

Carbonylbis{6,6'-[(3,3'-di-*tert*-butyl-5,5'-dimethoxy-1,1'-biphenyl-2,2'-diyl)bis(oxy)]bis(dibenzo-*[d,f]*[1,3,2]-dioxaphosphepine)}hydridorhodium(I) toluene-*d*₈ 2.25-solvate

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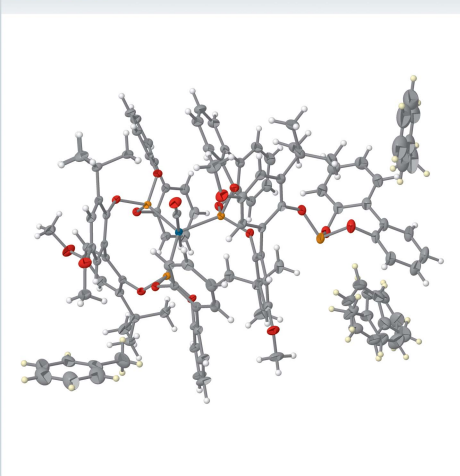
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Structural data: full structural data are available from iucrdata.iucr.org

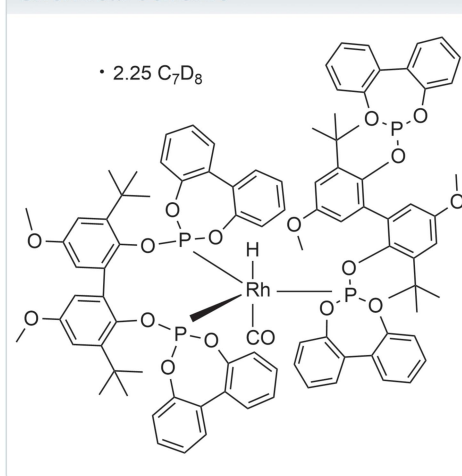
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The crystal-structure determination of the title compound, $[\text{RhH}(\text{C}_{46}\text{H}_{44}\text{O}_8\text{P}_2)(\text{CO})] \cdot 2.25\text{C}_7\text{D}_8$, is reported. The bisphosphite ligand, $\text{C}_{46}\text{H}_{44}\text{O}_8\text{P}_2$, is well known as Biphephos. One specific characteristic of this hydrido rhodium(I) monocarbonyl complex is that one bisphosphite ligand is coordinated in the expected bidentate mode and the other is coordinated in a monodentate mode. Thus, one phosphite moiety remains non-coordinating. All three coordinating phosphorus atoms occupy the equatorial positions in the trigonal-bipyramidal environment around the rhodium atom. The crystals of the hydrido rhodium(I) monocarbonyl complex contains deuterated solvent molecules (toluene-*d*₈). Most of them are included in the model, but the contributions of about 0.84 toluene per unit cell were removed from the diffraction data, using the SQUEEZE procedure in *PLATON* [Spek (2015). *Acta Cryst. C* **71**, 9–18].

3D view



Chemical scheme



Structure description

The crystal structure of the bisphosphite ligand Biphephos has recently been studied (Leidecker *et al.*, 2019). Biphephos is applied as a co-catalyst for the formation of the respective bisphosphite-modified hydrido rhodium(I) dicarbonyl complex $[\text{RhH}(\text{CO})_2(\text{Biphephos})]$ as catalyst for highly *n*-regioselective alkene hydroformylation (Börner & Franke, 2016; Moasser *et al.*, 1995). This rhodium dicarbonyl complex converts in the presence of an additional equivalent of free Biphephos and in the absence of

carbon monoxide into a monocarbonyl complex, during which the carbonyl ligand in the equatorial position is substituted by one phosphite moiety. The coordination environment around the rhodium(I) atom can be described as distorted trigonal–bipyramidal with three phosphorus atoms coordinating in the equatorial positions (Fig. 1). The occupation of the equatorial positions by the phosphorus atoms of the chelating Biphephos ligand is known from spectroscopic studies in solution (Moasser *et al.*, 1995). The preference for the coordination at the equatorial position of the third phosphorus atom belonging to the second ligand is caused by steric properties (Selent *et al.*, 2013; van der Veen *et al.*, 1998). The distances Rh1–P1 = 2.2325 (4) Å, Rh1–P2 = 2.2572 (4) Å and Rh1–P3 = 2.2600 (4) Å are comparable to those in complexes of the type [RhH(CO)₂(P(OP))], with bisphosphites as a ligand (van Rooy *et al.*, 1996; Selent *et al.*, 2012; Mormul *et al.*, 2015). The angle P1–Rh1–P2 = 118.79 (2)° is related to the chelating coordination mode of one ligand. The other P–Rh–P angles with P2–Rh1–P3 = 106.08 (2)° and P1–Rh1–P3 = 128.40 (2)° differ significantly from the ideal trigonal–bipyramidal geometry. The hydrido ligand and the carbonyl ligand coordinate at the axial positions. The crystals of the hydrido rhodium(I) monocarbonyl complex contain three sites including toluene-*d*₈ solvent molecules, two of which are partly occupied and disordered (Fig. 2). Additionally, the contributions of heavily disordered toluene-*d*₈ (0.84 molecules per unit cell) were removed from the diffraction data using the SQUEEZE procedure in PLATON (Spek, 2015).

Synthesis and crystallization

The bisphosphite Biphephos was provided by Evonik Operations GmbH (OxoPhos® 17). [Rh(acac)(CO)₂] (25.8 mg, 0.15 mmol) and Biphephos (157.36 mg, 0.20 mmol) were dissolved in 5 ml of toluene-*d*₈, transferred into a stainless-steel reactor (Swagelock®) and treated with synthesis gas

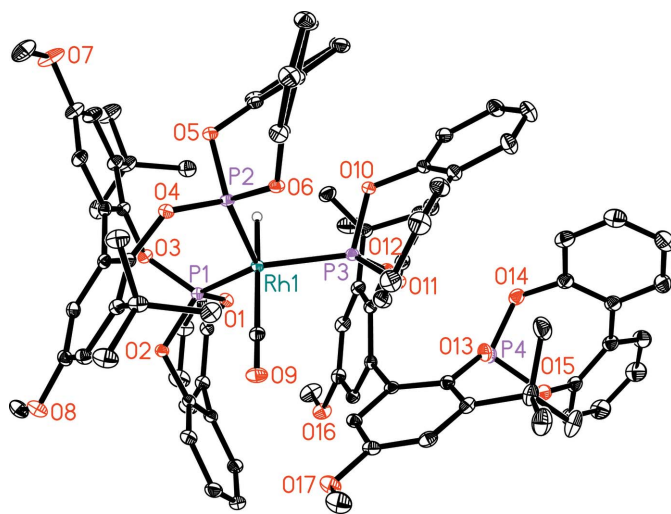


Figure 1
Molecular structure of the title compound with displacement ellipsoids drawn at 30% probability level. Co-crystallized solvent and C-bound hydrogen atoms are omitted for clarity.

Table 1
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | [RhH(C ₄₆ H ₄₄ O ₈ P ₂) ₂ (CO)]·2.25C ₇ D ₈ |
| <i>M_r</i> | 1930.84 |
| Crystal system, space group | Triclinic, <i>P</i> $\bar{1}$ |
| Temperature (K) | 150 |
| <i>a</i> , <i>b</i> , <i>c</i> (Å) | 13.5471 (10), 18.9745 (15), 19.8784 (16) |
| α , β , γ (°) | 77.0694 (17), 82.7785 (17), 77.2409 (17) |
| <i>V</i> (Å ³) | 4841.5 (7) |
| <i>Z</i> | 2 |
| Radiation type | Mo <i>K</i> α |
| μ (mm ⁻¹) | 0.31 |
| Crystal size (mm) | 0.43 × 0.28 × 0.22 |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (SADABS; Bruker, 2016) |
| <i>T_{min}</i> , <i>T_{max}</i> | 0.88, 0.94 |
| No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections | 143429, 23351, 20576 |
| <i>R_{int}</i> | 0.030 |
| (<i>sin</i> θ / λ) _{max} (Å ⁻¹) | 0.661 |
| Refinement | |
| <i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i> | 0.031, 0.087, 1.04 |
| No. of reflections | 23351 |
| No. of parameters | 1261 |
| No. of restraints | 258 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³) | 0.81, -0.79 |

Computer programs: APEX3 and SAINT (Bruker, 2019), SHELXT2014 (Sheldrick, 2015a), SHELXL2018 (Sheldrick, 2015b), XP in SHELXTL (Sheldrick, 2008) and publCIF (Westrip, 2010).

(20 bar) at 50°C for 2 h. After the reaction, the pressure was reduced to atmospheric pressure of the synthesis gas. Afterwards the sample was purged 12 times with pure hydrogen and the gas atmosphere completely exchanged and then cooled

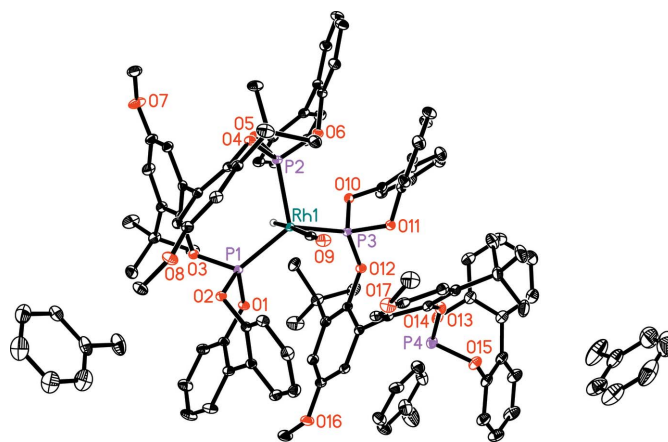


Figure 2
Molecular structure of the title compound with displacement ellipsoids drawn at 30% probability level. Deuterium and C-bound hydrogen atoms are omitted for clarity. Disordered solvent molecules are shown in only one orientation.

down to room temperature. During slow evaporation of toluene- d_8 at room temperature, fine colourless crystals were obtained and measured *via* single-crystal X-ray diffraction. The catalyst pre-formation starting from $[\text{Rh}(\text{acac})(\text{CO})_2]$ as a precursor in the presence of a bisphosphite ligand under *in situ* conditions at elevated pressures of synthesis gas (CO/H_2) is an established procedure (Börner & Franke, 2016). Toluene- d_8 was chosen because the highly concentrated catalyst solution was also used for further NMR-spectroscopic measurements. Crystallization of the carbonyl hydrido Rh^{I} complex might also be possible from other solvents such as non-deuterated benzene or toluene.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The hydride (H1) could be found from the difference-Fourier map and was refined with free coordinates. The crystals of the hydrido rhodium(I) mono-carbonyl complex contain solvent (toluene- d_8). The disordered solvent molecules were refined with the benzene rings constrained to have an idealized geometry (flat hexagon with C–C bond lengths of 1.39 Å). Moreover, disordered solvent molecules placed on the same site were restrained to have similar U_{ij} parameters, with standard deviation of 0.04 \AA^2 (Sheldrick, 2015b). The contributions of some additional disordered solvent were removed from the diffraction data using the SQUEEZE procedure in PLATON (Spek, 2015). SQUEEZE estimated the electron counts in the void of

197 \AA^3 volume to be 42, which corresponds to 0.84 disordered toluene molecules per triclinic unit cell.

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full crystallographic data

IUCrData (2023). **8**, x230083 [https://doi.org/10.1107/S2414314623000834]

Carbonylbis{6,6'-[(3,3'-di-*tert*-butyl-5,5'-dimethoxy-1,1'-biphenyl-2,2'-diyl)bis(oxy)]bis(dibenzo[*d,f*][1,3,2]-dioxaphosphepine)}hydridorhodium(I) toluene-*d*₈ 2.25-solvate

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Crystal data

[RhH(C₄₆H₄₄O₈P₂)₂(CO)]·2.25C₇D₈

M_r = 1930.84

Triclinic, *P* $\bar{1}$

a = 13.5471 (10) Å

b = 18.9745 (15) Å

c = 19.8784 (16) Å

α = 77.0694 (17)°

β = 82.7785 (17)°

γ = 77.2409 (17)°

V = 4841.5 (7) Å³

Z = 2

F(000) = 2001

D_x = 1.324 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 9835 reflections

θ = 2.3–30.6°

μ = 0.31 mm⁻¹

T = 150 K

Prism, colourless

0.43 × 0.28 × 0.22 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, 2016)

T_{min} = 0.88, *T_{max}* = 0.94

143429 measured reflections

23351 independent reflections

20576 reflections with *I* > 2σ(*I*)

R_{int} = 0.030

θ_{max} = 28.0°, θ_{min} = 1.7°

h = -17→17

k = -25→25

l = -26→26

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.031

wR(*F*²) = 0.087

S = 1.04

23351 reflections

1261 parameters

258 restraints

Primary atom site location: dual

Secondary atom site location: difference Fourier
map

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

w = 1/[σ²(*F_o*²) + (0.042*P*)² + 3.4299*P*]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} = 0.005

Δρ_{max} = 0.81 e Å⁻³

Δρ_{min} = -0.79 e Å⁻³

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 | 0.42212 (12) | 0.25587 (9) | 0.63980 (8) | 0.0195 (3) | |
| C2 | 0.32459 (13) | 0.24708 (10) | 0.66485 (9) | 0.0262 (3) | |
| H2 | 0.308763 | 0.231954 | 0.713155 | 0.031* | |
| C3 | 0.25002 (14) | 0.26048 (12) | 0.61908 (10) | 0.0342 (4) | |
| H3 | 0.183389 | 0.253338 | 0.635867 | 0.041* | |
| C4 | 0.27291 (14) | 0.28421 (13) | 0.54907 (10) | 0.0376 (5) | |
| H4 | 0.221752 | 0.293947 | 0.517751 | 0.045* | |
| C5 | 0.36990 (14) | 0.29378 (11) | 0.52460 (9) | 0.0301 (4) | |
| H5 | 0.384595 | 0.310262 | 0.476349 | 0.036* | |
| C6 | 0.44721 (12) | 0.27975 (9) | 0.56924 (8) | 0.0215 (3) | |
| C7 | 0.55070 (12) | 0.28787 (9) | 0.54017 (8) | 0.0200 (3) | |
| C8 | 0.56699 (14) | 0.34519 (9) | 0.48448 (8) | 0.0254 (3) | |
| H8 | 0.511279 | 0.383168 | 0.468993 | 0.030* | |
| C9 | 0.66276 (15) | 0.34736 (10) | 0.45171 (9) | 0.0285 (4) | |
| H9 | 0.672561 | 0.386993 | 0.414420 | 0.034* | |
| C10 | 0.74467 (14) | 0.29182 (10) | 0.47313 (9) | 0.0274 (4) | |
| H10 | 0.810079 | 0.292541 | 0.449590 | 0.033* | |
| C11 | 0.73085 (13) | 0.23522 (10) | 0.52898 (8) | 0.0229 (3) | |
| H11 | 0.786702 | 0.197205 | 0.544126 | 0.027* | |
| C12 | 0.63514 (12) | 0.23462 (8) | 0.56238 (8) | 0.0182 (3) | |
| C13 | 0.59038 (12) | 0.05302 (8) | 0.77726 (8) | 0.0179 (3) | |
| C14 | 0.51693 (12) | 0.02764 (9) | 0.82873 (9) | 0.0220 (3) | |
| C15 | 0.55128 (13) | −0.03125 (10) | 0.88114 (9) | 0.0286 (4) | |
| H15 | 0.503871 | −0.048132 | 0.917252 | 0.034* | |
| C16 | 0.65253 (13) | −0.06635 (10) | 0.88262 (9) | 0.0268 (4) | |
| C17 | 0.72217 (12) | −0.04354 (9) | 0.83031 (9) | 0.0220 (3) | |
| H17 | 0.791109 | −0.068632 | 0.830406 | 0.026* | |
| C18 | 0.69157 (12) | 0.01671 (8) | 0.77682 (8) | 0.0180 (3) | |
| C19 | 0.77139 (11) | 0.03281 (8) | 0.71980 (8) | 0.0171 (3) | |
| C20 | 0.75729 (12) | 0.02787 (8) | 0.65281 (8) | 0.0195 (3) | |
| H20 | 0.693878 | 0.021300 | 0.642210 | 0.023* | |
| C21 | 0.83651 (12) | 0.03264 (9) | 0.60206 (8) | 0.0210 (3) | |
| C22 | 0.93152 (12) | 0.03660 (9) | 0.61895 (8) | 0.0218 (3) | |
| H22 | 0.986484 | 0.035555 | 0.584192 | 0.026* | |
| C23 | 0.94881 (12) | 0.04204 (9) | 0.68493 (8) | 0.0187 (3) | |
| C24 | 0.86465 (11) | 0.04375 (8) | 0.73404 (8) | 0.0170 (3) | |
| C25 | 0.40242 (12) | 0.05992 (10) | 0.82745 (9) | 0.0260 (3) | |
| C26 | 0.34023 (15) | 0.01518 (13) | 0.88465 (12) | 0.0437 (5) | |
| H26A | 0.353568 | −0.036112 | 0.878863 | 0.066* | |
| H26B | 0.267748 | 0.036479 | 0.881478 | 0.066* | |
| H26C | 0.359760 | 0.016677 | 0.930063 | 0.066* | |
| C27 | 0.37977 (14) | 0.13918 (10) | 0.83949 (10) | 0.0297 (4) | |
| H27A | 0.397047 | 0.138879 | 0.885981 | 0.045* | |
| H27B | 0.307457 | 0.160421 | 0.835253 | 0.045* | |
| H27C | 0.420336 | 0.168886 | 0.804922 | 0.045* | |

| | | | | |
|------|--------------|---------------|--------------|------------|
| C28 | 0.36607 (14) | 0.05719 (11) | 0.75823 (11) | 0.0324 (4) |
| H28A | 0.401237 | 0.087404 | 0.720327 | 0.049* |
| H28B | 0.292704 | 0.076368 | 0.758271 | 0.049* |
| H28C | 0.381036 | 0.006049 | 0.751853 | 0.049* |
| C29 | 0.77303 (15) | -0.16684 (11) | 0.93774 (12) | 0.0399 (5) |
| H29A | 0.787523 | -0.188646 | 0.896416 | 0.060* |
| H29B | 0.778563 | -0.206213 | 0.979281 | 0.060* |
| H29C | 0.821925 | -0.135584 | 0.937322 | 0.060* |
| C30 | 0.73383 (14) | 0.02611 (11) | 0.51633 (9) | 0.0299 (4) |
| H30A | 0.716145 | -0.020522 | 0.541910 | 0.045* |
| H30B | 0.736870 | 0.027838 | 0.466486 | 0.045* |
| H30C | 0.682196 | 0.067450 | 0.528282 | 0.045* |
| C31 | 1.05574 (12) | 0.04355 (9) | 0.70251 (8) | 0.0217 (3) |
| C32 | 1.06044 (13) | 0.12047 (10) | 0.71223 (10) | 0.0268 (4) |
| H32A | 1.127850 | 0.119950 | 0.725598 | 0.040* |
| H32B | 1.008792 | 0.134563 | 0.748594 | 0.040* |
| H32C | 1.047704 | 0.156162 | 0.668712 | 0.040* |
| C33 | 1.13607 (13) | 0.02420 (12) | 0.64446 (9) | 0.0312 (4) |
| H33A | 1.203608 | 0.022885 | 0.658085 | 0.047* |
| H33B | 1.122918 | 0.061583 | 0.602033 | 0.047* |
| H33C | 1.133043 | -0.024244 | 0.636133 | 0.047* |
| C34 | 1.08489 (13) | -0.01414 (10) | 0.76818 (9) | 0.0279 (4) |
| H34A | 1.080646 | -0.063045 | 0.761656 | 0.042* |
| H34B | 1.038183 | -0.001826 | 0.807581 | 0.042* |
| H34C | 1.154439 | -0.014381 | 0.777220 | 0.042* |
| C35 | 0.70504 (12) | 0.12252 (9) | 0.94496 (8) | 0.0189 (3) |
| C36 | 0.59996 (13) | 0.13809 (9) | 0.95051 (8) | 0.0238 (3) |
| H36 | 0.563263 | 0.120983 | 0.921847 | 0.029* |
| C37 | 0.54907 (14) | 0.17908 (10) | 0.99859 (9) | 0.0291 (4) |
| H37 | 0.476961 | 0.190741 | 1.002691 | 0.035* |
| C38 | 0.60332 (14) | 0.20296 (10) | 1.04056 (9) | 0.0297 (4) |
| H38 | 0.568328 | 0.231872 | 1.072800 | 0.036* |
| C39 | 0.70817 (14) | 0.18500 (10) | 1.03584 (8) | 0.0261 (3) |
| H39 | 0.744436 | 0.200564 | 1.065900 | 0.031* |
| C40 | 0.76168 (12) | 0.14432 (9) | 0.98758 (8) | 0.0203 (3) |
| C41 | 0.87337 (12) | 0.12243 (9) | 0.98350 (8) | 0.0199 (3) |
| C42 | 0.92347 (14) | 0.09598 (10) | 1.04425 (8) | 0.0253 (3) |
| H42 | 0.885115 | 0.094826 | 1.087774 | 0.030* |
| C43 | 1.02729 (14) | 0.07153 (10) | 1.04241 (9) | 0.0286 (4) |
| H43 | 1.059743 | 0.053097 | 1.084296 | 0.034* |
| C44 | 1.08399 (13) | 0.07397 (10) | 0.97928 (9) | 0.0284 (4) |
| H44 | 1.155508 | 0.057008 | 0.977852 | 0.034* |
| C45 | 1.03679 (12) | 0.10109 (9) | 0.91807 (9) | 0.0234 (3) |
| H45 | 1.075807 | 0.103600 | 0.874725 | 0.028* |
| C46 | 0.93244 (12) | 0.12444 (9) | 0.92069 (8) | 0.0188 (3) |
| C47 | 0.81351 (12) | 0.23393 (8) | 0.68053 (8) | 0.0192 (3) |
| C48 | 0.70024 (13) | 0.35017 (9) | 0.91966 (8) | 0.0214 (3) |
| C49 | 0.61875 (14) | 0.37551 (10) | 0.96322 (9) | 0.0259 (3) |

| | | | | |
|------|--------------|--------------|--------------|------------|
| H49 | 0.553522 | 0.366098 | 0.960404 | 0.031* |
| C50 | 0.63297 (16) | 0.41482 (11) | 1.01110 (10) | 0.0336 (4) |
| H50 | 0.577531 | 0.432170 | 1.041466 | 0.040* |
| C51 | 0.72792 (17) | 0.42863 (12) | 1.01447 (10) | 0.0382 (5) |
| H51 | 0.737729 | 0.455574 | 1.047183 | 0.046* |
| C52 | 0.80860 (16) | 0.40344 (11) | 0.97050 (10) | 0.0339 (4) |
| H52 | 0.873341 | 0.413826 | 0.973041 | 0.041* |
| C53 | 0.79699 (13) | 0.36280 (9) | 0.92213 (8) | 0.0235 (3) |
| C54 | 0.88568 (13) | 0.33399 (9) | 0.87779 (8) | 0.0223 (3) |
| C55 | 0.98111 (14) | 0.30683 (11) | 0.90344 (10) | 0.0296 (4) |
| H55 | 0.988165 | 0.304236 | 0.950933 | 0.036* |
| C56 | 1.06532 (14) | 0.28370 (11) | 0.86118 (11) | 0.0334 (4) |
| H56 | 1.129470 | 0.265195 | 0.879742 | 0.040* |
| C57 | 1.05660 (14) | 0.28738 (11) | 0.79183 (10) | 0.0313 (4) |
| H57 | 1.114857 | 0.272016 | 0.762691 | 0.038* |
| C58 | 0.96267 (13) | 0.31353 (10) | 0.76485 (9) | 0.0256 (3) |
| H58 | 0.956162 | 0.316056 | 0.717294 | 0.031* |
| C59 | 0.87887 (12) | 0.33581 (9) | 0.80783 (8) | 0.0207 (3) |
| C60 | 0.54080 (12) | 0.41447 (8) | 0.72704 (8) | 0.0182 (3) |
| C61 | 0.43708 (12) | 0.41405 (9) | 0.74140 (8) | 0.0216 (3) |
| C62 | 0.37798 (13) | 0.43351 (9) | 0.68472 (9) | 0.0246 (3) |
| H62 | 0.307199 | 0.434093 | 0.692641 | 0.029* |
| C63 | 0.41949 (13) | 0.45192 (9) | 0.61750 (9) | 0.0231 (3) |
| C64 | 0.52104 (12) | 0.45603 (9) | 0.60494 (8) | 0.0207 (3) |
| H64 | 0.549071 | 0.470317 | 0.558895 | 0.025* |
| C65 | 0.58180 (12) | 0.43918 (8) | 0.65986 (8) | 0.0179 (3) |
| C66 | 0.68838 (12) | 0.45020 (8) | 0.64356 (8) | 0.0181 (3) |
| C67 | 0.75044 (12) | 0.41007 (9) | 0.59845 (8) | 0.0204 (3) |
| H67 | 0.724431 | 0.377046 | 0.579173 | 0.024* |
| C68 | 0.84993 (13) | 0.41801 (9) | 0.58152 (8) | 0.0230 (3) |
| C69 | 0.88908 (13) | 0.46384 (10) | 0.61169 (9) | 0.0250 (3) |
| H69 | 0.958743 | 0.466546 | 0.601667 | 0.030* |
| C70 | 0.82906 (13) | 0.50622 (9) | 0.65647 (9) | 0.0240 (3) |
| C71 | 0.72668 (12) | 0.50085 (9) | 0.66933 (8) | 0.0206 (3) |
| C72 | 0.38586 (13) | 0.39671 (10) | 0.81529 (9) | 0.0266 (4) |
| C73 | 0.42883 (15) | 0.31787 (10) | 0.85263 (10) | 0.0314 (4) |
| H73A | 0.499998 | 0.313809 | 0.860581 | 0.047* |
| H73B | 0.424437 | 0.282978 | 0.823994 | 0.047* |
| H73C | 0.389515 | 0.306474 | 0.897145 | 0.047* |
| C74 | 0.27127 (15) | 0.40266 (15) | 0.81441 (12) | 0.0474 (6) |
| H74A | 0.240722 | 0.392414 | 0.862048 | 0.071* |
| H74B | 0.259294 | 0.366778 | 0.789289 | 0.071* |
| H74C | 0.240548 | 0.452582 | 0.791326 | 0.071* |
| C75 | 0.40062 (16) | 0.45228 (10) | 0.85638 (10) | 0.0335 (4) |
| H75A | 0.370478 | 0.439930 | 0.903911 | 0.050* |
| H75B | 0.367508 | 0.502030 | 0.834459 | 0.050* |
| H75C | 0.473341 | 0.450477 | 0.857118 | 0.050* |
| C76 | 0.25979 (15) | 0.46869 (13) | 0.57090 (12) | 0.0414 (5) |

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|------|--------------|--------------|--------------|------------|
| H76A | 0.249057 | 0.420916 | 0.598562 | 0.062* |
| H76B | 0.231241 | 0.477393 | 0.526155 | 0.062* |
| H76C | 0.226127 | 0.507946 | 0.595569 | 0.062* |
| C77 | 1.01065 (15) | 0.36759 (13) | 0.53015 (12) | 0.0409 (5) |
| H77A | 1.032025 | 0.414601 | 0.510721 | 0.061* |
| H77B | 1.040316 | 0.332149 | 0.500469 | 0.061* |
| H77C | 1.033818 | 0.348279 | 0.576720 | 0.061* |
| C78 | 0.87709 (14) | 0.55480 (10) | 0.69058 (11) | 0.0319 (4) |
| C79 | 0.83163 (18) | 0.63643 (11) | 0.66452 (14) | 0.0458 (5) |
| H79A | 0.865554 | 0.667007 | 0.683988 | 0.069* |
| H79B | 0.758889 | 0.646113 | 0.679041 | 0.069* |
| H79C | 0.841367 | 0.648399 | 0.613868 | 0.069* |
| C80 | 0.99240 (16) | 0.54428 (13) | 0.67246 (13) | 0.0443 (5) |
| H80A | 1.006194 | 0.559798 | 0.622344 | 0.066* |
| H80B | 1.023801 | 0.492144 | 0.687024 | 0.066* |
| H80C | 1.020707 | 0.574199 | 0.696466 | 0.066* |
| C81 | 0.86080 (17) | 0.53374 (13) | 0.76978 (11) | 0.0416 (5) |
| H81A | 0.896973 | 0.483054 | 0.785786 | 0.062* |
| H81B | 0.788110 | 0.537268 | 0.783544 | 0.062* |
| H81C | 0.886922 | 0.567457 | 0.790575 | 0.062* |
| C82 | 0.56709 (14) | 0.62625 (10) | 0.82060 (9) | 0.0277 (4) |
| C83 | 0.62177 (16) | 0.58119 (11) | 0.87378 (10) | 0.0346 (4) |
| H83 | 0.628460 | 0.529143 | 0.881850 | 0.042* |
| C84 | 0.66649 (17) | 0.61277 (13) | 0.91499 (11) | 0.0421 (5) |
| H84 | 0.703504 | 0.582529 | 0.952145 | 0.051* |
| C85 | 0.65738 (18) | 0.68851 (13) | 0.90215 (12) | 0.0431 (5) |
| H85 | 0.688397 | 0.710069 | 0.930584 | 0.052* |
| C86 | 0.60366 (16) | 0.73313 (11) | 0.84842 (11) | 0.0363 (4) |
| H86 | 0.598933 | 0.785022 | 0.839838 | 0.044* |
| C87 | 0.55628 (14) | 0.70283 (10) | 0.80662 (9) | 0.0288 (4) |
| C88 | 0.49204 (15) | 0.74914 (10) | 0.75185 (10) | 0.0295 (4) |
| C89 | 0.42100 (18) | 0.81161 (11) | 0.76359 (11) | 0.0398 (5) |
| H89 | 0.417469 | 0.827126 | 0.806225 | 0.048* |
| C90 | 0.35577 (19) | 0.85117 (12) | 0.71406 (12) | 0.0473 (6) |
| H90 | 0.307318 | 0.893224 | 0.723052 | 0.057* |
| C91 | 0.36077 (18) | 0.82976 (12) | 0.65144 (12) | 0.0450 (5) |
| H91 | 0.314696 | 0.856348 | 0.617945 | 0.054* |
| C92 | 0.43314 (17) | 0.76938 (11) | 0.63753 (11) | 0.0367 (4) |
| H92 | 0.438276 | 0.755214 | 0.594113 | 0.044* |
| C93 | 0.49743 (14) | 0.73028 (9) | 0.68752 (9) | 0.0280 (4) |
| O1 | 0.49191 (8) | 0.24720 (6) | 0.68828 (5) | 0.0188 (2) |
| O2 | 0.62194 (8) | 0.17553 (6) | 0.61614 (5) | 0.0176 (2) |
| O3 | 0.55712 (8) | 0.11171 (6) | 0.72348 (6) | 0.0185 (2) |
| O4 | 0.87391 (8) | 0.05584 (6) | 0.79991 (5) | 0.0175 (2) |
| O5 | 0.75557 (8) | 0.08119 (6) | 0.89670 (5) | 0.0181 (2) |
| O6 | 0.88858 (8) | 0.15649 (6) | 0.85846 (5) | 0.0183 (2) |
| O7 | 0.67415 (10) | -0.12389 (8) | 0.93804 (8) | 0.0405 (4) |
| O8 | 0.83014 (9) | 0.03127 (7) | 0.53423 (6) | 0.0279 (3) |

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|------|--------------|--------------|--------------|-------------|-----------|
| O9 | 0.87726 (9) | 0.24214 (7) | 0.63851 (6) | 0.0277 (3) | |
| O10 | 0.68535 (9) | 0.30387 (6) | 0.87800 (5) | 0.0192 (2) | |
| O11 | 0.78705 (8) | 0.36703 (6) | 0.77893 (6) | 0.0203 (2) | |
| O12 | 0.60440 (8) | 0.39513 (6) | 0.78154 (5) | 0.0187 (2) | |
| O13 | 0.66483 (9) | 0.54450 (6) | 0.71242 (6) | 0.0248 (2) | |
| O14 | 0.51551 (10) | 0.59357 (7) | 0.78334 (7) | 0.0284 (3) | |
| O15 | 0.57300 (10) | 0.67130 (7) | 0.67288 (6) | 0.0292 (3) | |
| O16 | 0.36571 (10) | 0.46844 (7) | 0.55987 (7) | 0.0304 (3) | |
| O17 | 0.90379 (9) | 0.37875 (8) | 0.53378 (7) | 0.0309 (3) | |
| P1 | 0.59867 (3) | 0.18802 (2) | 0.69550 (2) | 0.01480 (7) | |
| P2 | 0.80453 (3) | 0.12767 (2) | 0.82633 (2) | 0.01506 (7) | |
| P3 | 0.69419 (3) | 0.32232 (2) | 0.79428 (2) | 0.01578 (8) | |
| P4 | 0.54796 (4) | 0.58775 (2) | 0.70301 (2) | 0.02573 (9) | |
| Rh1 | 0.70862 (2) | 0.21807 (2) | 0.75367 (2) | 0.01398 (3) | |
| H1 | 0.6205 (17) | 0.2069 (12) | 0.8086 (12) | 0.038 (6)* | |
| C94 | 0.81565 (17) | 0.83512 (10) | 0.63087 (10) | 0.0601 (7) | |
| C95 | 0.79998 (15) | 0.81955 (10) | 0.56840 (11) | 0.0711 (9) | |
| D95 | 0.736205 | 0.810153 | 0.561805 | 0.085* | |
| C96 | 0.8776 (2) | 0.81775 (12) | 0.51559 (9) | 0.0833 (10) | |
| D96 | 0.866909 | 0.807113 | 0.472901 | 0.100* | |
| C97 | 0.97093 (17) | 0.83150 (12) | 0.52525 (15) | 0.0923 (13) | |
| D97 | 1.023996 | 0.830271 | 0.489152 | 0.111* | |
| C98 | 0.98661 (15) | 0.84707 (12) | 0.58771 (18) | 0.1020 (14) | |
| D98 | 1.050382 | 0.856467 | 0.594307 | 0.122* | |
| C99 | 0.9090 (2) | 0.84887 (11) | 0.64052 (13) | 0.0929 (13) | |
| D99 | 0.919679 | 0.859507 | 0.683212 | 0.111* | |
| C100 | 0.7310 (3) | 0.83474 (18) | 0.6851 (2) | 0.0997 (14) | |
| D10A | 0.751266 | 0.846412 | 0.726276 | 0.150* | |
| D10B | 0.671988 | 0.871746 | 0.668021 | 0.150* | |
| D10C | 0.713345 | 0.785818 | 0.696971 | 0.150* | |
| C101 | 0.0868 (2) | 0.72891 (19) | 0.80410 (18) | 0.0514 (11) | 0.501 (3) |
| C102 | 0.08049 (19) | 0.7024 (2) | 0.74536 (17) | 0.0455 (12) | 0.501 (3) |
| D102 | 0.017986 | 0.713463 | 0.724560 | 0.055* | 0.501 (3) |
| C103 | 0.1656 (2) | 0.65960 (19) | 0.71705 (14) | 0.0407 (10) | 0.501 (3) |
| D103 | 0.161232 | 0.641464 | 0.676906 | 0.049* | 0.501 (3) |
| C104 | 0.2570 (2) | 0.64337 (17) | 0.74749 (16) | 0.0389 (11) | 0.501 (3) |
| D104 | 0.315178 | 0.614141 | 0.728140 | 0.047* | 0.501 (3) |
| C105 | 0.2634 (2) | 0.66991 (19) | 0.80623 (17) | 0.0454 (10) | 0.501 (3) |
| D105 | 0.325880 | 0.658818 | 0.827029 | 0.054* | 0.501 (3) |
| C106 | 0.1783 (3) | 0.7127 (2) | 0.83454 (15) | 0.0488 (12) | 0.501 (3) |
| D106 | 0.182634 | 0.730817 | 0.874685 | 0.059* | 0.501 (3) |
| C107 | -0.0019 (6) | 0.7740 (5) | 0.8369 (5) | 0.090 (2) | 0.501 (3) |
| D10D | 0.018388 | 0.787119 | 0.877379 | 0.134* | 0.501 (3) |
| D10E | -0.026704 | 0.819139 | 0.803505 | 0.134* | 0.501 (3) |
| D10F | -0.055912 | 0.745668 | 0.851386 | 0.134* | 0.501 (3) |
| C108 | 0.1602 (5) | 0.6854 (4) | 0.7735 (3) | 0.0411 (15) | 0.249 (3) |
| C109 | 0.1979 (4) | 0.6863 (4) | 0.8351 (4) | 0.0405 (18) | 0.249 (3) |
| D109 | 0.265558 | 0.662033 | 0.844174 | 0.049* | 0.249 (3) |

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|------|------------|---------------|--------------|-------------|-----------|
| C110 | 0.1367 (6) | 0.7228 (4) | 0.8834 (3) | 0.0535 (19) | 0.249 (3) |
| D110 | 0.162495 | 0.723402 | 0.925498 | 0.064* | 0.249 (3) |
| C111 | 0.0377 (6) | 0.7583 (5) | 0.8701 (4) | 0.065 (2) | 0.249 (3) |
| D111 | -0.004105 | 0.783247 | 0.903113 | 0.078* | 0.249 (3) |
| C112 | 0.0000 (5) | 0.7574 (5) | 0.8085 (4) | 0.070 (2) | 0.249 (3) |
| D112 | -0.067642 | 0.781723 | 0.799404 | 0.084* | 0.249 (3) |
| C113 | 0.0612 (5) | 0.7210 (5) | 0.7602 (3) | 0.050 (2) | 0.249 (3) |
| D113 | 0.035420 | 0.720354 | 0.718079 | 0.060* | 0.249 (3) |
| C114 | 0.2247 (9) | 0.6495 (7) | 0.7252 (6) | 0.049 (3) | 0.249 (3) |
| D11A | 0.188104 | 0.653322 | 0.684621 | 0.073* | 0.249 (3) |
| D11B | 0.283901 | 0.672750 | 0.710905 | 0.073* | 0.249 (3) |
| D11C | 0.247260 | 0.597402 | 0.746312 | 0.073* | 0.249 (3) |
| C115 | 0.4748 (3) | 0.02926 (18) | 0.51899 (18) | 0.0431 (10) | 0.5 |
| C116 | 0.5010 (3) | -0.04486 (19) | 0.55014 (15) | 0.0403 (17) | 0.5 |
| D116 | 0.493059 | -0.059641 | 0.599103 | 0.048* | 0.5 |
| C117 | 0.5388 (3) | -0.09735 (16) | 0.50964 (19) | 0.0517 (11) | 0.5 |
| D117 | 0.556675 | -0.148002 | 0.530924 | 0.062* | 0.5 |
| C118 | 0.5504 (4) | -0.07572 (19) | 0.43799 (19) | 0.064 (3) | 0.5 |
| D118 | 0.576206 | -0.111593 | 0.410313 | 0.076* | 0.5 |
| C119 | 0.5242 (3) | -0.0016 (2) | 0.40685 (15) | 0.0586 (13) | 0.5 |
| D119 | 0.532120 | 0.013178 | 0.357879 | 0.070* | 0.5 |
| C120 | 0.4864 (3) | 0.05089 (16) | 0.44734 (19) | 0.058 (2) | 0.5 |
| D120 | 0.468502 | 0.101540 | 0.426056 | 0.069* | 0.5 |
| C121 | 0.4341 (7) | 0.0849 (5) | 0.5626 (4) | 0.061 (3) | 0.5 |
| D12A | 0.419519 | 0.134131 | 0.532864 | 0.092* | 0.5 |
| D12B | 0.371454 | 0.073755 | 0.589152 | 0.092* | 0.5 |
| D12C | 0.484338 | 0.083650 | 0.594446 | 0.092* | 0.5 |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| C1 | 0.0165 (7) | 0.0192 (7) | 0.0213 (7) | 0.0018 (6) | -0.0056 (6) | -0.0041 (6) |
| C2 | 0.0183 (8) | 0.0314 (9) | 0.0258 (8) | -0.0018 (7) | -0.0025 (6) | -0.0019 (7) |
| C3 | 0.0166 (8) | 0.0467 (12) | 0.0373 (10) | -0.0038 (8) | -0.0053 (7) | -0.0047 (9) |
| C4 | 0.0219 (9) | 0.0551 (13) | 0.0341 (10) | -0.0005 (8) | -0.0131 (8) | -0.0065 (9) |
| C5 | 0.0243 (9) | 0.0393 (10) | 0.0232 (8) | 0.0014 (7) | -0.0073 (7) | -0.0034 (7) |
| C6 | 0.0190 (7) | 0.0217 (8) | 0.0216 (7) | 0.0005 (6) | -0.0038 (6) | -0.0034 (6) |
| C7 | 0.0225 (8) | 0.0207 (7) | 0.0164 (7) | -0.0025 (6) | -0.0022 (6) | -0.0043 (6) |
| C8 | 0.0316 (9) | 0.0218 (8) | 0.0201 (8) | -0.0018 (7) | -0.0033 (7) | -0.0016 (6) |
| C9 | 0.0389 (10) | 0.0259 (9) | 0.0201 (8) | -0.0104 (7) | 0.0016 (7) | -0.0018 (6) |
| C10 | 0.0281 (9) | 0.0338 (9) | 0.0216 (8) | -0.0106 (7) | 0.0042 (7) | -0.0071 (7) |
| C11 | 0.0212 (8) | 0.0271 (8) | 0.0197 (7) | -0.0027 (6) | -0.0008 (6) | -0.0056 (6) |
| C12 | 0.0218 (7) | 0.0185 (7) | 0.0151 (7) | -0.0040 (6) | -0.0023 (6) | -0.0041 (6) |
| C13 | 0.0174 (7) | 0.0166 (7) | 0.0193 (7) | -0.0045 (6) | -0.0014 (6) | -0.0015 (6) |
| C14 | 0.0164 (7) | 0.0220 (8) | 0.0258 (8) | -0.0049 (6) | 0.0009 (6) | -0.0011 (6) |
| C15 | 0.0223 (8) | 0.0284 (9) | 0.0303 (9) | -0.0091 (7) | 0.0034 (7) | 0.0051 (7) |
| C16 | 0.0242 (8) | 0.0218 (8) | 0.0299 (9) | -0.0057 (7) | -0.0042 (7) | 0.0062 (7) |
| C17 | 0.0180 (7) | 0.0184 (7) | 0.0274 (8) | -0.0028 (6) | -0.0018 (6) | -0.0009 (6) |

| | | | | | | |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| C18 | 0.0166 (7) | 0.0171 (7) | 0.0208 (7) | -0.0049 (6) | -0.0004 (6) | -0.0044 (6) |
| C19 | 0.0151 (7) | 0.0142 (7) | 0.0205 (7) | -0.0004 (5) | 0.0006 (5) | -0.0039 (5) |
| C20 | 0.0172 (7) | 0.0179 (7) | 0.0234 (8) | -0.0019 (6) | -0.0025 (6) | -0.0056 (6) |
| C21 | 0.0218 (8) | 0.0201 (7) | 0.0202 (7) | -0.0002 (6) | -0.0011 (6) | -0.0064 (6) |
| C22 | 0.0177 (7) | 0.0246 (8) | 0.0202 (7) | -0.0006 (6) | 0.0028 (6) | -0.0048 (6) |
| C23 | 0.0153 (7) | 0.0178 (7) | 0.0205 (7) | -0.0009 (6) | 0.0000 (6) | -0.0021 (6) |
| C24 | 0.0167 (7) | 0.0152 (7) | 0.0173 (7) | -0.0005 (5) | -0.0007 (5) | -0.0024 (5) |
| C25 | 0.0149 (7) | 0.0267 (9) | 0.0319 (9) | -0.0047 (6) | 0.0023 (6) | 0.0017 (7) |
| C26 | 0.0192 (9) | 0.0457 (12) | 0.0532 (13) | -0.0067 (8) | 0.0076 (8) | 0.0114 (10) |
| C27 | 0.0225 (8) | 0.0327 (9) | 0.0301 (9) | 0.0004 (7) | 0.0014 (7) | -0.0061 (7) |
| C28 | 0.0192 (8) | 0.0362 (10) | 0.0440 (11) | -0.0088 (7) | -0.0043 (7) | -0.0082 (8) |
| C29 | 0.0314 (10) | 0.0320 (10) | 0.0506 (12) | -0.0069 (8) | -0.0152 (9) | 0.0112 (9) |
| C30 | 0.0288 (9) | 0.0401 (10) | 0.0231 (8) | -0.0037 (8) | -0.0060 (7) | -0.0122 (7) |
| C31 | 0.0136 (7) | 0.0274 (8) | 0.0210 (7) | -0.0011 (6) | -0.0002 (6) | -0.0019 (6) |
| C32 | 0.0164 (8) | 0.0303 (9) | 0.0329 (9) | -0.0055 (7) | -0.0031 (6) | -0.0034 (7) |
| C33 | 0.0158 (8) | 0.0458 (11) | 0.0279 (9) | -0.0009 (7) | 0.0032 (7) | -0.0066 (8) |
| C34 | 0.0168 (8) | 0.0323 (9) | 0.0277 (9) | 0.0022 (7) | -0.0030 (6) | 0.0014 (7) |
| C35 | 0.0202 (7) | 0.0181 (7) | 0.0148 (7) | -0.0028 (6) | 0.0013 (6) | 0.0014 (5) |
| C36 | 0.0199 (8) | 0.0272 (8) | 0.0202 (7) | -0.0056 (6) | 0.0003 (6) | 0.0033 (6) |
| C37 | 0.0217 (8) | 0.0293 (9) | 0.0263 (8) | 0.0005 (7) | 0.0065 (7) | 0.0048 (7) |
| C38 | 0.0323 (9) | 0.0279 (9) | 0.0217 (8) | 0.0004 (7) | 0.0078 (7) | -0.0016 (7) |
| C39 | 0.0311 (9) | 0.0269 (9) | 0.0181 (7) | -0.0041 (7) | 0.0013 (6) | -0.0035 (6) |
| C40 | 0.0219 (8) | 0.0209 (7) | 0.0151 (7) | -0.0036 (6) | 0.0001 (6) | 0.0010 (6) |
| C41 | 0.0211 (8) | 0.0198 (7) | 0.0182 (7) | -0.0031 (6) | -0.0035 (6) | -0.0022 (6) |
| C42 | 0.0294 (9) | 0.0292 (9) | 0.0167 (7) | -0.0065 (7) | -0.0042 (6) | -0.0012 (6) |
| C43 | 0.0300 (9) | 0.0324 (9) | 0.0231 (8) | -0.0048 (7) | -0.0120 (7) | -0.0006 (7) |
| C44 | 0.0206 (8) | 0.0331 (9) | 0.0311 (9) | -0.0009 (7) | -0.0091 (7) | -0.0060 (7) |
| C45 | 0.0196 (8) | 0.0274 (8) | 0.0232 (8) | -0.0035 (6) | -0.0021 (6) | -0.0060 (6) |
| C46 | 0.0212 (8) | 0.0185 (7) | 0.0169 (7) | -0.0043 (6) | -0.0054 (6) | -0.0016 (6) |
| C47 | 0.0188 (7) | 0.0180 (7) | 0.0187 (7) | -0.0004 (6) | -0.0059 (6) | -0.0006 (6) |
| C48 | 0.0314 (9) | 0.0175 (7) | 0.0149 (7) | -0.0044 (6) | -0.0025 (6) | -0.0028 (6) |
| C49 | 0.0288 (9) | 0.0257 (8) | 0.0209 (8) | -0.0039 (7) | -0.0003 (6) | -0.0023 (6) |
| C50 | 0.0421 (11) | 0.0317 (10) | 0.0258 (9) | -0.0027 (8) | 0.0041 (8) | -0.0117 (7) |
| C51 | 0.0494 (12) | 0.0390 (11) | 0.0320 (10) | -0.0090 (9) | -0.0020 (9) | -0.0200 (8) |
| C52 | 0.0371 (10) | 0.0382 (10) | 0.0324 (9) | -0.0105 (8) | -0.0042 (8) | -0.0162 (8) |
| C53 | 0.0284 (9) | 0.0228 (8) | 0.0206 (7) | -0.0051 (7) | -0.0036 (6) | -0.0059 (6) |
| C54 | 0.0232 (8) | 0.0223 (8) | 0.0230 (8) | -0.0057 (6) | -0.0036 (6) | -0.0058 (6) |
| C55 | 0.0284 (9) | 0.0358 (10) | 0.0269 (9) | -0.0069 (8) | -0.0089 (7) | -0.0068 (7) |
| C56 | 0.0223 (9) | 0.0382 (10) | 0.0398 (10) | -0.0035 (8) | -0.0101 (8) | -0.0064 (8) |
| C57 | 0.0221 (8) | 0.0372 (10) | 0.0355 (10) | -0.0071 (7) | 0.0018 (7) | -0.0106 (8) |
| C58 | 0.0230 (8) | 0.0315 (9) | 0.0239 (8) | -0.0089 (7) | -0.0006 (6) | -0.0061 (7) |
| C59 | 0.0202 (8) | 0.0198 (7) | 0.0232 (8) | -0.0065 (6) | -0.0044 (6) | -0.0025 (6) |
| C60 | 0.0193 (7) | 0.0151 (7) | 0.0187 (7) | 0.0000 (6) | -0.0028 (6) | -0.0029 (5) |
| C61 | 0.0195 (8) | 0.0187 (7) | 0.0242 (8) | -0.0012 (6) | 0.0011 (6) | -0.0033 (6) |
| C62 | 0.0168 (7) | 0.0230 (8) | 0.0314 (9) | -0.0011 (6) | -0.0029 (6) | -0.0025 (7) |
| C63 | 0.0213 (8) | 0.0196 (8) | 0.0264 (8) | 0.0003 (6) | -0.0070 (6) | -0.0021 (6) |
| C64 | 0.0233 (8) | 0.0174 (7) | 0.0198 (7) | -0.0018 (6) | -0.0022 (6) | -0.0022 (6) |
| C65 | 0.0181 (7) | 0.0138 (7) | 0.0203 (7) | 0.0008 (5) | -0.0010 (6) | -0.0048 (5) |

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|-----|--------------|--------------|--------------|---------------|---------------|---------------|
| C66 | 0.0196 (7) | 0.0154 (7) | 0.0161 (7) | -0.0008 (6) | -0.0013 (6) | 0.0005 (5) |
| C67 | 0.0216 (8) | 0.0204 (7) | 0.0171 (7) | -0.0007 (6) | -0.0023 (6) | -0.0026 (6) |
| C68 | 0.0225 (8) | 0.0229 (8) | 0.0182 (7) | 0.0022 (6) | 0.0011 (6) | -0.0010 (6) |
| C69 | 0.0188 (8) | 0.0255 (8) | 0.0270 (8) | -0.0043 (6) | 0.0008 (6) | 0.0008 (7) |
| C70 | 0.0245 (8) | 0.0200 (8) | 0.0261 (8) | -0.0055 (6) | -0.0029 (6) | -0.0004 (6) |
| C71 | 0.0227 (8) | 0.0167 (7) | 0.0201 (7) | -0.0011 (6) | -0.0001 (6) | -0.0024 (6) |
| C72 | 0.0209 (8) | 0.0284 (9) | 0.0260 (8) | -0.0022 (7) | 0.0053 (6) | -0.0027 (7) |
| C73 | 0.0344 (10) | 0.0263 (9) | 0.0299 (9) | -0.0084 (7) | 0.0083 (7) | -0.0023 (7) |
| C74 | 0.0230 (10) | 0.0718 (16) | 0.0390 (11) | -0.0099 (10) | 0.0076 (8) | 0.0013 (11) |
| C75 | 0.0404 (11) | 0.0264 (9) | 0.0278 (9) | -0.0005 (8) | 0.0104 (8) | -0.0068 (7) |
| C76 | 0.0265 (10) | 0.0479 (12) | 0.0464 (12) | -0.0111 (9) | -0.0171 (9) | 0.0094 (10) |
| C77 | 0.0230 (9) | 0.0522 (13) | 0.0422 (11) | 0.0027 (9) | 0.0082 (8) | -0.0141 (10) |
| C78 | 0.0283 (9) | 0.0268 (9) | 0.0442 (11) | -0.0103 (7) | -0.0043 (8) | -0.0092 (8) |
| C79 | 0.0417 (12) | 0.0263 (10) | 0.0726 (16) | -0.0134 (9) | -0.0074 (11) | -0.0084 (10) |
| C80 | 0.0299 (10) | 0.0455 (12) | 0.0644 (15) | -0.0159 (9) | -0.0051 (10) | -0.0167 (11) |
| C81 | 0.0436 (12) | 0.0477 (12) | 0.0425 (11) | -0.0161 (10) | -0.0087 (9) | -0.0179 (10) |
| C82 | 0.0288 (9) | 0.0263 (9) | 0.0257 (8) | -0.0045 (7) | 0.0071 (7) | -0.0066 (7) |
| C83 | 0.0366 (10) | 0.0301 (10) | 0.0313 (9) | -0.0028 (8) | 0.0017 (8) | -0.0003 (8) |
| C84 | 0.0426 (12) | 0.0470 (12) | 0.0328 (10) | -0.0039 (10) | -0.0045 (9) | -0.0040 (9) |
| C85 | 0.0455 (12) | 0.0494 (13) | 0.0383 (11) | -0.0102 (10) | -0.0028 (9) | -0.0165 (10) |
| C86 | 0.0427 (11) | 0.0308 (10) | 0.0362 (10) | -0.0071 (8) | 0.0045 (8) | -0.0128 (8) |
| C87 | 0.0321 (9) | 0.0260 (9) | 0.0256 (8) | -0.0025 (7) | 0.0063 (7) | -0.0075 (7) |
| C88 | 0.0353 (10) | 0.0200 (8) | 0.0293 (9) | -0.0021 (7) | 0.0047 (7) | -0.0042 (7) |
| C89 | 0.0521 (13) | 0.0257 (9) | 0.0353 (10) | 0.0039 (9) | 0.0041 (9) | -0.0087 (8) |
| C90 | 0.0550 (14) | 0.0264 (10) | 0.0487 (13) | 0.0119 (9) | 0.0026 (11) | -0.0067 (9) |
| C91 | 0.0495 (13) | 0.0300 (10) | 0.0464 (12) | 0.0066 (9) | -0.0095 (10) | 0.0001 (9) |
| C92 | 0.0474 (12) | 0.0261 (9) | 0.0331 (10) | -0.0021 (8) | -0.0035 (9) | -0.0042 (8) |
| C93 | 0.0337 (9) | 0.0170 (8) | 0.0297 (9) | -0.0019 (7) | 0.0045 (7) | -0.0046 (7) |
| O1 | 0.0152 (5) | 0.0217 (5) | 0.0180 (5) | 0.0017 (4) | -0.0036 (4) | -0.0052 (4) |
| O2 | 0.0187 (5) | 0.0173 (5) | 0.0153 (5) | -0.0012 (4) | -0.0012 (4) | -0.0029 (4) |
| O3 | 0.0155 (5) | 0.0184 (5) | 0.0206 (5) | -0.0047 (4) | -0.0030 (4) | 0.0001 (4) |
| O4 | 0.0153 (5) | 0.0191 (5) | 0.0163 (5) | 0.0000 (4) | -0.0016 (4) | -0.0030 (4) |
| O5 | 0.0183 (5) | 0.0192 (5) | 0.0157 (5) | -0.0046 (4) | 0.0003 (4) | -0.0014 (4) |
| O6 | 0.0188 (5) | 0.0211 (5) | 0.0146 (5) | -0.0059 (4) | -0.0036 (4) | 0.0002 (4) |
| O7 | 0.0272 (7) | 0.0363 (8) | 0.0433 (8) | -0.0047 (6) | -0.0028 (6) | 0.0207 (6) |
| O8 | 0.0237 (6) | 0.0411 (7) | 0.0192 (6) | -0.0031 (5) | -0.0011 (5) | -0.0104 (5) |
| O9 | 0.0204 (6) | 0.0351 (7) | 0.0226 (6) | -0.0034 (5) | 0.0033 (5) | -0.0002 (5) |
| O10 | 0.0252 (6) | 0.0191 (5) | 0.0142 (5) | -0.0065 (4) | -0.0021 (4) | -0.0027 (4) |
| O11 | 0.0199 (5) | 0.0211 (5) | 0.0198 (5) | -0.0066 (4) | -0.0037 (4) | 0.0001 (4) |
| O12 | 0.0197 (5) | 0.0181 (5) | 0.0167 (5) | -0.0002 (4) | -0.0019 (4) | -0.0038 (4) |
| O13 | 0.0244 (6) | 0.0207 (6) | 0.0305 (6) | -0.0018 (5) | -0.0011 (5) | -0.0111 (5) |
| O14 | 0.0298 (7) | 0.0222 (6) | 0.0313 (6) | -0.0051 (5) | 0.0049 (5) | -0.0058 (5) |
| O15 | 0.0359 (7) | 0.0197 (6) | 0.0277 (6) | -0.0005 (5) | 0.0055 (5) | -0.0056 (5) |
| O16 | 0.0240 (6) | 0.0353 (7) | 0.0297 (6) | -0.0049 (5) | -0.0113 (5) | 0.0021 (5) |
| O17 | 0.0225 (6) | 0.0384 (7) | 0.0287 (6) | 0.0015 (5) | 0.0054 (5) | -0.0121 (5) |
| P1 | 0.01251 (17) | 0.01612 (18) | 0.01463 (17) | -0.00149 (13) | -0.00114 (13) | -0.00211 (13) |
| P2 | 0.01368 (17) | 0.01664 (18) | 0.01351 (16) | -0.00189 (14) | -0.00121 (13) | -0.00131 (13) |
| P3 | 0.01680 (18) | 0.01565 (18) | 0.01418 (17) | -0.00267 (14) | -0.00147 (13) | -0.00195 (13) |

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|------|-------------|-------------|-------------|--------------|---------------|---------------|
| P4 | 0.0258 (2) | 0.0190 (2) | 0.0313 (2) | 0.00000 (17) | -0.00118 (18) | -0.00767 (17) |
| Rh1 | 0.01282 (6) | 0.01477 (6) | 0.01325 (6) | -0.00160 (4) | -0.00098 (4) | -0.00170 (4) |
| C94 | 0.0768 (19) | 0.0263 (11) | 0.0703 (18) | -0.0067 (12) | 0.0020 (15) | -0.0032 (11) |
| C95 | 0.106 (3) | 0.0379 (14) | 0.0603 (17) | 0.0017 (15) | -0.0111 (17) | -0.0056 (12) |
| C96 | 0.104 (3) | 0.0506 (17) | 0.079 (2) | -0.0046 (18) | 0.007 (2) | 0.0022 (15) |
| C97 | 0.082 (3) | 0.0433 (17) | 0.133 (4) | -0.0092 (16) | 0.021 (2) | 0.0008 (19) |
| C98 | 0.086 (3) | 0.051 (2) | 0.168 (5) | -0.0130 (18) | -0.019 (3) | -0.017 (2) |
| C99 | 0.094 (3) | 0.0404 (16) | 0.148 (4) | -0.0042 (17) | -0.042 (3) | -0.016 (2) |
| C100 | 0.134 (3) | 0.0449 (17) | 0.099 (3) | -0.0099 (19) | 0.050 (2) | -0.0101 (17) |
| C101 | 0.042 (2) | 0.051 (2) | 0.065 (2) | -0.0079 (18) | -0.001 (2) | -0.021 (2) |
| C102 | 0.030 (2) | 0.055 (3) | 0.053 (3) | -0.0035 (19) | -0.0101 (19) | -0.014 (2) |
| C103 | 0.036 (2) | 0.055 (2) | 0.034 (2) | -0.015 (2) | -0.0036 (18) | -0.0082 (18) |
| C104 | 0.019 (2) | 0.048 (2) | 0.040 (2) | -0.0048 (18) | -0.0023 (17) | 0.010 (2) |
| C105 | 0.033 (2) | 0.052 (2) | 0.050 (2) | -0.0132 (19) | -0.0098 (18) | -0.0017 (19) |
| C106 | 0.051 (3) | 0.052 (3) | 0.054 (2) | -0.019 (2) | -0.007 (2) | -0.022 (2) |
| C107 | 0.065 (4) | 0.096 (5) | 0.126 (6) | 0.002 (4) | -0.004 (4) | -0.078 (5) |
| C108 | 0.035 (3) | 0.044 (3) | 0.044 (3) | -0.009 (3) | -0.009 (3) | -0.003 (3) |
| C109 | 0.043 (4) | 0.037 (4) | 0.046 (3) | -0.018 (3) | -0.015 (3) | -0.001 (3) |
| C110 | 0.067 (4) | 0.051 (4) | 0.054 (4) | -0.023 (3) | -0.012 (4) | -0.019 (3) |
| C111 | 0.078 (5) | 0.070 (5) | 0.054 (4) | 0.003 (4) | -0.020 (4) | -0.037 (4) |
| C112 | 0.065 (4) | 0.080 (5) | 0.059 (4) | 0.011 (4) | -0.018 (4) | -0.022 (4) |
| C113 | 0.047 (4) | 0.061 (4) | 0.040 (4) | 0.005 (3) | -0.013 (3) | -0.019 (3) |
| C114 | 0.029 (5) | 0.059 (5) | 0.040 (5) | 0.007 (5) | 0.002 (4) | 0.009 (4) |
| C115 | 0.032 (2) | 0.054 (3) | 0.055 (2) | -0.0189 (19) | 0.0003 (18) | -0.027 (2) |
| C116 | 0.040 (3) | 0.044 (3) | 0.043 (3) | -0.014 (3) | -0.011 (3) | -0.011 (3) |
| C117 | 0.051 (3) | 0.042 (2) | 0.065 (3) | -0.013 (2) | -0.002 (2) | -0.012 (2) |
| C118 | 0.061 (4) | 0.064 (5) | 0.070 (5) | -0.021 (4) | 0.015 (4) | -0.027 (4) |
| C119 | 0.069 (3) | 0.059 (3) | 0.050 (3) | -0.021 (3) | 0.015 (2) | -0.018 (2) |
| C120 | 0.053 (4) | 0.058 (4) | 0.060 (5) | -0.019 (3) | 0.017 (3) | -0.013 (4) |
| C121 | 0.064 (4) | 0.065 (5) | 0.070 (5) | -0.016 (4) | -0.001 (4) | -0.045 (4) |

Geometric parameters (Å, °)

| | | | |
|--------|-------------|----------|-------------|
| C1—C2 | 1.384 (2) | C67—C68 | 1.380 (2) |
| C1—O1 | 1.3925 (18) | C67—H67 | 0.9500 |
| C1—C6 | 1.397 (2) | C68—O17 | 1.375 (2) |
| C2—C3 | 1.388 (2) | C68—C69 | 1.384 (3) |
| C2—H2 | 0.9500 | C69—C70 | 1.396 (2) |
| C3—C4 | 1.381 (3) | C69—H69 | 0.9500 |
| C3—H3 | 0.9500 | C70—C71 | 1.400 (2) |
| C4—C5 | 1.379 (3) | C70—C78 | 1.546 (2) |
| C4—H4 | 0.9500 | C71—O13 | 1.3972 (19) |
| C5—C6 | 1.400 (2) | C72—C75 | 1.529 (3) |
| C5—H5 | 0.9500 | C72—C74 | 1.534 (3) |
| C6—C7 | 1.475 (2) | C72—C73 | 1.535 (3) |
| C7—C12 | 1.393 (2) | C73—H73A | 0.9800 |
| C7—C8 | 1.401 (2) | C73—H73B | 0.9800 |
| C8—C9 | 1.381 (3) | C73—H73C | 0.9800 |

| | | | |
|----------|-------------|----------|-----------|
| C8—H8 | 0.9500 | C74—H74A | 0.9800 |
| C9—C10 | 1.387 (3) | C74—H74B | 0.9800 |
| C9—H9 | 0.9500 | C74—H74C | 0.9800 |
| C10—C11 | 1.387 (2) | C75—H75A | 0.9800 |
| C10—H10 | 0.9500 | C75—H75B | 0.9800 |
| C11—C12 | 1.382 (2) | C75—H75C | 0.9800 |
| C11—H11 | 0.9500 | C76—O16 | 1.423 (2) |
| C12—O2 | 1.3911 (18) | C76—H76A | 0.9800 |
| C13—C18 | 1.392 (2) | C76—H76B | 0.9800 |
| C13—O3 | 1.3974 (18) | C76—H76C | 0.9800 |
| C13—C14 | 1.416 (2) | C77—O17 | 1.411 (2) |
| C14—C15 | 1.386 (2) | C77—H77A | 0.9800 |
| C14—C25 | 1.538 (2) | C77—H77B | 0.9800 |
| C15—C16 | 1.387 (2) | C77—H77C | 0.9800 |
| C15—H15 | 0.9500 | C78—C79 | 1.532 (3) |
| C16—C17 | 1.375 (2) | C78—C81 | 1.535 (3) |
| C16—O7 | 1.376 (2) | C78—C80 | 1.537 (3) |
| C17—C18 | 1.403 (2) | C79—H79A | 0.9800 |
| C17—H17 | 0.9500 | C79—H79B | 0.9800 |
| C18—C19 | 1.493 (2) | C79—H79C | 0.9800 |
| C19—C20 | 1.395 (2) | C80—H80A | 0.9800 |
| C19—C24 | 1.397 (2) | C80—H80B | 0.9800 |
| C20—C21 | 1.381 (2) | C80—H80C | 0.9800 |
| C20—H20 | 0.9500 | C81—H81A | 0.9800 |
| C21—O8 | 1.3682 (19) | C81—H81B | 0.9800 |
| C21—C22 | 1.392 (2) | C81—H81C | 0.9800 |
| C22—C23 | 1.391 (2) | C82—C83 | 1.382 (3) |
| C22—H22 | 0.9500 | C82—C87 | 1.395 (3) |
| C23—C24 | 1.404 (2) | C82—O14 | 1.396 (2) |
| C23—C31 | 1.540 (2) | C83—C84 | 1.379 (3) |
| C24—O4 | 1.4040 (18) | C83—H83 | 0.9500 |
| C25—C27 | 1.534 (3) | C84—C85 | 1.382 (3) |
| C25—C28 | 1.534 (3) | C84—H84 | 0.9500 |
| C25—C26 | 1.538 (2) | C85—C86 | 1.380 (3) |
| C26—H26A | 0.9800 | C85—H85 | 0.9500 |
| C26—H26B | 0.9800 | C86—C87 | 1.394 (3) |
| C26—H26C | 0.9800 | C86—H86 | 0.9500 |
| C27—H27A | 0.9800 | C87—C88 | 1.479 (3) |
| C27—H27B | 0.9800 | C88—C93 | 1.392 (3) |
| C27—H27C | 0.9800 | C88—C89 | 1.396 (3) |
| C28—H28A | 0.9800 | C89—C90 | 1.382 (3) |
| C28—H28B | 0.9800 | C89—H89 | 0.9500 |
| C28—H28C | 0.9800 | C90—C91 | 1.383 (3) |
| C29—O7 | 1.406 (2) | C90—H90 | 0.9500 |
| C29—H29A | 0.9800 | C91—C92 | 1.388 (3) |
| C29—H29B | 0.9800 | C91—H91 | 0.9500 |
| C29—H29C | 0.9800 | C92—C93 | 1.378 (3) |
| C30—O8 | 1.424 (2) | C92—H92 | 0.9500 |

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|----------|-------------|-----------|-------------|
| C30—H30A | 0.9800 | C93—O15 | 1.396 (2) |
| C30—H30B | 0.9800 | O1—P1 | 1.6237 (11) |
| C30—H30C | 0.9800 | O2—P1 | 1.6289 (11) |
| C31—C32 | 1.530 (2) | O3—P1 | 1.6258 (11) |
| C31—C33 | 1.532 (2) | O4—P2 | 1.6271 (11) |
| C31—C34 | 1.535 (2) | O5—P2 | 1.6270 (11) |
| C32—H32A | 0.9800 | O6—P2 | 1.6179 (11) |
| C32—H32B | 0.9800 | O10—P3 | 1.6168 (11) |
| C32—H32C | 0.9800 | O11—P3 | 1.6293 (11) |
| C33—H33A | 0.9800 | O12—P3 | 1.6221 (11) |
| C33—H33B | 0.9800 | O13—P4 | 1.6269 (13) |
| C33—H33C | 0.9800 | O14—P4 | 1.6237 (13) |
| C34—H34A | 0.9800 | O15—P4 | 1.6579 (13) |
| C34—H34B | 0.9800 | P1—Rh1 | 2.2325 (4) |
| C34—H34C | 0.9800 | P2—Rh1 | 2.2572 (4) |
| C35—C36 | 1.384 (2) | P3—Rh1 | 2.2600 (4) |
| C35—O5 | 1.3922 (19) | Rh1—H1 | 1.53 (2) |
| C35—C40 | 1.392 (2) | C94—C95 | 1.3900 |
| C36—C37 | 1.387 (2) | C94—C99 | 1.3900 |
| C36—H36 | 0.9500 | C94—C100 | 1.472 (4) |
| C37—C38 | 1.383 (3) | C95—C96 | 1.3900 |
| C37—H37 | 0.9500 | C95—D95 | 0.9500 |
| C38—C39 | 1.382 (3) | C96—C97 | 1.3900 |
| C38—H38 | 0.9500 | C96—D96 | 0.9500 |
| C39—C40 | 1.397 (2) | C97—C98 | 1.3900 |
| C39—H39 | 0.9500 | C97—D97 | 0.9500 |
| C40—C41 | 1.475 (2) | C98—C99 | 1.3900 |
| C41—C46 | 1.393 (2) | C98—D98 | 0.9500 |
| C41—C42 | 1.398 (2) | C99—D99 | 0.9500 |
| C42—C43 | 1.379 (3) | C100—D10A | 0.9800 |
| C42—H42 | 0.9500 | C100—D10B | 0.9800 |
| C43—C44 | 1.384 (3) | C100—D10C | 0.9800 |
| C43—H43 | 0.9500 | C101—C102 | 1.3900 |
| C44—C45 | 1.387 (2) | C101—C106 | 1.3900 |
| C44—H44 | 0.9500 | C101—C107 | 1.483 (7) |
| C45—C46 | 1.383 (2) | C102—C103 | 1.3900 |
| C45—H45 | 0.9500 | C102—D102 | 0.9500 |
| C46—O6 | 1.3935 (18) | C103—C104 | 1.3900 |
| C47—O9 | 1.135 (2) | C103—D103 | 0.9500 |
| C47—Rh1 | 1.9227 (16) | C104—C105 | 1.3900 |
| C48—C49 | 1.383 (2) | C104—D104 | 0.9500 |
| C48—C53 | 1.392 (2) | C105—C106 | 1.3900 |
| C48—O10 | 1.3943 (18) | C105—D105 | 0.9500 |
| C49—C50 | 1.388 (3) | C106—D106 | 0.9500 |
| C49—H49 | 0.9500 | C107—D10D | 0.9800 |
| C50—C51 | 1.381 (3) | C107—D10E | 0.9800 |
| C50—H50 | 0.9500 | C107—D10F | 0.9800 |
| C51—C52 | 1.379 (3) | C108—C109 | 1.3900 |

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| C51—H51 | 0.9500 | C108—C113 | 1.3900 |
| C52—C53 | 1.403 (2) | C108—C114 | 1.403 (12) |
| C52—H52 | 0.9500 | C109—C110 | 1.3900 |
| C53—C54 | 1.476 (2) | C109—D109 | 0.9500 |
| C54—C55 | 1.397 (2) | C110—C111 | 1.3900 |
| C54—C59 | 1.398 (2) | C110—D110 | 0.9500 |
| C55—C56 | 1.379 (3) | C111—C112 | 1.3900 |
| C55—H55 | 0.9500 | C111—D111 | 0.9500 |
| C56—C57 | 1.383 (3) | C112—C113 | 1.3900 |
| C56—H56 | 0.9500 | C112—D112 | 0.9500 |
| C57—C58 | 1.388 (3) | C113—D113 | 0.9500 |
| C57—H57 | 0.9500 | C114—D11A | 0.9800 |
| C58—C59 | 1.380 (2) | C114—D11B | 0.9800 |
| C58—H58 | 0.9500 | C114—D11C | 0.9800 |
| C59—O11 | 1.3892 (19) | C115—C116 | 1.3900 |
| C60—C61 | 1.400 (2) | C115—C120 | 1.3900 |
| C60—C65 | 1.400 (2) | C115—C121 | 1.484 (7) |
| C60—O12 | 1.4026 (18) | C116—C117 | 1.3900 |
| C61—C62 | 1.399 (2) | C116—D116 | 0.9500 |
| C61—C72 | 1.541 (2) | C117—C118 | 1.3900 |
| C62—C63 | 1.383 (2) | C117—D117 | 0.9500 |
| C62—H62 | 0.9500 | C118—C119 | 1.3900 |
| C63—O16 | 1.375 (2) | C118—D118 | 0.9500 |
| C63—C64 | 1.383 (2) | C119—C120 | 1.3900 |
| C64—C65 | 1.388 (2) | C119—D119 | 0.9500 |
| C64—H64 | 0.9500 | C120—D120 | 0.9500 |
| C65—C66 | 1.490 (2) | C121—D12A | 0.9800 |
| C66—C67 | 1.387 (2) | C121—D12B | 0.9800 |
| C66—C71 | 1.401 (2) | C121—D12C | 0.9800 |
| | | | |
| C2—C1—O1 | 117.29 (14) | C70—C71—C66 | 121.40 (15) |
| C2—C1—C6 | 121.52 (15) | C75—C72—C74 | 107.51 (17) |
| O1—C1—C6 | 120.88 (14) | C75—C72—C73 | 110.06 (16) |
| C1—C2—C3 | 119.71 (16) | C74—C72—C73 | 106.79 (16) |
| C1—C2—H2 | 120.1 | C75—C72—C61 | 109.59 (14) |
| C3—C2—H2 | 120.1 | C74—C72—C61 | 111.42 (15) |
| C4—C3—C2 | 119.86 (17) | C73—C72—C61 | 111.36 (14) |
| C4—C3—H3 | 120.1 | C72—C73—H73A | 109.5 |
| C2—C3—H3 | 120.1 | C72—C73—H73B | 109.5 |
| C5—C4—C3 | 120.09 (17) | H73A—C73—H73B | 109.5 |
| C5—C4—H4 | 120.0 | C72—C73—H73C | 109.5 |
| C3—C4—H4 | 120.0 | H73A—C73—H73C | 109.5 |
| C4—C5—C6 | 121.49 (17) | H73B—C73—H73C | 109.5 |
| C4—C5—H5 | 119.3 | C72—C74—H74A | 109.5 |
| C6—C5—H5 | 119.3 | C72—C74—H74B | 109.5 |
| C1—C6—C5 | 117.31 (15) | H74A—C74—H74B | 109.5 |
| C1—C6—C7 | 123.26 (14) | C72—C74—H74C | 109.5 |
| C5—C6—C7 | 119.39 (15) | H74A—C74—H74C | 109.5 |

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| C12—C7—C8 | 117.42 (15) | H74B—C74—H74C | 109.5 |
| C12—C7—C6 | 121.04 (14) | C72—C75—H75A | 109.5 |
| C8—C7—C6 | 121.22 (15) | C72—C75—H75B | 109.5 |
| C9—C8—C7 | 121.06 (16) | H75A—C75—H75B | 109.5 |
| C9—C8—H8 | 119.5 | C72—C75—H75C | 109.5 |
| C7—C8—H8 | 119.5 | H75A—C75—H75C | 109.5 |
| C8—C9—C10 | 120.17 (16) | H75B—C75—H75C | 109.5 |
| C8—C9—H9 | 119.9 | O16—C76—H76A | 109.5 |
| C10—C9—H9 | 119.9 | O16—C76—H76B | 109.5 |
| C11—C10—C9 | 119.85 (16) | H76A—C76—H76B | 109.5 |
| C11—C10—H10 | 120.1 | O16—C76—H76C | 109.5 |
| C9—C10—H10 | 120.1 | H76A—C76—H76C | 109.5 |
| C12—C11—C10 | 119.42 (16) | H76B—C76—H76C | 109.5 |
| C12—C11—H11 | 120.3 | O17—C77—H77A | 109.5 |
| C10—C11—H11 | 120.3 | O17—C77—H77B | 109.5 |
| C11—C12—O2 | 118.51 (14) | H77A—C77—H77B | 109.5 |
| C11—C12—C7 | 121.99 (15) | O17—C77—H77C | 109.5 |
| O2—C12—C7 | 119.28 (14) | H77A—C77—H77C | 109.5 |
| C18—C13—O3 | 120.63 (13) | H77B—C77—H77C | 109.5 |
| C18—C13—C14 | 121.01 (14) | C79—C78—C81 | 110.80 (18) |
| O3—C13—C14 | 118.13 (13) | C79—C78—C80 | 107.26 (17) |
| C15—C14—C13 | 117.25 (15) | C81—C78—C80 | 106.73 (18) |
| C15—C14—C25 | 119.27 (14) | C79—C78—C70 | 109.91 (16) |
| C13—C14—C25 | 123.43 (14) | C81—C78—C70 | 110.40 (15) |
| C14—C15—C16 | 122.21 (16) | C80—C78—C70 | 111.65 (16) |
| C14—C15—H15 | 118.9 | C78—C79—H79A | 109.5 |
| C16—C15—H15 | 118.9 | C78—C79—H79B | 109.5 |
| C17—C16—O7 | 125.11 (16) | H79A—C79—H79B | 109.5 |
| C17—C16—C15 | 119.86 (15) | C78—C79—H79C | 109.5 |
| O7—C16—C15 | 115.02 (15) | H79A—C79—H79C | 109.5 |
| C16—C17—C18 | 120.09 (15) | H79B—C79—H79C | 109.5 |
| C16—C17—H17 | 120.0 | C78—C80—H80A | 109.5 |
| C18—C17—H17 | 120.0 | C78—C80—H80B | 109.5 |
| C13—C18—C17 | 119.42 (14) | H80A—C80—H80B | 109.5 |
| C13—C18—C19 | 124.85 (14) | C78—C80—H80C | 109.5 |
| C17—C18—C19 | 115.54 (14) | H80A—C80—H80C | 109.5 |
| C20—C19—C24 | 119.47 (14) | H80B—C80—H80C | 109.5 |
| C20—C19—C18 | 119.25 (14) | C78—C81—H81A | 109.5 |
| C24—C19—C18 | 120.82 (14) | C78—C81—H81B | 109.5 |
| C21—C20—C19 | 119.29 (14) | H81A—C81—H81B | 109.5 |
| C21—C20—H20 | 120.4 | C78—C81—H81C | 109.5 |
| C19—C20—H20 | 120.4 | H81A—C81—H81C | 109.5 |
| O8—C21—C20 | 124.31 (15) | H81B—C81—H81C | 109.5 |
| O8—C21—C22 | 115.53 (14) | C83—C82—C87 | 122.22 (18) |
| C20—C21—C22 | 120.12 (15) | C83—C82—O14 | 118.04 (16) |
| C23—C22—C21 | 122.30 (15) | C87—C82—O14 | 119.58 (17) |
| C23—C22—H22 | 118.8 | C84—C83—C82 | 119.14 (19) |
| C21—C22—H22 | 118.8 | C84—C83—H83 | 120.4 |

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| C22—C23—C24 | 116.31 (14) | C82—C83—H83 | 120.4 |
| C22—C23—C31 | 120.93 (14) | C83—C84—C85 | 119.9 (2) |
| C24—C23—C31 | 122.74 (14) | C83—C84—H84 | 120.1 |
| C19—C24—O4 | 118.45 (13) | C85—C84—H84 | 120.1 |
| C19—C24—C23 | 121.96 (14) | C86—C85—C84 | 120.7 (2) |
| O4—C24—C23 | 119.58 (13) | C86—C85—H85 | 119.7 |
| C27—C25—C28 | 111.02 (15) | C84—C85—H85 | 119.7 |
| C27—C25—C14 | 110.16 (14) | C85—C86—C87 | 120.69 (19) |
| C28—C25—C14 | 109.83 (15) | C85—C86—H86 | 119.7 |
| C27—C25—C26 | 107.27 (16) | C87—C86—H86 | 119.7 |
| C28—C25—C26 | 106.76 (16) | C86—C87—C82 | 117.38 (18) |
| C14—C25—C26 | 111.75 (14) | C86—C87—C88 | 122.22 (17) |
| C25—C26—H26A | 109.5 | C82—C87—C88 | 120.31 (17) |
| C25—C26—H26B | 109.5 | C93—C88—C89 | 117.54 (18) |
| H26A—C26—H26B | 109.5 | C93—C88—C87 | 121.07 (16) |
| C25—C26—H26C | 109.5 | C89—C88—C87 | 121.34 (17) |
| H26A—C26—H26C | 109.5 | C90—C89—C88 | 120.9 (2) |
| H26B—C26—H26C | 109.5 | C90—C89—H89 | 119.5 |
| C25—C27—H27A | 109.5 | C88—C89—H89 | 119.5 |
| C25—C27—H27B | 109.5 | C89—C90—C91 | 120.22 (19) |
| H27A—C27—H27B | 109.5 | C89—C90—H90 | 119.9 |
| C25—C27—H27C | 109.5 | C91—C90—H90 | 119.9 |
| H27A—C27—H27C | 109.5 | C90—C91—C92 | 120.0 (2) |
| H27B—C27—H27C | 109.5 | C90—C91—H91 | 120.0 |
| C25—C28—H28A | 109.5 | C92—C91—H91 | 120.0 |
| C25—C28—H28B | 109.5 | C93—C92—C91 | 119.14 (19) |
| H28A—C28—H28B | 109.5 | C93—C92—H92 | 120.4 |
| C25—C28—H28C | 109.5 | C91—C92—H92 | 120.4 |
| H28A—C28—H28C | 109.5 | C92—C93—C88 | 122.14 (17) |
| H28B—C28—H28C | 109.5 | C92—C93—O15 | 119.42 (17) |
| O7—C29—H29A | 109.5 | C88—C93—O15 | 118.40 (16) |
| O7—C29—H29B | 109.5 | C1—O1—P1 | 126.60 (10) |
| H29A—C29—H29B | 109.5 | C12—O2—P1 | 119.87 (9) |
| O7—C29—H29C | 109.5 | C13—O3—P1 | 128.64 (10) |
| H29A—C29—H29C | 109.5 | C24—O4—P2 | 120.30 (9) |
| H29B—C29—H29C | 109.5 | C35—O5—P2 | 115.59 (9) |
| O8—C30—H30A | 109.5 | C46—O6—P2 | 126.53 (10) |
| O8—C30—H30B | 109.5 | C16—O7—C29 | 117.25 (15) |
| H30A—C30—H30B | 109.5 | C21—O8—C30 | 116.22 (13) |
| O8—C30—H30C | 109.5 | C48—O10—P3 | 125.20 (10) |
| H30A—C30—H30C | 109.5 | C59—O11—P3 | 120.47 (10) |
| H30B—C30—H30C | 109.5 | C60—O12—P3 | 125.01 (10) |
| C32—C31—C33 | 107.86 (14) | C71—O13—P4 | 127.26 (11) |
| C32—C31—C34 | 110.15 (14) | C82—O14—P4 | 123.17 (11) |
| C33—C31—C34 | 106.63 (14) | C93—O15—P4 | 116.16 (11) |
| C32—C31—C23 | 110.42 (13) | C63—O16—C76 | 117.26 (15) |
| C33—C31—C23 | 111.20 (14) | C68—O17—C77 | 117.24 (15) |
| C34—C31—C23 | 110.47 (13) | O1—P1—O3 | 100.33 (6) |

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| C31—C32—H32A | 109.5 | O1—P1—O2 | 99.78 (6) |
| C31—C32—H32B | 109.5 | O3—P1—O2 | 93.64 (6) |
| H32A—C32—H32B | 109.5 | O1—P1—Rh1 | 113.71 (4) |
| C31—C32—H32C | 109.5 | O3—P1—Rh1 | 120.63 (4) |
| H32A—C32—H32C | 109.5 | O2—P1—Rh1 | 124.12 (4) |
| H32B—C32—H32C | 109.5 | O6—P2—O5 | 99.93 (6) |
| C31—C33—H33A | 109.5 | O6—P2—O4 | 100.91 (6) |
| C31—C33—H33B | 109.5 | O5—P2—O4 | 95.49 (6) |
| H33A—C33—H33B | 109.5 | O6—P2—Rh1 | 113.09 (4) |
| C31—C33—H33C | 109.5 | O5—P2—Rh1 | 122.18 (4) |
| H33A—C33—H33C | 109.5 | O4—P2—Rh1 | 121.13 (4) |
| H33B—C33—H33C | 109.5 | O10—P3—O12 | 99.18 (6) |
| C31—C34—H34A | 109.5 | O10—P3—O11 | 100.23 (6) |
| C31—C34—H34B | 109.5 | O12—P3—O11 | 95.66 (6) |
| H34A—C34—H34B | 109.5 | O10—P3—Rh1 | 110.13 (4) |
| C31—C34—H34C | 109.5 | O12—P3—Rh1 | 126.79 (4) |
| H34A—C34—H34C | 109.5 | O11—P3—Rh1 | 120.20 (5) |
| H34B—C34—H34C | 109.5 | O14—P4—O13 | 97.63 (7) |
| C36—C35—O5 | 118.61 (14) | O14—P4—O15 | 99.05 (6) |
| C36—C35—C40 | 122.36 (15) | O13—P4—O15 | 96.77 (7) |
| O5—C35—C40 | 118.99 (14) | C47—Rh1—P1 | 99.54 (5) |
| C35—C36—C37 | 118.95 (16) | C47—Rh1—P2 | 97.23 (5) |
| C35—C36—H36 | 120.5 | P1—Rh1—P2 | 118.789 (15) |
| C37—C36—H36 | 120.5 | C47—Rh1—P3 | 98.70 (5) |
| C38—C37—C36 | 119.99 (16) | P1—Rh1—P3 | 128.401 (15) |
| C38—C37—H37 | 120.0 | P2—Rh1—P3 | 106.081 (15) |
| C36—C37—H37 | 120.0 | C47—Rh1—H1 | 176.5 (8) |
| C39—C38—C37 | 120.34 (16) | P1—Rh1—H1 | 77.5 (8) |
| C39—C38—H38 | 119.8 | P2—Rh1—H1 | 85.8 (8) |
| C37—C38—H38 | 119.8 | P3—Rh1—H1 | 82.0 (8) |
| C38—C39—C40 | 121.05 (17) | C95—C94—C99 | 120.0 |
| C38—C39—H39 | 119.5 | C95—C94—C100 | 117.2 (3) |
| C40—C39—H39 | 119.5 | C99—C94—C100 | 122.8 (3) |
| C35—C40—C39 | 117.27 (15) | C94—C95—C96 | 120.0 |
| C35—C40—C41 | 120.93 (14) | C94—C95—D95 | 120.0 |
| C39—C40—C41 | 121.76 (15) | C96—C95—D95 | 120.0 |
| C46—C41—C42 | 117.55 (15) | C97—C96—C95 | 120.0 |
| C46—C41—C40 | 122.54 (14) | C97—C96—D96 | 120.0 |
| C42—C41—C40 | 119.87 (14) | C95—C96—D96 | 120.0 |
| C43—C42—C41 | 121.49 (16) | C98—C97—C96 | 120.0 |
| C43—C42—H42 | 119.3 | C98—C97—D97 | 120.0 |
| C41—C42—H42 | 119.3 | C96—C97—D97 | 120.0 |
| C42—C43—C44 | 119.69 (16) | C97—C98—C99 | 120.0 |
| C42—C43—H43 | 120.2 | C97—C98—D98 | 120.0 |
| C44—C43—H43 | 120.2 | C99—C98—D98 | 120.0 |
| C43—C44—C45 | 120.24 (16) | C98—C99—C94 | 120.0 |
| C43—C44—H44 | 119.9 | C98—C99—D99 | 120.0 |
| C45—C44—H44 | 119.9 | C94—C99—D99 | 120.0 |

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| C46—C45—C44 | 119.44 (16) | C94—C100—D10A | 109.5 |
| C46—C45—H45 | 120.3 | C94—C100—D10B | 109.5 |
| C44—C45—H45 | 120.3 | D10A—C100—D10B | 109.5 |
| C45—C46—C41 | 121.59 (14) | C94—C100—D10C | 109.5 |
| C45—C46—O6 | 117.75 (14) | D10A—C100—D10C | 109.5 |
| C41—C46—O6 | 120.42 (14) | D10B—C100—D10C | 109.5 |
| O9—C47—Rh1 | 178.18 (14) | C102—C101—C106 | 120.0 |
| C49—C48—C53 | 122.03 (15) | C102—C101—C107 | 122.2 (4) |
| C49—C48—O10 | 117.51 (15) | C106—C101—C107 | 117.8 (4) |
| C53—C48—O10 | 120.07 (14) | C103—C102—C101 | 120.0 |
| C48—C49—C50 | 119.49 (17) | C103—C102—D102 | 120.0 |
| C48—C49—H49 | 120.3 | C101—C102—D102 | 120.0 |
| C50—C49—H49 | 120.3 | C102—C103—C104 | 120.0 |
| C51—C50—C49 | 119.80 (18) | C102—C103—D103 | 120.0 |
| C51—C50—H50 | 120.1 | C104—C103—D103 | 120.0 |
| C49—C50—H50 | 120.1 | C105—C104—C103 | 120.0 |
| C52—C51—C50 | 120.24 (18) | C105—C104—D104 | 120.0 |
| C52—C51—H51 | 119.9 | C103—C104—D104 | 120.0 |
| C50—C51—H51 | 119.9 | C104—C105—C106 | 120.0 |
| C51—C52—C53 | 121.33 (18) | C104—C105—D105 | 120.0 |
| C51—C52—H52 | 119.3 | C106—C105—D105 | 120.0 |
| C53—C52—H52 | 119.3 | C105—C106—C101 | 120.0 |
| C48—C53—C52 | 117.10 (16) | C105—C106—D106 | 120.0 |
| C48—C53—C54 | 122.85 (15) | C101—C106—D106 | 120.0 |
| C52—C53—C54 | 120.03 (16) | C101—C107—D10D | 109.5 |
| C55—C54—C59 | 117.24 (16) | C101—C107—D10E | 109.5 |
| C55—C54—C53 | 121.13 (15) | D10D—C107—D10E | 109.5 |
| C59—C54—C53 | 121.56 (15) | C101—C107—D10F | 109.5 |
| C56—C55—C54 | 121.30 (17) | D10D—C107—D10F | 109.5 |
| C56—C55—H55 | 119.4 | D10E—C107—D10F | 109.5 |
| C54—C55—H55 | 119.4 | C109—C108—C113 | 120.0 |
| C55—C56—C57 | 120.16 (17) | C109—C108—C114 | 118.5 (7) |
| C55—C56—H56 | 119.9 | C113—C108—C114 | 121.5 (7) |
| C57—C56—H56 | 119.9 | C108—C109—C110 | 120.0 |
| C56—C57—C58 | 119.96 (17) | C108—C109—D109 | 120.0 |
| C56—C57—H57 | 120.0 | C110—C109—D109 | 120.0 |
| C58—C57—H57 | 120.0 | C109—C110—C111 | 120.0 |
| C59—C58—C57 | 119.29 (16) | C109—C110—D110 | 120.0 |
| C59—C58—H58 | 120.4 | C111—C110—D110 | 120.0 |
| C57—C58—H58 | 120.4 | C112—C111—C110 | 120.0 |
| C58—C59—O11 | 118.50 (14) | C112—C111—D111 | 120.0 |
| C58—C59—C54 | 122.03 (15) | C110—C111—D111 | 120.0 |
| O11—C59—C54 | 119.22 (15) | C113—C112—C111 | 120.0 |
| C61—C60—C65 | 121.49 (14) | C113—C112—D112 | 120.0 |
| C61—C60—O12 | 119.68 (14) | C111—C112—D112 | 120.0 |
| C65—C60—O12 | 118.65 (14) | C112—C113—C108 | 120.0 |
| C62—C61—C60 | 116.82 (15) | C112—C113—D113 | 120.0 |
| C62—C61—C72 | 119.58 (15) | C108—C113—D113 | 120.0 |

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| C60—C61—C72 | 123.55 (15) | C108—C114—D11A | 109.5 |
| C63—C62—C61 | 121.98 (15) | C108—C114—D11B | 109.5 |
| C63—C62—H62 | 119.0 | D11A—C114—D11B | 109.5 |
| C61—C62—H62 | 119.0 | C108—C114—D11C | 109.5 |
| O16—C63—C62 | 124.31 (15) | D11A—C114—D11C | 109.5 |
| O16—C63—C64 | 115.61 (15) | D11B—C114—D11C | 109.5 |
| C62—C63—C64 | 120.08 (15) | C116—C115—C120 | 120.0 |
| C63—C64—C65 | 119.73 (15) | C116—C115—C121 | 119.7 (4) |
| C63—C64—H64 | 120.1 | C120—C115—C121 | 120.3 (4) |
| C65—C64—H64 | 120.1 | C117—C116—C115 | 120.0 |
| C64—C65—C60 | 119.50 (15) | C117—C116—D116 | 120.0 |
| C64—C65—C66 | 117.14 (14) | C115—C116—D116 | 120.0 |
| C60—C65—C66 | 123.34 (14) | C116—C117—C118 | 120.0 |
| C67—C66—C71 | 119.21 (15) | C116—C117—D117 | 120.0 |
| C67—C66—C65 | 117.61 (14) | C118—C117—D117 | 120.0 |
| C71—C66—C65 | 123.14 (14) | C117—C118—C119 | 120.0 |
| C68—C67—C66 | 120.13 (15) | C117—C118—D118 | 120.0 |
| C68—C67—H67 | 119.9 | C119—C118—D118 | 120.0 |
| C66—C67—H67 | 119.9 | C120—C119—C118 | 120.0 |
| O17—C68—C67 | 115.78 (15) | C120—C119—D119 | 120.0 |
| O17—C68—C69 | 124.23 (15) | C118—C119—D119 | 120.0 |
| C67—C68—C69 | 119.98 (15) | C119—C120—C115 | 120.0 |
| C68—C69—C70 | 121.84 (16) | C119—C120—D120 | 120.0 |
| C68—C69—H69 | 119.1 | C115—C120—D120 | 120.0 |
| C70—C69—H69 | 119.1 | C115—C121—D12A | 109.5 |
| C69—C70—C71 | 117.07 (15) | C115—C121—D12B | 109.5 |
| C69—C70—C78 | 119.88 (16) | D12A—C121—D12B | 109.5 |
| C71—C70—C78 | 123.04 (16) | C115—C121—D12C | 109.5 |
| O13—C71—C70 | 117.83 (14) | D12A—C121—D12C | 109.5 |
| O13—C71—C66 | 120.66 (14) | D12B—C121—D12C | 109.5 |
| O1—C1—C2—C3 | 175.21 (16) | C66—C67—C68—C69 | 2.6 (2) |
| C6—C1—C2—C3 | 1.6 (3) | O17—C68—C69—C70 | 175.70 (15) |
| C1—C2—C3—C4 | -1.6 (3) | C67—C68—C69—C70 | -3.7 (3) |
| C2—C3—C4—C5 | 0.7 (3) | C68—C69—C70—C71 | -0.5 (2) |
| C3—C4—C5—C6 | 0.2 (3) | C68—C69—C70—C78 | 178.19 (16) |
| C2—C1—C6—C5 | -0.7 (3) | C69—C70—C71—O13 | -178.17 (14) |
| O1—C1—C6—C5 | -174.08 (15) | C78—C70—C71—O13 | 3.2 (2) |
| C2—C1—C6—C7 | -178.26 (16) | C69—C70—C71—C66 | 5.7 (2) |
| O1—C1—C6—C7 | 8.3 (2) | C78—C70—C71—C66 | -172.86 (16) |
| C4—C5—C6—C1 | -0.2 (3) | C67—C66—C71—O13 | 177.16 (14) |
| C4—C5—C6—C7 | 177.48 (18) | C65—C66—C71—O13 | -0.2 (2) |
| C1—C6—C7—C12 | 42.9 (2) | C67—C66—C71—C70 | -6.9 (2) |
| C5—C6—C7—C12 | -134.62 (17) | C65—C66—C71—C70 | 175.81 (15) |
| C1—C6—C7—C8 | -143.71 (17) | C62—C61—C72—C75 | -117.75 (18) |
| C5—C6—C7—C8 | 38.7 (2) | C60—C61—C72—C75 | 59.5 (2) |
| C12—C7—C8—C9 | 1.9 (2) | C62—C61—C72—C74 | 1.1 (2) |
| C6—C7—C8—C9 | -171.71 (16) | C60—C61—C72—C74 | 178.41 (18) |

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| C7—C8—C9—C10 | 0.8 (3) | C62—C61—C72—C73 | 120.23 (18) |
| C8—C9—C10—C11 | -2.0 (3) | C60—C61—C72—C73 | -62.5 (2) |
| C9—C10—C11—C12 | 0.5 (3) | C69—C70—C78—C79 | 114.9 (2) |
| C10—C11—C12—O2 | 176.97 (14) | C71—C70—C78—C79 | -66.5 (2) |
| C10—C11—C12—C7 | 2.4 (2) | C69—C70—C78—C81 | -122.57 (18) |
| C8—C7—C12—C11 | -3.5 (2) | C71—C70—C78—C81 | 56.0 (2) |
| C6—C7—C12—C11 | 170.10 (15) | C69—C70—C78—C80 | -4.0 (2) |
| C8—C7—C12—O2 | -178.05 (14) | C71—C70—C78—C80 | 174.55 (17) |
| C6—C7—C12—O2 | -4.5 (2) | C87—C82—C83—C84 | 0.6 (3) |
| C18—C13—C14—C15 | 4.6 (2) | O14—C82—C83—C84 | -174.73 (17) |
| O3—C13—C14—C15 | 179.17 (15) | C82—C83—C84—C85 | -0.9 (3) |
| C18—C13—C14—C25 | -172.95 (15) | C83—C84—C85—C86 | 0.1 (3) |
| O3—C13—C14—C25 | 1.7 (2) | C84—C85—C86—C87 | 0.9 (3) |
| C13—C14—C15—C16 | -2.3 (3) | C85—C86—C87—C82 | -1.1 (3) |
| C25—C14—C15—C16 | 175.28 (17) | C85—C86—C87—C88 | 175.52 (19) |
| C14—C15—C16—C17 | -1.0 (3) | C83—C82—C87—C86 | 0.4 (3) |
| C14—C15—C16—O7 | -179.87 (17) | O14—C82—C87—C86 | 175.67 (16) |
| O7—C16—C17—C18 | -179.04 (17) | C83—C82—C87—C88 | -176.36 (17) |
| C15—C16—C17—C18 | 2.2 (3) | O14—C82—C87—C88 | -1.1 (2) |
| O3—C13—C18—C17 | -177.95 (14) | C86—C87—C88—C93 | 138.6 (2) |
| C14—C13—C18—C17 | -3.5 (2) | C82—C87—C88—C93 | -44.8 (3) |
| O3—C13—C18—C19 | -3.3 (2) | C86—C87—C88—C89 | -44.0 (3) |
| C14—C13—C18—C19 | 171.24 (15) | C82—C87—C88—C89 | 132.6 (2) |
| C16—C17—C18—C13 | 0.0 (2) | C93—C88—C89—C90 | 2.7 (3) |
| C16—C17—C18—C19 | -175.17 (15) | C87—C88—C89—C90 | -174.8 (2) |
| C13—C18—C19—C20 | -57.3 (2) | C88—C89—C90—C91 | -0.7 (4) |
| C17—C18—C19—C20 | 117.56 (16) | C89—C90—C91—C92 | -1.6 (4) |
| C13—C18—C19—C24 | 130.59 (17) | C90—C91—C92—C93 | 1.8 (3) |
| C17—C18—C19—C24 | -54.5 (2) | C91—C92—C93—C88 | 0.2 (3) |
| C24—C19—C20—C21 | 1.1 (2) | C91—C92—C93—O15 | -177.48 (19) |
| C18—C19—C20—C21 | -171.10 (14) | C89—C88—C93—C92 | -2.4 (3) |
| C19—C20—C21—O8 | -177.46 (15) | C87—C88—C93—C92 | 175.04 (18) |
| C19—C20—C21—C22 | 4.9 (2) | C89—C88—C93—O15 | 175.30 (17) |
| O8—C21—C22—C23 | 176.80 (15) | C87—C88—C93—O15 | -7.2 (3) |
| C20—C21—C22—C23 | -5.4 (3) | C2—C1—O1—P1 | 121.05 (15) |
| C21—C22—C23—C24 | -0.3 (2) | C6—C1—O1—P1 | -65.25 (19) |
| C21—C22—C23—C31 | 177.82 (15) | C11—C12—O2—P1 | 110.45 (14) |
| C20—C19—C24—O4 | 173.79 (13) | C7—C12—O2—P1 | -74.80 (16) |
| C18—C19—C24—O4 | -14.1 (2) | C18—C13—O3—P1 | -56.55 (19) |
| C20—C19—C24—C23 | -7.0 (2) | C14—C13—O3—P1 | 128.80 (14) |
| C18—C19—C24—C23 | 165.06 (14) | C19—C24—O4—P2 | -62.22 (17) |
| C22—C23—C24—C19 | 6.5 (2) | C23—C24—O4—P2 | 118.58 (13) |
| C31—C23—C24—C19 | -171.59 (14) | C36—C35—O5—P2 | 103.54 (14) |
| C22—C23—C24—O4 | -174.29 (14) | C40—C35—O5—P2 | -78.83 (15) |
| C31—C23—C24—O4 | 7.6 (2) | C45—C46—O6—P2 | 120.59 (14) |
| C15—C14—C25—C27 | 114.46 (18) | C41—C46—O6—P2 | -65.06 (19) |
| C13—C14—C25—C27 | -68.1 (2) | C17—C16—O7—C29 | -6.2 (3) |
| C15—C14—C25—C28 | -122.95 (18) | C15—C16—O7—C29 | 172.64 (18) |

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| C13—C14—C25—C28 | 54.5 (2) | C20—C21—O8—C30 | 1.4 (2) |
| C15—C14—C25—C26 | -4.7 (2) | C22—C21—O8—C30 | 179.10 (15) |
| C13—C14—C25—C26 | 172.79 (18) | C49—C48—O10—P3 | 117.57 (14) |
| C22—C23—C31—C32 | 109.21 (17) | C53—C48—O10—P3 | -69.48 (19) |
| C24—C23—C31—C32 | -72.75 (19) | C58—C59—O11—P3 | 109.54 (15) |
| C22—C23—C31—C33 | -10.5 (2) | C54—C59—O11—P3 | -76.13 (17) |
| C24—C23—C31—C33 | 167.54 (15) | C61—C60—O12—P3 | 113.49 (14) |
| C22—C23—C31—C34 | -128.68 (16) | C65—C60—O12—P3 | -71.29 (17) |
| C24—C23—C31—C34 | 49.3 (2) | C70—C71—O13—P4 | 140.53 (13) |
| O5—C35—C36—C37 | 179.84 (14) | C66—C71—O13—P4 | -43.4 (2) |
| C40—C35—C36—C37 | 2.3 (2) | C83—C82—O14—P4 | -111.33 (17) |
| C35—C36—C37—C38 | -0.7 (2) | C87—C82—O14—P4 | 73.18 (19) |
| C36—C37—C38—C39 | -1.3 (3) | C92—C93—O15—P4 | -99.77 (18) |
| C37—C38—C39—C40 | 1.8 (3) | C88—C93—O15—P4 | 82.43 (19) |
| C36—C35—C40—C39 | -1.8 (2) | C62—C63—O16—C76 | 2.1 (3) |
| O5—C35—C40—C39 | -179.30 (14) | C64—C63—O16—C76 | -176.72 (17) |
| C36—C35—C40—C41 | 175.77 (15) | C67—C68—O17—C77 | -161.75 (16) |
| O5—C35—C40—C41 | -1.8 (2) | C69—C68—O17—C77 | 18.8 (2) |
| C38—C39—C40—C35 | -0.3 (2) | C1—O1—P1—O3 | -69.81 (13) |
| C38—C39—C40—C41 | -177.82 (15) | C1—O1—P1—O2 | 25.75 (13) |
| C35—C40—C41—C46 | 42.8 (2) | C1—O1—P1—Rh1 | 159.97 (11) |
| C39—C40—C41—C46 | -139.72 (17) | C13—O3—P1—O1 | -134.97 (12) |
| C35—C40—C41—C42 | -134.81 (17) | C13—O3—P1—O2 | 124.39 (13) |
| C39—C40—C41—C42 | 42.6 (2) | C13—O3—P1—Rh1 | -9.31 (14) |
| C46—C41—C42—C43 | -1.1 (3) | C12—O2—P1—O1 | 61.61 (12) |
| C40—C41—C42—C43 | 176.69 (16) | C12—O2—P1—O3 | 162.76 (11) |
| C41—C42—C43—C44 | 0.9 (3) | C12—O2—P1—Rh1 | -65.95 (12) |
| C42—C43—C44—C45 | 0.2 (3) | C46—O6—P2—O5 | 23.49 (13) |
| C43—C44—C45—C46 | -1.1 (3) | C46—O6—P2—O4 | -74.13 (13) |
| C44—C45—C46—C41 | 1.0 (3) | C46—O6—P2—Rh1 | 154.98 (11) |
| C44—C45—C46—O6 | 175.23 (15) | C35—O5—P2—O6 | 64.68 (11) |
| C42—C41—C46—C45 | 0.1 (2) | C35—O5—P2—O4 | 166.79 (10) |
| C40—C41—C46—C45 | -177.57 (15) | C35—O5—P2—Rh1 | -60.82 (11) |
| C42—C41—C46—O6 | -173.99 (14) | C24—O4—P2—O6 | -134.54 (11) |
| C40—C41—C46—O6 | 8.3 (2) | C24—O4—P2—O5 | 124.21 (11) |
| C53—C48—C49—C50 | 0.0 (3) | C24—O4—P2—Rh1 | -8.87 (12) |
| O10—C48—C49—C50 | 172.80 (15) | C48—O10—P3—O12 | -61.69 (13) |
| C48—C49—C50—C51 | 0.4 (3) | C48—O10—P3—O11 | 35.82 (14) |
| C49—C50—C51—C52 | -0.1 (3) | C48—O10—P3—Rh1 | 163.45 (11) |
| C50—C51—C52—C53 | -0.7 (3) | C60—O12—P3—O10 | -145.21 (12) |
| C49—C48—C53—C52 | -0.7 (3) | C60—O12—P3—O11 | 113.45 (12) |
| O10—C48—C53—C52 | -173.36 (15) | C60—O12—P3—Rh1 | -21.42 (14) |
| C49—C48—C53—C54 | 177.79 (16) | C59—O11—P3—O10 | 53.92 (12) |
| O10—C48—C53—C54 | 5.2 (2) | C59—O11—P3—O12 | 154.33 (12) |
| C51—C52—C53—C48 | 1.1 (3) | C59—O11—P3—Rh1 | -66.72 (12) |
| C51—C52—C53—C54 | -177.48 (18) | C82—O14—P4—O13 | 56.31 (14) |
| C48—C53—C54—C55 | -140.80 (18) | C82—O14—P4—O15 | -41.83 (14) |
| C52—C53—C54—C55 | 37.7 (3) | C71—O13—P4—O14 | 156.89 (13) |

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| C48—C53—C54—C59 | 42.1 (2) | C71—O13—P4—O15 | -103.00 (13) |
| C52—C53—C54—C59 | -139.37 (18) | C93—O15—P4—O14 | -51.64 (14) |
| C59—C54—C55—C56 | 0.8 (3) | C93—O15—P4—O13 | -150.51 (13) |
| C53—C54—C55—C56 | -176.33 (17) | C99—C94—C95—C96 | 0.0 |
| C54—C55—C56—C57 | 0.3 (3) | C100—C94—C95—C96 | -178.8 (2) |
| C55—C56—C57—C58 | -0.8 (3) | C94—C95—C96—C97 | 0.0 |
| C56—C57—C58—C59 | 0.2 (3) | C95—C96—C97—C98 | 0.0 |
| C57—C58—C59—O11 | 175.17 (15) | C96—C97—C98—C99 | 0.0 |
| C57—C58—C59—C54 | 1.0 (3) | C97—C98—C99—C94 | 0.0 |
| C55—C54—C59—C58 | -1.5 (2) | C95—C94—C99—C98 | 0.0 |
| C53—C54—C59—C58 | 175.65 (16) | C100—C94—C99—C98 | 178.8 (2) |
| C55—C54—C59—O11 | -175.62 (15) | C106—C101—C102—C103 | 0.0 |
| C53—C54—C59—O11 | 1.5 (2) | C107—C101—C102—C103 | -179.3 (6) |
| C65—C60—C61—C62 | 5.2 (2) | C101—C102—C103—C104 | 0.0 |
| O12—C60—C61—C62 | -179.67 (14) | C102—C103—C104—C105 | 0.0 |
| C65—C60—C61—C72 | -172.12 (15) | C103—C104—C105—C106 | 0.0 |
| O12—C60—C61—C72 | 3.0 (2) | C104—C105—C106—C101 | 0.0 |
| C60—C61—C62—C63 | 0.4 (2) | C102—C101—C106—C105 | 0.0 |
| C72—C61—C62—C63 | 177.87 (16) | C107—C101—C106—C105 | 179.3 (5) |
| C61—C62—C63—O16 | 177.17 (16) | C113—C108—C109—C110 | 0.0 |
| C61—C62—C63—C64 | -4.1 (3) | C114—C108—C109—C110 | 178.6 (8) |
| O16—C63—C64—C65 | -179.00 (14) | C108—C109—C110—C111 | 0.0 |
| C62—C63—C64—C65 | 2.2 (2) | C109—C110—C111—C112 | 0.0 |
| C63—C64—C65—C60 | 3.3 (2) | C110—C111—C112—C113 | 0.0 |
| C63—C64—C65—C66 | -175.42 (14) | C111—C112—C113—C108 | 0.0 |
| C61—C60—C65—C64 | -7.2 (2) | C109—C108—C113—C112 | 0.0 |
| O12—C60—C65—C64 | 177.68 (13) | C114—C108—C113—C112 | -178.6 (9) |
| C61—C60—C65—C66 | 171.49 (14) | C120—C115—C116—C117 | 0.0 |
| O12—C60—C65—C66 | -3.6 (2) | C121—C115—C116—C117 | 179.7 (6) |
| C64—C65—C66—C67 | -60.49 (19) | C115—C116—C117—C118 | 0.0 |
| C60—C65—C66—C67 | 120.80 (17) | C116—C117—C118—C119 | 0.0 |
| C64—C65—C66—C71 | 116.88 (17) | C117—C118—C119—C120 | 0.0 |
| C60—C65—C66—C71 | -61.8 (2) | C118—C119—C120—C115 | 0.0 |
| C71—C66—C67—C68 | 2.6 (2) | C116—C115—C120—C119 | 0.0 |
| C65—C66—C67—C68 | -179.96 (14) | C121—C115—C120—C119 | -179.7 (6) |
| C66—C67—C68—O17 | -176.85 (14) | | |
