0.0039 (9)
C8	0.0254 (11)	0.0306 (12)	0.0446 (14)	-0.0049 (9)	-0.0070 (10)	-0.0024 (10)
C9	0.0422 (14)	0.0353 (13)	0.0460 (15)	-0.0175 (11)	0.0058 (12)	0.0057 (11)
C10	0.0377 (13)	0.0227 (11)	0.0439 (14)	-0.0013 (9)	0.0032 (11)	-0.0012 (10)
C11	0.0241 (10)	0.0406 (12)	0.0190 (10)	-0.0027 (9)	0.0033 (8)	0.0070 (9)
C12	0.0445 (14)	0.0520 (16)	0.0246 (11)	-0.0113 (12)	0.0078 (10)	0.0095 (11)
C13	0.0305 (13)	0.085 (2)	0.0242 (12)	0.0076 (13)	-0.0002 (10)	0.0161 (13)
C14	0.0470 (15)	0.0473 (15)	0.0218 (11)	-0.0068 (12)	0.0087 (10)	-0.0011 (10)
C15	0.0172 (9)	0.0245 (10)	0.0190 (9)	0.0007 (7)	0.0018 (7)	0.0038 (7)
C16	0.0245 (10)	0.0302 (11)	0.0214 (10)	-0.0018 (8)	-0.0051 (8)	0.0017 (8)
C17	0.0405 (13)	0.0290 (11)	0.0271 (11)	-0.0070 (10)	-0.0089 (10)	0.0003 (9)
C18	0.0451 (14)	0.0260 (11)	0.0305 (12)	-0.0016 (10)	-0.0088 (10)	0.0030 (9)
C19	0.0331 (11)	0.0282 (11)	0.0237 (10)	0.0009 (9)	-0.0070 (9)	0.0030 (8)
C20	0.0175 (9)	0.0268 (10)	0.0191 (9)	0.0006 (7)	-0.0004 (7)	0.0008 (8)
C21	0.087 (2)	0.0254 (12)	0.0453 (16)	-0.0051 (13)	-0.0271 (16)	0.0071 (11)
C22	0.119 (3)	0.0499 (19)	0.061 (2)	-0.036 (2)	-0.019 (2)	0.0220 (17)
C23	0.151 (4)	0.0299 (15)	0.078 (3)	-0.006 (2)	-0.068 (3)	0.0163 (16)

C24	0.104 (3)	0.0302 (15)	0.077 (2)	0.0103 (17)	-0.028 (2)	-0.0040 (15)
C25	0.0207 (9)	0.0254 (10)	0.0211 (9)	0.0007 (8)	-0.0041 (8)	0.0020 (8)
C26	0.0309 (11)	0.0326 (12)	0.0281 (11)	0.0002 (9)	-0.0123 (9)	0.0022 (9)
C27	0.0233 (10)	0.0375 (12)	0.0345 (12)	-0.0066 (9)	-0.0016 (9)	0.0020 (10)
C28	0.0319 (11)	0.0326 (12)	0.0224 (10)	0.0053 (9)	-0.0026 (9)	-0.0027 (9)
C29	0.0172 (9)	0.0224 (9)	0.0186 (9)	-0.0009 (7)	-0.0019 (7)	0.0015 (7)
C30	0.0229 (10)	0.0235 (10)	0.0204 (9)	-0.0006 (8)	0.0019 (8)	-0.0010 (8)
C31	0.0212 (10)	0.0267 (10)	0.0260 (10)	0.0011 (8)	0.0041 (8)	0.0021 (8)
C32	0.0221 (10)	0.0244 (10)	0.0275 (10)	-0.0040 (8)	-0.0012 (8)	0.0032 (8)
C33	0.0252 (10)	0.0254 (10)	0.0254 (10)	-0.0015 (8)	-0.0019 (8)	-0.0033 (8)
C34	0.0219 (10)	0.0255 (10)	0.0203 (9)	0.0024 (8)	-0.0004 (8)	-0.0014 (8)
C35	0.0226 (10)	0.0318 (12)	0.0396 (13)	-0.0076 (9)	0.0016 (9)	-0.0012 (10)
C36A	0.030 (2)	0.054 (2)	0.079 (3)	-0.0072 (19)	-0.006 (2)	-0.002 (2)
C37A	0.0324 (19)	0.049 (2)	0.070 (3)	-0.0182 (18)	0.001 (2)	-0.015 (2)
C38A	0.045 (2)	0.053 (2)	0.070 (3)	-0.0262 (19)	0.008 (2)	0.003 (2)
C36B	0.032 (2)	0.058 (3)	0.064 (3)	-0.013 (2)	-0.004 (2)	0.003 (2)
C37B	0.037 (2)	0.043 (2)	0.077 (3)	-0.017 (2)	0.006 (2)	0.002 (2)
C38B	0.034 (2)	0.058 (3)	0.070 (3)	-0.020 (2)	0.011 (2)	-0.005 (2)
C39	0.0251 (10)	0.0322 (11)	0.0249 (10)	0.0040 (9)	0.0015 (8)	-0.0068 (9)
C40	0.0390 (14)	0.0458 (15)	0.0388 (14)	0.0044 (11)	0.0041 (11)	-0.0192 (12)
C41	0.0275 (11)	0.0347 (12)	0.0332 (12)	0.0095 (9)	0.0007 (9)	-0.0010 (10)
C42	0.0274 (11)	0.0449 (14)	0.0237 (10)	0.0063 (10)	0.0048 (9)	-0.0017 (10)
C43	0.0137 (8)	0.0241 (9)	0.0159 (8)	0.0013 (7)	0.0039 (7)	-0.0006 (7)
C44	0.0134 (8)	0.0215 (9)	0.0174 (9)	0.0027 (7)	0.0023 (7)	0.0000 (7)
C45	0.0148 (8)	0.0245 (10)	0.0212 (9)	0.0011 (7)	-0.0015 (7)	0.0014 (8)
C46	0.0219 (10)	0.0284 (10)	0.0206 (9)	0.0039 (8)	0.0015 (8)	0.0016 (8)
C47	0.0326 (12)	0.0335 (12)	0.0228 (10)	0.0064 (9)	-0.0011 (9)	0.0055 (9)
C48	0.0284 (11)	0.0332 (12)	0.0343 (12)	0.0094 (9)	-0.0058 (9)	0.0054 (10)
C49	0.0190 (10)	0.0344 (12)	0.0362 (12)	0.0066 (9)	0.0024 (9)	0.0011 (10)
C50	0.0186 (9)	0.0294 (11)	0.0262 (10)	0.0029 (8)	0.0037 (8)	0.0030 (8)
C51	0.0149 (8)	0.0250 (10)	0.0200 (9)	0.0012 (7)	0.0044 (7)	0.0025 (7)
C52	0.0181 (9)	0.0300 (11)	0.0264 (10)	0.0001 (8)	-0.0011 (8)	0.0038 (8)
C53	0.0218 (10)	0.0351 (12)	0.0395 (13)	-0.0072 (9)	0.0017 (9)	0.0024 (10)
C54	0.0312 (12)	0.0327 (12)	0.0336 (12)	-0.0068 (9)	0.0099 (9)	0.0061 (10)
C55	0.0327 (12)	0.0332 (12)	0.0226 (10)	0.0001 (9)	0.0047 (9)	0.0066 (9)
C56	0.0200 (9)	0.0302 (11)	0.0211 (10)	-0.0007 (8)	0.0015 (8)	0.0013 (8)
C57	0.0227 (9)	0.0231 (9)	0.0181 (9)	0.0043 (8)	0.0034 (7)	0.0004 (7)
C58	0.0255 (11)	0.0398 (12)	0.0238 (10)	0.0039 (9)	0.0059 (8)	-0.0024 (9)
C59	0.0384 (13)	0.0461 (14)	0.0268 (11)	0.0060 (11)	0.0142 (10)	-0.0020 (10)
C60	0.0533 (15)	0.0360 (13)	0.0192 (10)	0.0066 (11)	0.0077 (10)	-0.0025 (9)
C61	0.0430 (14)	0.0357 (12)	0.0243 (11)	-0.0020 (10)	-0.0012 (10)	-0.0063 (9)
C62	0.0267 (10)	0.0317 (11)	0.0241 (10)	0.0004 (9)	0.0031 (8)	-0.0036 (9)
C63	0.0206 (9)	0.0214 (9)	0.0170 (9)	0.0004 (7)	0.0005 (7)	-0.0005 (7)
C64	0.0243 (10)	0.0269 (11)	0.0315 (11)	0.0031 (8)	0.0029 (9)	0.0011 (9)
C65	0.0367 (12)	0.0246 (11)	0.0393 (13)	0.0068 (9)	0.0011 (10)	0.0014 (9)
C66	0.0456 (14)	0.0224 (11)	0.0315 (12)	-0.0034 (10)	0.0054 (10)	0.0047 (9)
C67	0.0319 (11)	0.0288 (11)	0.0289 (11)	-0.0048 (9)	0.0092 (9)	0.0007 (9)
C68	0.0229 (10)	0.0221 (9)	0.0219 (9)	0.0003 (8)	0.0029 (8)	-0.0011 (8)

C69	0.0176 (8)	0.0185 (9)	0.0149 (8)	0.0018 (7)	0.0018 (7)	0.0011 (7)
C70	0.0230 (9)	0.0202 (9)	0.0168 (9)	-0.0007 (7)	0.0012 (7)	0.0002 (7)
C71	0.0298 (11)	0.0180 (9)	0.0232 (10)	0.0024 (8)	0.0009 (8)	-0.0017 (8)
C72	0.0251 (10)	0.0222 (10)	0.0211 (9)	0.0066 (8)	0.0006 (8)	0.0012 (8)
C73	0.0215 (9)	0.0259 (10)	0.0178 (9)	0.0026 (8)	-0.0012 (7)	-0.0004 (8)
C74	0.0191 (9)	0.0191 (9)	0.0153 (8)	-0.0003 (7)	0.0034 (7)	0.0008 (7)
C75	0.0164 (8)	0.0203 (9)	0.0149 (8)	0.0025 (7)	-0.0023 (7)	0.0000 (7)
C76	0.0155 (8)	0.0222 (9)	0.0134 (8)	0.0032 (7)	0.0006 (7)	0.0005 (7)
C77	0.0181 (9)	0.0221 (9)	0.0174 (9)	0.0014 (7)	-0.0007 (7)	-0.0010 (7)
C78	0.0249 (10)	0.0250 (10)	0.0186 (9)	-0.0003 (8)	0.0019 (8)	-0.0050 (8)
C79	0.0234 (10)	0.0289 (10)	0.0158 (9)	0.0024 (8)	0.0044 (7)	-0.0010 (8)
C80	0.0186 (9)	0.0237 (10)	0.0176 (9)	0.0016 (7)	0.0016 (7)	0.0014 (7)
C81	0.0282 (11)	0.0222 (10)	0.0269 (10)	-0.0014 (8)	-0.0050 (8)	-0.0020 (8)
C82	0.0537 (17)	0.0268 (12)	0.0649 (19)	-0.0088 (12)	-0.0272 (14)	0.0000 (12)
C83	0.0546 (17)	0.0549 (17)	0.0260 (12)	-0.0079 (13)	-0.0132 (11)	0.0020 (11)
C84	0.0247 (12)	0.0544 (17)	0.073 (2)	-0.0045 (11)	-0.0053 (13)	-0.0295 (15)
C85	0.0469 (15)	0.0411 (14)	0.0425 (14)	0.0228 (12)	-0.0203 (12)	-0.0068 (11)
C86	0.0223 (10)	0.0224 (10)	0.0226 (10)	-0.0036 (8)	0.0009 (8)	-0.0038 (8)
C87	0.0373 (13)	0.0302 (12)	0.0374 (13)	-0.0102 (10)	0.0082 (10)	-0.0126 (10)
C88	0.0217 (11)	0.0361 (13)	0.0501 (15)	-0.0048 (9)	0.0015 (10)	-0.0111 (11)
C89	0.0533 (16)	0.0285 (12)	0.0330 (12)	-0.0114 (11)	-0.0054 (11)	0.0064 (10)
C90	0.0364 (13)	0.0484 (15)	0.0254 (11)	-0.0083 (11)	0.0149 (10)	-0.0042 (10)
C91	0.0125 (8)	0.0216 (9)	0.0178 (9)	0.0011 (7)	0.0018 (7)	-0.0007 (7)
C92	0.0120 (8)	0.0209 (9)	0.0183 (9)	0.0009 (7)	0.0013 (7)	0.0004 (7)
C93	0.0183 (9)	0.0210 (9)	0.0173 (9)	-0.0002 (7)	0.0012 (7)	-0.0021 (7)
C94	0.0185 (9)	0.0316 (11)	0.0212 (10)	0.0015 (8)	0.0016 (7)	-0.0047 (8)
C95	0.0239 (10)	0.0420 (13)	0.0224 (10)	0.0063 (9)	-0.0034 (8)	-0.0053 (9)
C96	0.0341 (12)	0.0443 (13)	0.0172 (10)	0.0052 (10)	0.0013 (9)	-0.0050 (9)
C97	0.0263 (11)	0.0392 (12)	0.0230 (10)	0.0031 (9)	0.0073 (8)	-0.0058 (9)
C98	0.0175 (9)	0.0296 (11)	0.0239 (10)	0.0024 (8)	0.0015 (8)	-0.0038 (8)
C99	0.0229 (9)	0.0213 (9)	0.0184 (9)	0.0030 (7)	0.0010 (7)	-0.0012 (7)
C100	0.0279 (11)	0.0232 (10)	0.0298 (11)	0.0003 (8)	0.0067 (9)	-0.0027 (8)
C101	0.0494 (15)	0.0215 (11)	0.0404 (13)	0.0004 (10)	0.0122 (11)	-0.0008 (9)
C102	0.0542 (16)	0.0259 (11)	0.0388 (13)	0.0153 (11)	0.0051 (12)	0.0036 (10)
C103	0.0348 (12)	0.0340 (12)	0.0366 (13)	0.0159 (10)	-0.0017 (10)	0.0011 (10)
C104	0.0232 (10)	0.0289 (11)	0.0296 (11)	0.0049 (8)	-0.0009 (8)	0.0005 (9)
C105	0.0134 (8)	0.0279 (10)	0.0180 (9)	0.0030 (7)	0.0001 (7)	-0.0010 (7)
C106	0.0170 (9)	0.0373 (12)	0.0226 (10)	-0.0039 (8)	0.0014 (8)	-0.0036 (9)
C107	0.0180 (10)	0.0572 (16)	0.0267 (11)	-0.0057 (10)	0.0006 (8)	-0.0113 (10)
C108	0.0240 (11)	0.0637 (17)	0.0200 (10)	0.0071 (11)	-0.0052 (8)	-0.0057 (10)
C109	0.0337 (12)	0.0423 (13)	0.0203 (10)	0.0108 (10)	0.0002 (9)	0.0044 (9)
C110	0.0247 (10)	0.0283 (11)	0.0215 (10)	0.0033 (8)	0.0012 (8)	0.0011 (8)
C111	0.0159 (9)	0.0219 (9)	0.0190 (9)	-0.0019 (7)	0.0038 (7)	-0.0020 (7)
C112	0.0181 (9)	0.0241 (10)	0.0217 (9)	-0.0002 (7)	0.0034 (7)	-0.0005 (8)
C113	0.0277 (11)	0.0329 (11)	0.0230 (10)	0.0017 (9)	0.0061 (8)	0.0050 (9)
C114	0.0276 (11)	0.0394 (13)	0.0289 (11)	-0.0036 (9)	0.0126 (9)	0.0017 (10)
C115	0.0163 (9)	0.0394 (12)	0.0320 (11)	-0.0021 (8)	0.0071 (8)	-0.0026 (9)
C116	0.0168 (9)	0.0291 (10)	0.0236 (10)	0.0000 (8)	0.0015 (8)	-0.0012 (8)

C117	0.028 (2)	0.026 (2)	0.029 (2)	0.0067 (17)	0.0080 (18)	0.0048 (17)
C118	0.056 (3)	0.029 (2)	0.023 (2)	0.015 (2)	0.007 (2)	0.0054 (18)
C119	0.058 (4)	0.060 (4)	0.066 (4)	0.026 (3)	0.040 (4)	0.035 (3)
C120	0.033 (3)	0.084 (5)	0.102 (6)	-0.021 (3)	-0.005 (4)	0.053 (5)
C121	0.088 (6)	0.101 (7)	0.071 (5)	-0.032 (5)	-0.007 (5)	-0.025 (5)
C122	0.056 (4)	0.098 (6)	0.042 (3)	-0.023 (4)	0.012 (3)	-0.032 (4)
C123	0.035 (3)	0.082 (5)	0.064 (4)	0.011 (3)	0.004 (3)	0.030 (4)
C124	0.0540 (18)	0.0552 (19)	0.061 (2)	-0.0006 (15)	0.0048 (15)	0.0025 (15)
C125	0.0519 (17)	0.0447 (16)	0.0617 (19)	-0.0107 (13)	0.0096 (15)	0.0076 (14)
C126	0.065 (2)	0.0508 (18)	0.065 (2)	0.0019 (16)	0.0169 (17)	0.0057 (16)
C127	0.066 (2)	0.061 (2)	0.060 (2)	-0.0050 (17)	-0.0024 (17)	-0.0084 (16)
C128	0.064 (2)	0.0565 (19)	0.058 (2)	-0.0094 (16)	0.0179 (17)	-0.0006 (16)
C129	0.0489 (17)	0.0398 (15)	0.081 (2)	-0.0074 (13)	0.0251 (16)	-0.0074 (15)
C130	0.086 (3)	0.099 (3)	0.092 (3)	-0.012 (3)	-0.024 (3)	0.007 (3)
O1	0.0153 (6)	0.0327 (8)	0.0156 (6)	-0.0042 (6)	0.0012 (5)	0.0008 (6)
O2	0.0152 (6)	0.0222 (7)	0.0212 (7)	0.0013 (5)	-0.0012 (5)	0.0037 (5)
O3	0.0157 (6)	0.0242 (7)	0.0240 (7)	-0.0007 (5)	-0.0002 (5)	-0.0038 (6)
O4	0.0117 (6)	0.0238 (7)	0.0169 (6)	0.0019 (5)	0.0014 (5)	-0.0006 (5)
O5	0.0141 (6)	0.0204 (6)	0.0173 (6)	0.0024 (5)	0.0001 (5)	-0.0015 (5)
O6	0.0155 (6)	0.0187 (6)	0.0209 (7)	0.0007 (5)	0.0024 (5)	0.0026 (5)
O7	0.0355 (9)	0.0249 (8)	0.0328 (8)	0.0120 (7)	-0.0082 (7)	-0.0014 (6)
O8	0.0150 (6)	0.0257 (7)	0.0135 (6)	0.0011 (5)	0.0015 (5)	-0.0014 (5)
O9	0.0332 (8)	0.0385 (9)	0.0204 (7)	-0.0063 (7)	0.0116 (6)	-0.0078 (6)
O10	0.0143 (6)	0.0199 (6)	0.0186 (6)	-0.0004 (5)	0.0031 (5)	-0.0012 (5)
O11	0.0115 (6)	0.0185 (6)	0.0187 (6)	0.0008 (5)	0.0018 (5)	-0.0001 (5)
P1	0.0127 (2)	0.0231 (2)	0.0150 (2)	-0.00064 (17)	0.00033 (17)	0.00077 (18)
P2	0.0126 (2)	0.0180 (2)	0.0149 (2)	0.00055 (17)	0.00090 (17)	0.00089 (17)
P3	0.0122 (2)	0.0183 (2)	0.0140 (2)	-0.00004 (17)	0.00104 (16)	-0.00021 (17)
Rh1	0.01143 (7)	0.02012 (8)	0.01394 (7)	-0.00024 (5)	0.00080 (5)	0.00152 (5)

Geometric parameters (Å, °)

C1—C6	1.400 (3)	C74—C75	1.495 (3)
C1—C2	1.403 (3)	C75—C76	1.381 (3)
C1—O1	1.414 (2)	C75—C80	1.406 (3)
C2—C3	1.392 (3)	C76—O8	1.397 (2)
C2—Rh1	2.0705 (19)	C76—C77	1.422 (3)
C3—C4	1.396 (3)	C77—C78	1.387 (3)
C3—H3	0.9500	C77—C86	1.534 (3)
C4—C5	1.391 (3)	C78—C79	1.388 (3)
C4—C7	1.537 (3)	C78—H78	0.9500
C5—C6	1.400 (3)	C79—O9	1.369 (2)
C5—H5	0.9500	C79—C80	1.376 (3)
C6—C11	1.542 (3)	C80—H80	0.9500
C7—C9	1.528 (3)	C81—C84	1.521 (3)
C7—C10	1.533 (3)	C81—C83	1.524 (3)
C7—C8	1.536 (3)	C81—C82	1.536 (3)
C8—H8A	0.9800	C82—H82A	0.9800

C8—H8B	0.9800	C82—H82B	0.9800
C8—H8C	0.9800	C82—H82C	0.9800
C9—H9A	0.9800	C83—H83A	0.9800
C9—H9B	0.9800	C83—H83B	0.9800
C9—H9C	0.9800	C83—H83C	0.9800
C10—H10A	0.9800	C84—H84A	0.9800
C10—H10B	0.9800	C84—H84B	0.9800
C10—H10C	0.9800	C84—H84C	0.9800
C11—C14	1.528 (4)	C85—O7	1.422 (3)
C11—C13	1.530 (3)	C85—H85A	0.9800
C11—C12	1.537 (3)	C85—H85B	0.9800
C12—H12A	0.9800	C85—H85C	0.9800
C12—H12B	0.9800	C86—C89	1.526 (3)
C12—H12C	0.9800	C86—C88	1.529 (3)
C13—H13A	0.9800	C86—C87	1.532 (3)
C13—H13B	0.9800	C87—H87A	0.9800
C13—H13C	0.9800	C87—H87B	0.9800
C14—H14A	0.9800	C87—H87C	0.9800
C14—H14B	0.9800	C88—H88A	0.9800
C14—H14C	0.9800	C88—H88B	0.9800
C15—C16	1.379 (3)	C88—H88C	0.9800
C15—O2	1.402 (2)	C89—H89A	0.9800
C15—C20	1.403 (3)	C89—H89B	0.9800
C16—C17	1.377 (3)	C89—H89C	0.9800
C16—H16	0.9500	C90—O9	1.418 (3)
C17—C18	1.384 (3)	C90—H90A	0.9800
C17—H17	0.9500	C90—H90B	0.9800
C18—C19	1.395 (3)	C90—H90C	0.9800
C18—C21	1.536 (3)	C91—O10	1.458 (2)
C19—C20	1.397 (3)	C91—C99	1.526 (3)
C19—H19	0.9500	C91—C93	1.538 (3)
C20—C25	1.538 (3)	C91—C92	1.600 (3)
C21—C24	1.521 (5)	C92—O11	1.467 (2)
C21—C23	1.527 (4)	C92—C111	1.532 (3)
C21—C22	1.536 (5)	C92—C105	1.536 (3)
C22—H22A	0.9800	C93—C94	1.384 (3)
C22—H22B	0.9800	C93—C98	1.399 (3)
C22—H22C	0.9800	C94—C95	1.389 (3)
C23—H23A	0.9800	C94—H94	0.9500
C23—H23B	0.9800	C95—C96	1.376 (3)
C23—H23C	0.9800	C95—H95	0.9500
C24—H24A	0.9800	C96—C97	1.382 (3)
C24—H24B	0.9800	C96—H96	0.9500
C24—H24C	0.9800	C97—C98	1.379 (3)
C25—C27	1.531 (3)	C97—H97	0.9500
C25—C28	1.533 (3)	C98—H98	0.9500
C25—C26	1.535 (3)	C99—C100	1.389 (3)
C26—H26A	0.9800	C99—C104	1.392 (3)

C26—H26B	0.9800	C100—C101	1.386 (3)
C26—H26C	0.9800	C100—H100	0.9500
C27—H27A	0.9800	C101—C102	1.384 (4)
C27—H27B	0.9800	C101—H101	0.9500
C27—H27C	0.9800	C102—C103	1.384 (4)
C28—H28A	0.9800	C102—H102	0.9500
C28—H28B	0.9800	C103—C104	1.387 (3)
C28—H28C	0.9800	C103—H103	0.9500
C29—C30	1.382 (3)	C104—H104	0.9500
C29—C34	1.404 (3)	C105—C110	1.394 (3)
C29—O3	1.407 (2)	C105—C106	1.395 (3)
C30—C31	1.381 (3)	C106—C107	1.394 (3)
C30—H30	0.9500	C106—H106	0.9500
C31—C32	1.390 (3)	C107—C108	1.377 (4)
C31—H31	0.9500	C107—H107	0.9500
C32—C33	1.395 (3)	C108—C109	1.380 (4)
C32—C35	1.533 (3)	C108—H108	0.9500
C33—C34	1.399 (3)	C109—C110	1.385 (3)
C33—H33	0.9500	C109—H109	0.9500
C34—C39	1.540 (3)	C110—H110	0.9500
C35—C36A	1.522 (3)	C111—C112	1.393 (3)
C35—C37B	1.523 (3)	C111—C116	1.396 (3)
C35—C38A	1.523 (3)	C112—C113	1.387 (3)
C35—C36B	1.524 (3)	C112—H112	0.9500
C35—C38B	1.526 (3)	C113—C114	1.384 (3)
C35—C37A	1.527 (3)	C113—H113	0.9500
C36A—H36A	0.9800	C114—C115	1.383 (3)
C36A—H36B	0.9800	C114—H114	0.9500
C36A—H36C	0.9800	C115—C116	1.388 (3)
C37A—H37A	0.9800	C115—H115	0.9500
C37A—H37B	0.9800	C116—H116	0.9500
C37A—H37C	0.9800	C117—C118	1.3900
C38A—H38A	0.9800	C117—C122	1.3900
C38A—H38B	0.9800	C117—C123	1.505 (2)
C38A—H38C	0.9800	C118—C119	1.3900
C36B—H36D	0.9800	C118—D118	0.9500
C36B—H36E	0.9800	C119—C120	1.3900
C36B—H36F	0.9800	C119—D119	0.9500
C37B—H37D	0.9800	C120—C121	1.3900
C37B—H37E	0.9800	C120—D120	0.9500
C37B—H37F	0.9800	C121—C122	1.3900
C38B—H38D	0.9800	C121—D121	0.9500
C38B—H38E	0.9800	C122—D122	0.9500
C38B—H38F	0.9800	C123—D12D	0.9800
C39—C42	1.536 (3)	C123—D12E	0.9800
C39—C41	1.538 (3)	C123—D12F	0.9800
C39—C40	1.538 (3)	C217—C218	1.3900
C40—H40A	0.9800	C217—C222	1.3900

C40—H40B	0.9800	C217—C223	1.5058 (13)
C40—H40C	0.9800	C218—C219	1.3900
C41—H41A	0.9800	C218—D218	0.9500
C41—H41B	0.9800	C219—C220	1.3900
C41—H41C	0.9800	C219—D219	0.9500
C42—H42A	0.9800	C220—C221	1.3900
C42—H42B	0.9800	C220—D220	0.9500
C42—H42C	0.9800	C221—C222	1.3900
C43—O4	1.471 (2)	C221—D221	0.9500
C43—C45	1.527 (3)	C222—D222	0.9500
C43—C51	1.534 (3)	C223—D22D	0.9800
C43—C44	1.590 (3)	C223—D22E	0.9800
C44—O5	1.455 (2)	C223—D22F	0.9800
C44—C57	1.536 (3)	C124—C125	1.3900
C44—C63	1.543 (3)	C124—C129	1.3900
C45—C46	1.386 (3)	C124—C130	1.472 (4)
C45—C50	1.396 (3)	C125—C126	1.3900
C46—C47	1.391 (3)	C125—D125	0.9500
C46—H46	0.9500	C126—C127	1.3900
C47—C48	1.387 (3)	C126—D126	0.9500
C47—H47	0.9500	C127—C128	1.3900
C48—C49	1.380 (3)	C127—D127	0.9500
C48—H48	0.9500	C128—C129	1.3900
C49—C50	1.389 (3)	C128—D128	0.9500
C49—H49	0.9500	C129—D129	0.9500
C50—H50	0.9500	C130—D13D	0.9800
C51—C56	1.392 (3)	C130—D13E	0.9800
C51—C52	1.394 (3)	C130—D13F	0.9800
C52—C53	1.387 (3)	O1—P1	1.6231 (14)
C52—H52	0.9500	O2—P1	1.6302 (14)
C53—C54	1.381 (3)	O3—P1	1.6121 (15)
C53—H53	0.9500	O4—P2	1.6208 (13)
C54—C55	1.383 (3)	O5—P2	1.6296 (14)
C54—H54	0.9500	O6—P2	1.6218 (14)
C55—C56	1.387 (3)	O8—P3	1.6241 (14)
C55—H55	0.9500	O10—P3	1.6226 (14)
C56—H56	0.9500	O11—P3	1.6153 (13)
C57—C58	1.388 (3)	P1—Rh1	2.2430 (5)
C57—C62	1.393 (3)	P2—Rh1	2.2469 (5)
C58—C59	1.391 (3)	P3—Rh1	2.2768 (5)
C58—H58	0.9500	C131—C132	1.3900
C59—C60	1.374 (4)	C131—C136	1.3900
C59—H59	0.9500	C131—C137	1.507 (2)
C60—C61	1.379 (4)	C132—C133	1.3900
C60—H60	0.9500	C132—D132	0.9500
C61—C62	1.381 (3)	C133—C134	1.3900
C61—H61	0.9500	C133—D133	0.9500
C62—H62	0.9500	C134—C135	1.3900

C63—C68	1.387 (3)	C134—D134	0.9500
C63—C64	1.395 (3)	C135—C136	1.3900
C64—C65	1.381 (3)	C135—D135	0.9500
C64—H64	0.9500	C136—D136	0.9500
C65—C66	1.388 (3)	C137—D13G	0.9800
C65—H65	0.9500	C137—D13H	0.9800
C66—C67	1.377 (3)	C137—D13I	0.9800
C66—H66	0.9500	C231—C232	1.3900
C67—C68	1.395 (3)	C231—C236	1.3900
C67—H67	0.9500	C231—C237	1.5059 (13)
C68—H68	0.9500	C232—C233	1.3900
C69—C74	1.390 (3)	C232—D232	0.9500
C69—O6	1.398 (2)	C233—C234	1.3900
C69—C70	1.416 (3)	C233—D233	0.9500
C70—C71	1.386 (3)	C234—C235	1.3900
C70—C81	1.536 (3)	C234—D234	0.9500
C71—C72	1.389 (3)	C235—C236	1.3900
C71—H71	0.9500	C235—D235	0.9500
C72—O7	1.373 (2)	C236—D236	0.9500
C72—C73	1.376 (3)	C237—D23D	0.9800
C73—C74	1.399 (3)	C237—D23E	0.9800
C73—H73	0.9500	C237—D23F	0.9800
C6—C1—C2	124.31 (18)	C69—C74—C73	120.28 (18)
C6—C1—O1	119.50 (17)	C69—C74—C75	122.87 (17)
C2—C1—O1	116.13 (17)	C73—C74—C75	115.88 (17)
C3—C2—C1	116.46 (17)	C76—C75—C80	120.59 (18)
C3—C2—Rh1	122.31 (14)	C76—C75—C74	123.77 (17)
C1—C2—Rh1	120.72 (14)	C80—C75—C74	115.02 (17)
C2—C3—C4	122.48 (18)	C75—C76—O8	119.47 (17)
C2—C3—H3	118.8	C75—C76—C77	120.95 (17)
C4—C3—H3	118.8	O8—C76—C77	119.18 (17)
C5—C4—C3	117.78 (19)	C78—C77—C76	116.35 (18)
C5—C4—C7	123.16 (18)	C78—C77—C86	119.45 (17)
C3—C4—C7	119.05 (18)	C76—C77—C86	124.20 (17)
C4—C5—C6	123.46 (19)	C77—C78—C79	123.17 (19)
C4—C5—H5	118.3	C77—C78—H78	118.4
C6—C5—H5	118.3	C79—C78—H78	118.4
C1—C6—C5	115.36 (18)	O9—C79—C80	125.24 (19)
C1—C6—C11	123.94 (19)	O9—C79—C78	115.06 (18)
C5—C6—C11	120.70 (18)	C80—C79—C78	119.69 (18)
C9—C7—C10	109.0 (2)	C79—C80—C75	119.15 (18)
C9—C7—C8	108.03 (19)	C79—C80—H80	120.4
C10—C7—C8	108.7 (2)	C75—C80—H80	120.4
C9—C7—C4	112.12 (19)	C84—C81—C83	110.8 (2)
C10—C7—C4	108.50 (18)	C84—C81—C70	113.28 (19)
C8—C7—C4	110.46 (18)	C83—C81—C70	106.87 (19)
C7—C8—H8A	109.5	C84—C81—C82	106.4 (2)

C7—C8—H8B	109.5	C83—C81—C82	107.7 (2)
H8A—C8—H8B	109.5	C70—C81—C82	111.70 (18)
C7—C8—H8C	109.5	C81—C82—H82A	109.5
H8A—C8—H8C	109.5	C81—C82—H82B	109.5
H8B—C8—H8C	109.5	H82A—C82—H82B	109.5
C7—C9—H9A	109.5	C81—C82—H82C	109.5
C7—C9—H9B	109.5	H82A—C82—H82C	109.5
H9A—C9—H9B	109.5	H82B—C82—H82C	109.5
C7—C9—H9C	109.5	C81—C83—H83A	109.5
H9A—C9—H9C	109.5	C81—C83—H83B	109.5
H9B—C9—H9C	109.5	H83A—C83—H83B	109.5
C7—C10—H10A	109.5	C81—C83—H83C	109.5
C7—C10—H10B	109.5	H83A—C83—H83C	109.5
H10A—C10—H10B	109.5	H83B—C83—H83C	109.5
C7—C10—H10C	109.5	C81—C84—H84A	109.5
H10A—C10—H10C	109.5	C81—C84—H84B	109.5
H10B—C10—H10C	109.5	H84A—C84—H84B	109.5
C14—C11—C13	109.5 (2)	C81—C84—H84C	109.5
C14—C11—C12	107.3 (2)	H84A—C84—H84C	109.5
C13—C11—C12	107.5 (2)	H84B—C84—H84C	109.5
C14—C11—C6	110.74 (18)	O7—C85—H85A	109.5
C13—C11—C6	110.21 (18)	O7—C85—H85B	109.5
C12—C11—C6	111.48 (19)	H85A—C85—H85B	109.5
C11—C12—H12A	109.5	O7—C85—H85C	109.5
C11—C12—H12B	109.5	H85A—C85—H85C	109.5
H12A—C12—H12B	109.5	H85B—C85—H85C	109.5
C11—C12—H12C	109.5	C89—C86—C88	110.5 (2)
H12A—C12—H12C	109.5	C89—C86—C87	107.03 (19)
H12B—C12—H12C	109.5	C88—C86—C87	107.31 (18)
C11—C13—H13A	109.5	C89—C86—C77	109.54 (17)
C11—C13—H13B	109.5	C88—C86—C77	110.39 (17)
H13A—C13—H13B	109.5	C87—C86—C77	112.05 (17)
C11—C13—H13C	109.5	C86—C87—H87A	109.5
H13A—C13—H13C	109.5	C86—C87—H87B	109.5
H13B—C13—H13C	109.5	H87A—C87—H87B	109.5
C11—C14—H14A	109.5	C86—C87—H87C	109.5
C11—C14—H14B	109.5	H87A—C87—H87C	109.5
H14A—C14—H14B	109.5	H87B—C87—H87C	109.5
C11—C14—H14C	109.5	C86—C88—H88A	109.5
H14A—C14—H14C	109.5	C86—C88—H88B	109.5
H14B—C14—H14C	109.5	H88A—C88—H88B	109.5
C16—C15—O2	118.95 (17)	C86—C88—H88C	109.5
C16—C15—C20	121.90 (19)	H88A—C88—H88C	109.5
O2—C15—C20	119.11 (18)	H88B—C88—H88C	109.5
C17—C16—C15	120.18 (19)	C86—C89—H89A	109.5
C17—C16—H16	119.9	C86—C89—H89B	109.5
C15—C16—H16	119.9	H89A—C89—H89B	109.5
C16—C17—C18	121.1 (2)	C86—C89—H89C	109.5

C16—C17—H17	119.4	H89A—C89—H89C	109.5
C18—C17—H17	119.4	H89B—C89—H89C	109.5
C17—C18—C19	117.1 (2)	O9—C90—H90A	109.5
C17—C18—C21	119.9 (2)	O9—C90—H90B	109.5
C19—C18—C21	123.0 (2)	H90A—C90—H90B	109.5
C18—C19—C20	124.2 (2)	O9—C90—H90C	109.5
C18—C19—H19	117.9	H90A—C90—H90C	109.5
C20—C19—H19	117.9	H90B—C90—H90C	109.5
C19—C20—C15	115.44 (19)	O10—C91—C99	107.43 (15)
C19—C20—C25	121.01 (18)	O10—C91—C93	109.36 (15)
C15—C20—C25	123.53 (18)	C99—C91—C93	105.75 (15)
C24—C21—C23	108.9 (3)	O10—C91—C92	103.72 (14)
C24—C21—C22	109.1 (3)	C99—C91—C92	118.46 (15)
C23—C21—C22	108.4 (3)	C93—C91—C92	111.85 (15)
C24—C21—C18	109.2 (3)	O11—C92—C111	105.49 (15)
C23—C21—C18	112.2 (2)	O11—C92—C105	107.40 (14)
C22—C21—C18	109.0 (3)	C111—C92—C105	112.92 (15)
C21—C22—H22A	109.5	O11—C92—C91	101.84 (13)
C21—C22—H22B	109.5	C111—C92—C91	111.94 (15)
H22A—C22—H22B	109.5	C105—C92—C91	115.94 (16)
C21—C22—H22C	109.5	C94—C93—C98	118.41 (18)
H22A—C22—H22C	109.5	C94—C93—C91	121.27 (17)
H22B—C22—H22C	109.5	C98—C93—C91	120.31 (17)
C21—C23—H23A	109.5	C93—C94—C95	120.23 (19)
C21—C23—H23B	109.5	C93—C94—H94	119.9
H23A—C23—H23B	109.5	C95—C94—H94	119.9
C21—C23—H23C	109.5	C96—C95—C94	120.6 (2)
H23A—C23—H23C	109.5	C96—C95—H95	119.7
H23B—C23—H23C	109.5	C94—C95—H95	119.7
C21—C24—H24A	109.5	C95—C96—C97	119.7 (2)
C21—C24—H24B	109.5	C95—C96—H96	120.1
H24A—C24—H24B	109.5	C97—C96—H96	120.1
C21—C24—H24C	109.5	C98—C97—C96	119.8 (2)
H24A—C24—H24C	109.5	C98—C97—H97	120.1
H24B—C24—H24C	109.5	C96—C97—H97	120.1
C27—C25—C28	110.05 (19)	C97—C98—C93	120.99 (19)
C27—C25—C26	107.94 (18)	C97—C98—H98	119.5
C28—C25—C26	106.10 (18)	C93—C98—H98	119.5
C27—C25—C20	109.35 (17)	C100—C99—C104	118.78 (19)
C28—C25—C20	111.31 (17)	C100—C99—C91	118.34 (18)
C26—C25—C20	111.99 (17)	C104—C99—C91	122.57 (18)
C25—C26—H26A	109.5	C101—C100—C99	120.5 (2)
C25—C26—H26B	109.5	C101—C100—H100	119.7
H26A—C26—H26B	109.5	C99—C100—H100	119.7
C25—C26—H26C	109.5	C102—C101—C100	120.3 (2)
H26A—C26—H26C	109.5	C102—C101—H101	119.9
H26B—C26—H26C	109.5	C100—C101—H101	119.9
C25—C27—H27A	109.5	C103—C102—C101	119.8 (2)

C25—C27—H27B	109.5	C103—C102—H102	120.1
H27A—C27—H27B	109.5	C101—C102—H102	120.1
C25—C27—H27C	109.5	C102—C103—C104	119.9 (2)
H27A—C27—H27C	109.5	C102—C103—H103	120.0
H27B—C27—H27C	109.5	C104—C103—H103	120.0
C25—C28—H28A	109.5	C103—C104—C99	120.7 (2)
C25—C28—H28B	109.5	C103—C104—H104	119.6
H28A—C28—H28B	109.5	C99—C104—H104	119.6
C25—C28—H28C	109.5	C110—C105—C106	117.68 (19)
H28A—C28—H28C	109.5	C110—C105—C92	123.23 (18)
H28B—C28—H28C	109.5	C106—C105—C92	118.84 (18)
C30—C29—C34	121.28 (18)	C107—C106—C105	121.1 (2)
C30—C29—O3	119.95 (17)	C107—C106—H106	119.4
C34—C29—O3	118.68 (17)	C105—C106—H106	119.4
C31—C30—C29	120.69 (19)	C108—C107—C106	120.0 (2)
C31—C30—H30	119.7	C108—C107—H107	120.0
C29—C30—H30	119.7	C106—C107—H107	120.0
C30—C31—C32	120.93 (19)	C107—C108—C109	119.5 (2)
C30—C31—H31	119.5	C107—C108—H108	120.2
C32—C31—H31	119.5	C109—C108—H108	120.2
C31—C32—C33	116.90 (19)	C108—C109—C110	120.6 (2)
C31—C32—C35	121.31 (19)	C108—C109—H109	119.7
C33—C32—C35	121.79 (19)	C110—C109—H109	119.7
C32—C33—C34	124.4 (2)	C109—C110—C105	121.0 (2)
C32—C33—H33	117.8	C109—C110—H110	119.5
C34—C33—H33	117.8	C105—C110—H110	119.5
C33—C34—C29	115.74 (18)	C112—C111—C116	118.15 (18)
C33—C34—C39	120.49 (19)	C112—C111—C92	119.71 (17)
C29—C34—C39	123.67 (18)	C116—C111—C92	122.05 (18)
C36A—C35—C38A	112.6 (4)	C113—C112—C111	120.69 (19)
C37B—C35—C36B	111.8 (4)	C113—C112—H112	119.7
C37B—C35—C38B	105.1 (4)	C111—C112—H112	119.7
C36B—C35—C38B	106.7 (4)	C114—C113—C112	120.6 (2)
C36A—C35—C37A	106.8 (4)	C114—C113—H113	119.7
C38A—C35—C37A	107.4 (4)	C112—C113—H113	119.7
C36A—C35—C32	109.2 (2)	C115—C114—C113	119.3 (2)
C37B—C35—C32	110.1 (3)	C115—C114—H114	120.4
C38A—C35—C32	108.8 (2)	C113—C114—H114	120.4
C36B—C35—C32	110.4 (3)	C114—C115—C116	120.3 (2)
C38B—C35—C32	112.6 (3)	C114—C115—H115	119.9
C37A—C35—C32	112.2 (2)	C116—C115—H115	119.9
C35—C36A—H36A	109.5	C115—C116—C111	121.0 (2)
C35—C36A—H36B	109.5	C115—C116—H116	119.5
H36A—C36A—H36B	109.5	C111—C116—H116	119.5
C35—C36A—H36C	109.5	C118—C117—C122	120.0
H36A—C36A—H36C	109.5	C118—C117—C123	120.5 (4)
H36B—C36A—H36C	109.5	C122—C117—C123	119.4 (4)
C35—C37A—H37A	109.5	C119—C118—C117	120.0

C35—C37A—H37B	109.5	C119—C118—D118	120.0
H37A—C37A—H37B	109.5	C117—C118—D118	120.0
C35—C37A—H37C	109.5	C120—C119—C118	120.0
H37A—C37A—H37C	109.5	C120—C119—D119	120.0
H37B—C37A—H37C	109.5	C118—C119—D119	120.0
C35—C38A—H38A	109.5	C119—C120—C121	120.0
C35—C38A—H38B	109.5	C119—C120—D120	120.0
H38A—C38A—H38B	109.5	C121—C120—D120	120.0
C35—C38A—H38C	109.5	C122—C121—C120	120.0
H38A—C38A—H38C	109.5	C122—C121—D121	120.0
H38B—C38A—H38C	109.5	C120—C121—D121	120.0
C35—C36B—H36D	109.5	C121—C122—C117	120.0
C35—C36B—H36E	109.5	C121—C122—D122	120.0
H36D—C36B—H36E	109.5	C117—C122—D122	120.0
C35—C36B—H36F	109.5	C117—C123—D12D	109.5
H36D—C36B—H36F	109.5	C117—C123—D12E	109.5
H36E—C36B—H36F	109.5	D12D—C123—D12E	109.5
C35—C37B—H37D	109.5	C117—C123—D12F	109.5
C35—C37B—H37E	109.5	D12D—C123—D12F	109.5
H37D—C37B—H37E	109.5	D12E—C123—D12F	109.5
C35—C37B—H37F	109.5	C218—C217—C222	120.0
H37D—C37B—H37F	109.5	C218—C217—C223	120.01 (12)
H37E—C37B—H37F	109.5	C222—C217—C223	119.97 (12)
C35—C38B—H38D	109.5	C219—C218—C217	120.0
C35—C38B—H38E	109.5	C219—C218—D218	120.0
H38D—C38B—H38E	109.5	C217—C218—D218	120.0
C35—C38B—H38F	109.5	C218—C219—C220	120.0
H38D—C38B—H38F	109.5	C218—C219—D219	120.0
H38E—C38B—H38F	109.5	C220—C219—D219	120.0
C42—C39—C41	111.16 (19)	C219—C220—C221	120.0
C42—C39—C40	107.43 (19)	C219—C220—D220	120.0
C41—C39—C40	106.35 (19)	C221—C220—D220	120.0
C42—C39—C34	111.00 (18)	C220—C221—C222	120.0
C41—C39—C34	108.75 (18)	C220—C221—D221	120.0
C40—C39—C34	112.08 (19)	C222—C221—D221	120.0
C39—C40—H40A	109.5	C221—C222—C217	120.0
C39—C40—H40B	109.5	C221—C222—D222	120.0
H40A—C40—H40B	109.5	C217—C222—D222	120.0
C39—C40—H40C	109.5	C217—C223—D22D	109.5
H40A—C40—H40C	109.5	C217—C223—D22E	109.5
H40B—C40—H40C	109.5	D22D—C223—D22E	109.5
C39—C41—H41A	109.5	C217—C223—D22F	109.5
C39—C41—H41B	109.5	D22D—C223—D22F	109.5
H41A—C41—H41B	109.5	D22E—C223—D22F	109.5
C39—C41—H41C	109.5	C125—C124—C129	120.0
H41A—C41—H41C	109.5	C125—C124—C130	119.8 (2)
H41B—C41—H41C	109.5	C129—C124—C130	120.2 (2)
C39—C42—H42A	109.5	C126—C125—C124	120.0

C39—C42—H42B	109.5	C126—C125—D125	120.0
H42A—C42—H42B	109.5	C124—C125—D125	120.0
C39—C42—H42C	109.5	C127—C126—C125	120.0
H42A—C42—H42C	109.5	C127—C126—D126	120.0
H42B—C42—H42C	109.5	C125—C126—D126	120.0
O4—C43—C45	106.74 (15)	C126—C127—C128	120.0
O4—C43—C51	105.58 (15)	C126—C127—D127	120.0
C45—C43—C51	113.40 (16)	C128—C127—D127	120.0
O4—C43—C44	101.18 (13)	C129—C128—C127	120.0
C45—C43—C44	111.79 (16)	C129—C128—D128	120.0
C51—C43—C44	116.66 (15)	C127—C128—D128	120.0
O5—C44—C57	107.08 (15)	C128—C129—C124	120.0
O5—C44—C63	108.66 (14)	C128—C129—D129	120.0
C57—C44—C63	104.76 (15)	C124—C129—D129	120.0
O5—C44—C43	102.83 (14)	C124—C130—D13D	109.5
C57—C44—C43	119.08 (15)	C124—C130—D13E	109.5
C63—C44—C43	113.96 (15)	D13D—C130—D13E	109.5
C46—C45—C50	118.38 (18)	C124—C130—D13F	109.5
C46—C45—C43	120.56 (17)	D13D—C130—D13F	109.5
C50—C45—C43	120.76 (18)	D13E—C130—D13F	109.5
C45—C46—C47	120.89 (19)	C1—O1—P1	112.83 (12)
C45—C46—H46	119.6	C15—O2—P1	124.83 (12)
C47—C46—H46	119.6	C29—O3—P1	128.55 (13)
C48—C47—C46	120.1 (2)	C43—O4—P2	114.47 (11)
C48—C47—H47	119.9	C44—O5—P2	114.21 (11)
C46—C47—H47	119.9	C69—O6—P2	129.22 (12)
C49—C48—C47	119.5 (2)	C72—O7—C85	116.75 (18)
C49—C48—H48	120.2	C76—O8—P3	133.12 (12)
C47—C48—H48	120.2	C79—O9—C90	117.42 (17)
C48—C49—C50	120.3 (2)	C91—O10—P3	115.16 (11)
C48—C49—H49	119.9	C92—O11—P3	115.16 (11)
C50—C49—H49	119.9	O3—P1—O1	97.62 (8)
C49—C50—C45	120.7 (2)	O3—P1—O2	97.30 (7)
C49—C50—H50	119.6	O1—P1—O2	100.85 (7)
C45—C50—H50	119.6	O3—P1—Rh1	117.86 (6)
C56—C51—C52	117.94 (19)	O1—P1—Rh1	106.77 (5)
C56—C51—C43	123.02 (18)	O2—P1—Rh1	130.81 (6)
C52—C51—C43	118.80 (18)	O4—P2—O6	99.95 (7)
C53—C52—C51	121.2 (2)	O4—P2—O5	93.68 (7)
C53—C52—H52	119.4	O6—P2—O5	102.33 (7)
C51—C52—H52	119.4	O4—P2—Rh1	114.21 (5)
C54—C53—C52	120.0 (2)	O6—P2—Rh1	128.14 (5)
C54—C53—H53	120.0	O5—P2—Rh1	112.54 (5)
C52—C53—H53	120.0	O11—P3—O10	94.10 (7)
C53—C54—C55	119.6 (2)	O11—P3—O8	98.08 (7)
C53—C54—H54	120.2	O10—P3—O8	102.44 (7)
C55—C54—H54	120.2	O11—P3—Rh1	118.44 (5)
C54—C55—C56	120.3 (2)	O10—P3—Rh1	113.01 (5)

C54—C55—H55	119.8	O8—P3—Rh1	125.32 (5)
C56—C55—H55	119.8	C2—Rh1—P1	77.71 (5)
C55—C56—C51	120.9 (2)	C2—Rh1—P2	159.49 (6)
C55—C56—H56	119.6	P1—Rh1—P2	102.172 (18)
C51—C56—H56	119.6	C2—Rh1—P3	90.23 (5)
C58—C57—C62	118.33 (19)	P1—Rh1—P3	143.592 (18)
C58—C57—C44	125.30 (19)	P2—Rh1—P3	100.696 (18)
C62—C57—C44	116.06 (17)	C132—C131—C136	120.0
C57—C58—C59	120.2 (2)	C132—C131—C137	123.0 (7)
C57—C58—H58	119.9	C136—C131—C137	117.0 (7)
C59—C58—H58	119.9	C131—C132—C133	120.0
C60—C59—C58	120.8 (2)	C131—C132—D132	120.0
C60—C59—H59	119.6	C133—C132—D132	120.0
C58—C59—H59	119.6	C134—C133—C132	120.0
C59—C60—C61	119.5 (2)	C134—C133—D133	120.0
C59—C60—H60	120.3	C132—C133—D133	120.0
C61—C60—H60	120.3	C135—C134—C133	120.0
C60—C61—C62	120.1 (2)	C135—C134—D134	120.0
C60—C61—H61	119.9	C133—C134—D134	120.0
C62—C61—H61	119.9	C134—C135—C136	120.0
C61—C62—C57	121.1 (2)	C134—C135—D135	120.0
C61—C62—H62	119.5	C136—C135—D135	120.0
C57—C62—H62	119.5	C135—C136—C131	120.0
C68—C63—C64	118.23 (19)	C135—C136—D136	120.0
C68—C63—C44	121.54 (17)	C131—C136—D136	120.0
C64—C63—C44	119.90 (18)	C131—C137—D13G	109.5
C65—C64—C63	120.9 (2)	C131—C137—D13H	109.5
C65—C64—H64	119.5	D13G—C137—D13H	109.5
C63—C64—H64	119.5	C131—C137—D13I	109.5
C64—C65—C66	120.4 (2)	D13G—C137—D13I	109.5
C64—C65—H65	119.8	D13H—C137—D13I	109.5
C66—C65—H65	119.8	C232—C231—C236	120.0
C67—C66—C65	119.3 (2)	C232—C231—C237	120.05 (11)
C67—C66—H66	120.3	C236—C231—C237	119.95 (11)
C65—C66—H66	120.3	C231—C232—C233	120.0
C66—C67—C68	120.3 (2)	C231—C232—D232	120.0
C66—C67—H67	119.8	C233—C232—D232	120.0
C68—C67—H67	119.8	C234—C233—C232	120.0
C63—C68—C67	120.80 (19)	C234—C233—D233	120.0
C63—C68—H68	119.6	C232—C233—D233	120.0
C67—C68—H68	119.6	C233—C234—C235	120.0
C74—C69—O6	119.44 (16)	C233—C234—D234	120.0
C74—C69—C70	121.01 (17)	C235—C234—D234	120.0
O6—C69—C70	119.18 (16)	C234—C235—C236	120.0
C71—C70—C69	116.51 (18)	C234—C235—D235	120.0
C71—C70—C81	119.22 (18)	C236—C235—D235	120.0
C69—C70—C81	124.23 (17)	C235—C236—C231	120.0
C70—C71—C72	122.88 (19)	C235—C236—D236	120.0

C70—C71—H71	118.6	C231—C236—D236	120.0
C72—C71—H71	118.6	C231—C237—D23D	109.5
O7—C72—C73	125.30 (19)	C231—C237—D23E	109.5
O7—C72—C71	114.81 (18)	D23D—C237—D23E	109.5
C73—C72—C71	119.88 (18)	C231—C237—D23F	109.5
C72—C73—C74	119.29 (18)	D23D—C237—D23F	109.5
C72—C73—H73	120.4	D23E—C237—D23F	109.5
C74—C73—H73	120.4		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C30—H30 \cdots O4	0.95	2.35	3.234 (2)	155
C46—H46 \cdots O2	0.95	2.52	3.405 (2)	155
C56—H56 \cdots O5	0.95	2.56	3.136 (3)	120