



metal-organic compounds

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

***trans*-Carbonylchloridobis[tris(naphthalen-1-yl)phosphane-κP]rhodium(I) acetone trisolvate**

Reinout Meijboom

Research Centre for Synthesis and Catalysis, Department of Chemistry, University of Johannesburg, PO Box 524, Auckland Park, 2006, Johannesburg, South Africa
Correspondence e-mail: rmeijboom@uj.ac.za

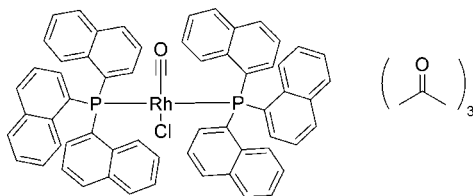
Received 23 August 2011; accepted 20 September 2011

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.046; wR factor = 0.098; data-to-parameter ratio = 19.6.

In the title compound, *trans*-[RhCl{P(C₁₀H₇)₃}₂(CO)]·3C₃H₆O, where P(C₁₀H₇)₃ is trinaphthylphosphine, the Rh—P bond lengths are 2.3360 (10) and 2.3258 (10) Å, while the Rh—Cl bond length is 2.3525 (11) Å. The coordination around the Rh atom shows a slightly distorted square-planar arrangement.

Related literature

For related compounds see: Otto (2001); Otto *et al.* (2000); Chen *et al.* (1991); Kuwabara & Bau (1994). Symmetrical square-planar complexes of Rh, Ir, Pd and Pt often crystallize with the metal atom on a crystallographic centre of symmetry, thus imposing a disordered packing arrangement. The present study is part of an ongoing investigation into determining which factors govern a disordered packing mode. The title compound is one of the few examples which does not show disorder along the carbonyl/chlorido axis. For similar non-disordered compounds, see: Burgoyne *et al.* (2010); Makhoba *et al.* (2011).



Experimental

Crystal data

[RhCl(C₃₀H₂₁P)₂(CO)]·3C₃H₆O
 $M_r = 1165.48$
Monoclinic, Cc
 $a = 10.1306$ (15) Å
 $b = 27.673$ (4) Å
 $c = 20.201$ (3) Å
 $\beta = 94.610$ (4)°
 $V = 5645.0$ (14) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.46$ mm⁻¹
 $T = 100$ K
 $0.34 \times 0.22 \times 0.04$ mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (SADABS; Bruker; 2004)
 $T_{\min} = 0.888$, $T_{\max} = 0.983$
31682 measured reflections
13902 independent reflections
11679 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.057$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.098$
 $S = 0.99$
13902 reflections
709 parameters
2 restraints
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.90$ e Å⁻³
 $\Delta\rho_{\min} = -0.56$ e Å⁻³
Absolute structure: Flack (1983), 6894 Friedel pairs
Flack parameter: -0.001 (19)

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT-Plus (Bruker, 2004); data reduction: SAINT-Plus and XPREP (Bruker, 2004); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 2005); software used to prepare material for publication: WinGX (Farrugia, 1999).

Financial assistance from the South African National Research Foundation (SA NRF), the Research Fund of the University of Johannesburg and SASOL is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MW2021).

References

- Brandenburg, K. (2005). DIAMOND. Crystal Impact GbR, Bonn, Germany.
Bruker (2004). SAINT-Plus XPREP and SADABS. Bruker AXS Inc, Madison, Wisconsin, USA.
Bruker (2005). APEX2. BrukerAXS Inc, Madison, Wisconsin, USA.
Burgoyne, A. R., Meijboom, R., Muller, A. & Omondi, B. O. (2010). *Acta Cryst.* E66, m1380–m1381.
Chen, Y.-J., Wang, J.-C. & Wang, Y. (1991). *Acta Cryst.* C47, 2441–2442.
Farrugia, L. J. (1999). *J. Appl. Cryst.* 32, 837–838.
Flack, H. D. (1983). *Acta Cryst.* A39, 876–881.
Kuwabara, E. & Bau, R. (1994). *Acta Cryst.* C50, 1409–1411.
Makhoba, S., Muller, A., Meijboom, R. & Omondi, B. (2011). *Acta Cryst.* E67, m1286–m1287.
Otto, S. (2001). *Acta Cryst.* C57, 793–795.
Otto, S., Roodt, A. & Smith, J. (2000). *Inorg. Chim. Acta*, 303, 295–299.
Sheldrick, G. M. (2008). *Acta Cryst.* A64, 112–122.

supplementary materials

Acta Cryst. (2011). E67, m1438 [doi:10.1107/S1600536811038505]

***trans*-Carbonylchloridobis[tris(naphthalen-1-yl)phosphane- κ P]rhodium(I) acetone trisolvate**

R. Meijboom

Comment

Symmetrical square-planar complexes of Rh, Ir, Pd and Pt often crystallize with the metal atom on a crystallographic centre of symmetry, thus imposing a disordered packing arrangement (Otto, 2001; Otto *et al.*, 2000; Chen *et al.*, 1991; Kuwabara & Bau, 1994). The present study is part of an ongoing investigation into determining which factors govern a disordered packing mode and reports the structure of *trans*-carbonylchloridobis(trinaphthylphosphine)rhodium(I). The compound is one of the few crystallographic examples of these complexes which does not show disorder along the carbonyl/chloro axis (Burgoyne *et al.*, 2010; Makhoba *et al.*, 2011). The coordination around the Rh atom shows a slightly distorted square-planar arrangement.

Experimental

Tri-naphthylphosphine (0.08 g, 0.21 mmol) was dissolved in acetone (5 cm³). A solution of dichlorotetracarbonyldirrhodium(I) (0.02 g, 0.05 mmol) in acetone (5 cm³) was added to the phosphine solution. The mixture was stirred for 5 minutes, after which the solution was left to crystallize. Yellow crystals of the title compound were obtained.

Refinement

The aromatic, and methyl H atoms were placed in geometrically idealized positions (C—H = 0.95–0.98) and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms respectively. Methyl torsion angles were refined from electron density.

Figures

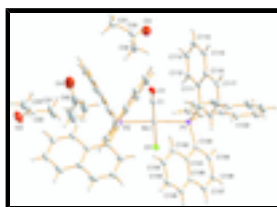


Fig. 1. The structure of the title compound, showing 50% probability displacement ellipsoids. For the C atoms, the first digit indicates ring number and the second digit indicates the position of the atom in the ring. Some labels have been omitted for clarity, all rings have been numbered in the same, systematic manner.

***trans*-Carbonylchloridobis[tris(naphthalen-1-yl)phosphane- κ P]rhodium(I) acetone trisolvate**

Crystal data

[RhCl(C₃₀H₂₁P)₂(CO)]·3C₃H₆O

$M_r = 1165.48$

Monoclinic, *Cc*

$F(000) = 2416$

$D_x = 1.371 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

supplementary materials

Hall symbol: C -2yc
 $a = 10.1306$ (15) Å
 $b = 27.673$ (4) Å
 $c = 20.201$ (3) Å
 $\beta = 94.610$ (4)°
 $V = 5645.0$ (14) Å³
 $Z = 4$

Cell parameters from 5353 reflections
 $\theta = 2.3$ – 25.8 °
 $\mu = 0.46$ mm⁻¹
 $T = 100$ K
Plate, yellow
 $0.34 \times 0.22 \times 0.04$ mm

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: sealed tube
graphite

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker; 2004)

$T_{\min} = 0.888$, $T_{\max} = 0.983$

31682 measured reflections

13902 independent reflections

11679 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.057$

$\theta_{\max} = 28.3$ °, $\theta_{\min} = 1.5$ °

$h = -13$ → 13

$k = -34$ → 36

$l = -26$ → 26

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.098$

$S = 0.99$

13902 reflections

709 parameters

2 restraints

Primary atom site location: structure-invariant direct
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring
sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2]$

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

$(\Delta/\sigma)_{\max} = 0.003$

$\Delta\rho_{\max} = 0.90$ e Å⁻³

$\Delta\rho_{\min} = -0.56$ e Å⁻³

Absolute structure: Flack (1983), 6894 Friedel pairs

Flack parameter: -0.001 (19)

Special details

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

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

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|-------------|--------------|--------------|----------------------------------|
| C1 | 0.5700 (4) | 0.70768 (13) | 0.71336 (19) | 0.0197 (8) |
| C10 | 0.4720 (4) | 0.75940 (14) | 0.90434 (19) | 0.0189 (8) |
| H10 | 0.5327 | 0.7468 | 0.9368 | 0.023* |
| C21 | 0.3148 (6) | 0.91871 (18) | 0.8501 (3) | 0.0592 (16) |
| H21A | 0.2548 | 0.8918 | 0.8483 | 0.089* |
| H21B | 0.394 | 0.9104 | 0.877 | 0.089* |
| H21C | 0.3369 | 0.9266 | 0.8061 | 0.089* |
| C22 | 0.2511 (5) | 0.96117 (15) | 0.8796 (2) | 0.0351 (11) |
| C23 | 0.1343 (6) | 0.9827 (2) | 0.8417 (3) | 0.0630 (17) |
| H23A | 0.1624 | 0.9997 | 0.8038 | 0.094* |
| H23B | 0.0915 | 1.0049 | 0.8696 | 0.094* |
| H23C | 0.0735 | 0.9576 | 0.8271 | 0.094* |
| C31 | 0.1743 (5) | 0.63458 (18) | 0.9130 (2) | 0.0402 (12) |
| H31A | 0.1715 | 0.6102 | 0.9467 | 0.06* |
| H31B | 0.0865 | 0.6401 | 0.8928 | 0.06* |
| H31C | 0.2087 | 0.664 | 0.9326 | 0.06* |
| C32 | 0.2779 (5) | 0.65282 (16) | 0.8050 (2) | 0.0368 (11) |
| H32A | 0.3291 | 0.6379 | 0.7726 | 0.055* |
| H32B | 0.3225 | 0.6814 | 0.822 | 0.055* |
| H32C | 0.1922 | 0.6614 | 0.7846 | 0.055* |
| C33 | 0.2621 (4) | 0.61795 (16) | 0.8611 (2) | 0.0309 (9) |
| C41 | 0.1187 (8) | 0.9664 (2) | 0.6213 (3) | 0.080 (2) |
| H41A | 0.1095 | 0.958 | 0.6667 | 0.12* |
| H41B | 0.1449 | 0.9996 | 0.6187 | 0.12* |
| H41C | 0.1848 | 0.9462 | 0.6038 | 0.12* |
| C42 | -0.0094 (7) | 0.95927 (17) | 0.5819 (3) | 0.0521 (16) |
| O4 | -0.1061 (6) | 0.94247 (14) | 0.6066 (2) | 0.0895 (17) |
| C110 | 0.6912 (4) | 0.63432 (13) | 0.61001 (18) | 0.0184 (7) |
| C111 | 0.5784 (4) | 0.60753 (12) | 0.62852 (18) | 0.0176 (7) |
| C112 | 0.5610 (4) | 0.59302 (13) | 0.6952 (2) | 0.0218 (9) |
| H112 | 0.6255 | 0.6008 | 0.7289 | 0.026* |
| C113 | 0.4520 (4) | 0.56801 (13) | 0.7101 (2) | 0.0245 (8) |
| H113 | 0.443 | 0.5589 | 0.7538 | 0.029* |
| C114 | 0.3527 (4) | 0.55567 (13) | 0.6605 (2) | 0.0247 (9) |
| H114 | 0.2779 | 0.539 | 0.6715 | 0.03* |
| C115 | 0.3664 (4) | 0.56821 (13) | 0.5966 (2) | 0.0252 (9) |
| H115 | 0.3007 | 0.5597 | 0.5639 | 0.03* |
| C116 | 0.4795 (4) | 0.59413 (13) | 0.57838 (19) | 0.0210 (8) |
| C117 | 0.4953 (4) | 0.60580 (13) | 0.51121 (19) | 0.0232 (8) |
| H117 | 0.4315 | 0.5963 | 0.4781 | 0.028* |
| C118 | 0.6040 (4) | 0.63101 (14) | 0.4950 (2) | 0.0218 (9) |
| H118 | 0.6135 | 0.6387 | 0.4509 | 0.026* |
| C119 | 0.7015 (4) | 0.64540 (13) | 0.54427 (17) | 0.0193 (8) |
| H119 | 0.7744 | 0.6628 | 0.5323 | 0.023* |
| C120 | 0.8843 (4) | 0.60061 (13) | 0.71304 (18) | 0.0187 (7) |

supplementary materials

| | | | | |
|------|------------|--------------|--------------|-------------|
| C121 | 0.9266 (4) | 0.55858 (13) | 0.67798 (19) | 0.0208 (8) |
| C122 | 0.9226 (4) | 0.55473 (14) | 0.60798 (19) | 0.0242 (8) |
| H122 | 0.8889 | 0.5803 | 0.5821 | 0.029* |
| C123 | 0.9668 (4) | 0.51458 (14) | 0.5774 (2) | 0.0305 (10) |
| H123 | 0.9624 | 0.5129 | 0.5313 | 0.037* |
| C124 | 1.0194 (5) | 0.47556 (15) | 0.6160 (2) | 0.0365 (11) |
| H124 | 1.0524 | 0.4486 | 0.5953 | 0.044* |
| C125 | 1.0220 (5) | 0.47715 (15) | 0.6830 (2) | 0.0344 (10) |
| H125 | 1.0537 | 0.4507 | 0.7079 | 0.041* |
| C126 | 0.9767 (4) | 0.51870 (14) | 0.7157 (2) | 0.0247 (9) |
| C127 | 0.9821 (4) | 0.52022 (14) | 0.7864 (2) | 0.0302 (9) |
| H127 | 1.0148 | 0.4938 | 0.811 | 0.036* |
| C128 | 0.9401 (4) | 0.55975 (15) | 0.8181 (2) | 0.0281 (9) |
| H128 | 0.9425 | 0.5602 | 0.8642 | 0.034* |
| C129 | 0.8928 (4) | 0.60008 (14) | 0.78146 (19) | 0.0210 (9) |
| H129 | 0.8665 | 0.6273 | 0.804 | 0.025* |
| C130 | 0.9467 (4) | 0.68404 (13) | 0.63052 (17) | 0.0172 (7) |
| C131 | 0.9307 (4) | 0.73167 (12) | 0.60455 (17) | 0.0166 (7) |
| C132 | 0.8109 (4) | 0.75808 (13) | 0.60300 (18) | 0.0191 (8) |
| H132 | 0.7358 | 0.7434 | 0.6175 | 0.023* |
| C133 | 0.8031 (4) | 0.80487 (14) | 0.58056 (19) | 0.0219 (8) |
| H133 | 0.7233 | 0.8215 | 0.5805 | 0.026* |
| C134 | 0.9140 (4) | 0.82788 (14) | 0.55780 (18) | 0.0242 (8) |
| H134 | 0.9077 | 0.8596 | 0.5429 | 0.029* |
| C135 | 1.0306 (4) | 0.80377 (14) | 0.55755 (18) | 0.0231 (8) |
| H135 | 1.1034 | 0.8191 | 0.5417 | 0.028* |
| C136 | 1.0428 (4) | 0.75567 (14) | 0.58109 (18) | 0.0200 (9) |
| C137 | 1.1648 (4) | 0.73095 (14) | 0.58231 (19) | 0.0234 (8) |
| H137 | 1.2378 | 0.7462 | 0.5664 | 0.028* |
| C138 | 1.1768 (4) | 0.68526 (14) | 0.60638 (19) | 0.0233 (8) |
| H138 | 1.2576 | 0.6693 | 0.6064 | 0.028* |
| C139 | 1.0687 (4) | 0.66206 (13) | 0.63110 (18) | 0.0203 (8) |
| H139 | 1.0794 | 0.631 | 0.6484 | 0.024* |
| C210 | 0.5165 (4) | 0.77527 (13) | 0.84513 (18) | 0.0178 (7) |
| C211 | 0.4235 (4) | 0.79589 (12) | 0.79625 (18) | 0.0184 (7) |
| C213 | 0.4599 (4) | 0.81645 (13) | 0.73540 (18) | 0.0214 (8) |
| H213 | 0.5483 | 0.8165 | 0.7261 | 0.026* |
| C214 | 0.3672 (4) | 0.83595 (14) | 0.69095 (19) | 0.0260 (9) |
| H214 | 0.3935 | 0.8499 | 0.6522 | 0.031* |
| C215 | 0.2317 (4) | 0.83552 (14) | 0.70244 (19) | 0.0283 (9) |
| H215 | 0.1691 | 0.8485 | 0.6712 | 0.034* |
| C216 | 0.1933 (4) | 0.81590 (14) | 0.7596 (2) | 0.0262 (9) |
| H216 | 0.1038 | 0.8152 | 0.7668 | 0.031* |
| C217 | 0.2870 (4) | 0.79663 (12) | 0.80827 (18) | 0.0195 (8) |
| C218 | 0.2472 (4) | 0.77876 (13) | 0.86930 (19) | 0.0229 (8) |
| H218 | 0.158 | 0.7786 | 0.8771 | 0.027* |
| C219 | 0.3391 (4) | 0.76176 (13) | 0.91667 (18) | 0.0204 (8) |
| H219 | 0.3126 | 0.7517 | 0.9575 | 0.024* |
| C220 | 0.7764 (4) | 0.74587 (13) | 0.90737 (18) | 0.0183 (7) |

| | | | | |
|------|--------------|--------------|---------------|--------------|
| C221 | 0.7635 (4) | 0.69568 (14) | 0.92564 (18) | 0.0204 (8) |
| C222 | 0.6681 (4) | 0.66430 (14) | 0.89414 (19) | 0.0225 (8) |
| H222 | 0.6079 | 0.6763 | 0.8609 | 0.027* |
| C223 | 0.6626 (5) | 0.61682 (15) | 0.9116 (2) | 0.0283 (10) |
| H223 | 0.5984 | 0.5969 | 0.8905 | 0.034* |
| C224 | 0.7539 (5) | 0.59760 (15) | 0.9616 (2) | 0.0323 (10) |
| H224 | 0.7519 | 0.5649 | 0.9723 | 0.039* |
| C225 | 0.8447 (5) | 0.62740 (15) | 0.9938 (2) | 0.0276 (10) |
| H225 | 0.903 | 0.6149 | 1.0275 | 0.033* |
| C226 | 0.8523 (4) | 0.67687 (14) | 0.97734 (18) | 0.0220 (8) |
| C227 | 0.9478 (4) | 0.70750 (15) | 1.01019 (19) | 0.0265 (9) |
| H227 | 1.0053 | 0.6952 | 1.0443 | 0.032* |
| C228 | 0.9567 (4) | 0.75456 (15) | 0.99269 (19) | 0.0244 (9) |
| H228 | 1.0188 | 0.7745 | 1.0155 | 0.029* |
| C229 | 0.8729 (4) | 0.77340 (13) | 0.94048 (18) | 0.0210 (8) |
| H229 | 0.883 | 0.8054 | 0.9279 | 0.025* |
| C230 | 0.7504 (4) | 0.82926 (13) | 0.81709 (18) | 0.0191 (8) |
| C231 | 0.7240 (4) | 0.86965 (13) | 0.85781 (18) | 0.0192 (8) |
| C232 | 0.6607 (4) | 0.86690 (14) | 0.91772 (19) | 0.0230 (8) |
| H232 | 0.6353 | 0.8369 | 0.9329 | 0.028* |
| C233 | 0.6359 (4) | 0.90717 (14) | 0.9537 (2) | 0.0266 (9) |
| H233 | 0.593 | 0.9042 | 0.9925 | 0.032* |
| C234 | 0.6745 (4) | 0.95301 (15) | 0.9329 (2) | 0.0323 (10) |
| H234 | 0.6566 | 0.9803 | 0.9575 | 0.039* |
| C235 | 0.7385 (4) | 0.95739 (14) | 0.8763 (2) | 0.0300 (10) |
| H235 | 0.7655 | 0.9878 | 0.8633 | 0.036* |
| C236 | 0.7646 (4) | 0.91686 (13) | 0.8371 (2) | 0.0240 (8) |
| C237 | 0.8269 (4) | 0.92113 (15) | 0.7772 (2) | 0.0311 (10) |
| H237 | 0.8497 | 0.9516 | 0.7625 | 0.037* |
| C238 | 0.8541 (4) | 0.88163 (15) | 0.74067 (19) | 0.0272 (9) |
| H238 | 0.8979 | 0.8852 | 0.7022 | 0.033* |
| C239 | 0.8161 (4) | 0.83557 (14) | 0.76091 (19) | 0.0236 (8) |
| H239 | 0.8359 | 0.8088 | 0.7358 | 0.028* |
| O1 | 0.4643 (3) | 0.70580 (10) | 0.69001 (15) | 0.0304 (7) |
| O2 | 0.2950 (4) | 0.97818 (12) | 0.93165 (17) | 0.0539 (10) |
| O3 | 0.3165 (4) | 0.57932 (12) | 0.86447 (18) | 0.0503 (9) |
| C43 | -0.0219 (6) | 0.97133 (19) | 0.5102 (2) | 0.0549 (15) |
| H43A | -0.0012 | 0.9434 | 0.4849 | 0.082* |
| H43B | 0.0383 | 0.997 | 0.5018 | 0.082* |
| H43C | -0.111 | 0.9814 | 0.4974 | 0.082* |
| P1 | 0.81469 (9) | 0.65586 (3) | 0.67416 (5) | 0.01594 (19) |
| P2 | 0.69062 (9) | 0.76754 (3) | 0.82986 (5) | 0.01584 (19) |
| Cl1 | 0.96409 (10) | 0.72128 (4) | 0.78862 (5) | 0.0230 (2) |
| Rh1 | 0.74079 (2) | 0.712399 (9) | 0.748699 (15) | 0.01574 (6) |

Atomic displacement parameters (\AA^2)

U^{11}

U^{22}

U^{33}

U^{12}

U^{13}

U^{23}

supplementary materials

| | | | | | | |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| C1 | 0.025 (2) | 0.0116 (18) | 0.0235 (19) | 0.0012 (15) | 0.0063 (17) | -0.0043 (15) |
| C10 | 0.021 (2) | 0.0191 (19) | 0.0158 (18) | -0.0001 (16) | -0.0021 (15) | 0.0008 (15) |
| C21 | 0.066 (4) | 0.036 (3) | 0.072 (4) | 0.010 (3) | -0.014 (3) | -0.022 (3) |
| C22 | 0.045 (3) | 0.025 (2) | 0.034 (2) | -0.016 (2) | -0.003 (2) | -0.0010 (18) |
| C23 | 0.034 (3) | 0.065 (4) | 0.088 (5) | 0.001 (3) | -0.008 (3) | -0.012 (3) |
| C31 | 0.043 (3) | 0.050 (3) | 0.028 (2) | -0.014 (2) | 0.005 (2) | -0.010 (2) |
| C32 | 0.043 (3) | 0.030 (2) | 0.038 (2) | 0.008 (2) | 0.013 (2) | 0.0009 (19) |
| C33 | 0.025 (2) | 0.032 (2) | 0.035 (2) | -0.0050 (19) | -0.0013 (19) | -0.0030 (19) |
| C41 | 0.114 (7) | 0.058 (4) | 0.065 (4) | 0.029 (4) | -0.009 (4) | -0.014 (3) |
| C42 | 0.090 (5) | 0.020 (2) | 0.049 (3) | 0.005 (3) | 0.029 (3) | -0.002 (2) |
| O4 | 0.147 (5) | 0.035 (2) | 0.096 (3) | -0.006 (3) | 0.071 (3) | 0.006 (2) |
| C110 | 0.0137 (18) | 0.0176 (18) | 0.0234 (18) | 0.0017 (14) | -0.0009 (15) | -0.0011 (15) |
| C111 | 0.0167 (18) | 0.0091 (16) | 0.0266 (19) | 0.0036 (14) | -0.0013 (15) | -0.0014 (14) |
| C112 | 0.024 (2) | 0.0182 (19) | 0.023 (2) | -0.0004 (16) | 0.0022 (17) | -0.0019 (16) |
| C113 | 0.026 (2) | 0.0181 (19) | 0.030 (2) | -0.0016 (16) | 0.0035 (17) | -0.0002 (16) |
| C114 | 0.020 (2) | 0.0164 (19) | 0.038 (2) | -0.0047 (16) | 0.0043 (17) | 0.0019 (17) |
| C115 | 0.019 (2) | 0.0167 (19) | 0.038 (2) | -0.0020 (15) | -0.0074 (17) | -0.0010 (17) |
| C116 | 0.020 (2) | 0.0140 (17) | 0.028 (2) | -0.0014 (15) | -0.0047 (16) | -0.0013 (15) |
| C117 | 0.023 (2) | 0.0172 (19) | 0.027 (2) | -0.0009 (16) | -0.0126 (16) | -0.0029 (16) |
| C118 | 0.025 (2) | 0.020 (2) | 0.0199 (19) | -0.0008 (17) | -0.0060 (16) | 0.0028 (16) |
| C119 | 0.0201 (19) | 0.0168 (18) | 0.0204 (18) | -0.0006 (15) | -0.0024 (15) | 0.0016 (15) |
| C120 | 0.0178 (19) | 0.0179 (18) | 0.0199 (18) | -0.0030 (15) | -0.0013 (15) | 0.0029 (15) |
| C121 | 0.0171 (19) | 0.0182 (19) | 0.0262 (19) | -0.0038 (15) | -0.0035 (15) | 0.0021 (15) |
| C122 | 0.025 (2) | 0.023 (2) | 0.0239 (19) | 0.0032 (17) | -0.0004 (16) | -0.0006 (16) |
| C123 | 0.034 (3) | 0.025 (2) | 0.032 (2) | 0.0002 (18) | -0.0005 (19) | -0.0054 (17) |
| C124 | 0.033 (3) | 0.022 (2) | 0.053 (3) | 0.0102 (19) | -0.006 (2) | -0.005 (2) |
| C125 | 0.036 (3) | 0.022 (2) | 0.043 (3) | 0.0028 (19) | -0.010 (2) | 0.0048 (19) |
| C126 | 0.022 (2) | 0.021 (2) | 0.030 (2) | -0.0021 (16) | -0.0054 (17) | 0.0023 (16) |
| C127 | 0.029 (2) | 0.022 (2) | 0.038 (2) | -0.0035 (18) | -0.0058 (19) | 0.0123 (18) |
| C128 | 0.028 (2) | 0.030 (2) | 0.025 (2) | 0.0008 (18) | -0.0033 (17) | 0.0029 (17) |
| C129 | 0.022 (2) | 0.0195 (19) | 0.021 (2) | -0.0006 (16) | -0.0005 (16) | 0.0015 (16) |
| C130 | 0.0160 (18) | 0.0176 (18) | 0.0179 (17) | -0.0054 (14) | 0.0000 (14) | -0.0004 (14) |
| C131 | 0.022 (2) | 0.0123 (16) | 0.0151 (16) | -0.0047 (15) | -0.0031 (14) | -0.0024 (14) |
| C132 | 0.020 (2) | 0.0214 (19) | 0.0156 (17) | -0.0045 (16) | -0.0014 (15) | -0.0012 (15) |
| C133 | 0.022 (2) | 0.0194 (19) | 0.024 (2) | 0.0002 (16) | -0.0034 (16) | -0.0022 (16) |
| C134 | 0.032 (2) | 0.0180 (19) | 0.0214 (19) | -0.0020 (17) | -0.0032 (17) | 0.0009 (15) |
| C135 | 0.026 (2) | 0.0226 (19) | 0.0200 (18) | -0.0088 (16) | 0.0008 (16) | -0.0007 (15) |
| C136 | 0.023 (2) | 0.021 (2) | 0.0153 (18) | -0.0053 (16) | -0.0001 (16) | -0.0064 (15) |
| C137 | 0.021 (2) | 0.027 (2) | 0.0223 (19) | -0.0079 (17) | 0.0047 (16) | -0.0023 (16) |
| C138 | 0.020 (2) | 0.023 (2) | 0.027 (2) | 0.0020 (16) | 0.0017 (16) | -0.0060 (16) |
| C139 | 0.020 (2) | 0.0191 (18) | 0.0210 (19) | 0.0017 (15) | -0.0021 (15) | -0.0064 (15) |
| C210 | 0.0165 (18) | 0.0185 (18) | 0.0180 (17) | -0.0011 (14) | -0.0005 (14) | 0.0002 (14) |
| C211 | 0.0225 (19) | 0.0129 (17) | 0.0193 (17) | -0.0019 (14) | -0.0023 (15) | -0.0016 (14) |
| C213 | 0.020 (2) | 0.0203 (19) | 0.0232 (19) | 0.0009 (15) | -0.0005 (16) | 0.0005 (15) |
| C214 | 0.033 (2) | 0.026 (2) | 0.0179 (18) | -0.0027 (18) | -0.0045 (17) | 0.0017 (16) |
| C215 | 0.034 (2) | 0.026 (2) | 0.0224 (19) | 0.0061 (18) | -0.0145 (17) | -0.0009 (17) |
| C216 | 0.019 (2) | 0.024 (2) | 0.034 (2) | 0.0003 (16) | -0.0084 (17) | -0.0060 (17) |
| C217 | 0.022 (2) | 0.0135 (18) | 0.0223 (18) | 0.0013 (14) | -0.0013 (15) | -0.0048 (14) |
| C218 | 0.0185 (19) | 0.022 (2) | 0.028 (2) | -0.0036 (15) | -0.0006 (16) | -0.0090 (16) |

| | | | | | | |
|------|--------------|--------------|--------------|---------------|--------------|---------------|
| C219 | 0.021 (2) | 0.0213 (19) | 0.0191 (18) | -0.0071 (16) | 0.0028 (15) | -0.0022 (15) |
| C220 | 0.0144 (18) | 0.0207 (18) | 0.0197 (18) | 0.0038 (15) | 0.0010 (14) | 0.0006 (15) |
| C221 | 0.022 (2) | 0.0205 (18) | 0.0194 (18) | 0.0026 (16) | 0.0064 (15) | 0.0007 (15) |
| C222 | 0.029 (2) | 0.021 (2) | 0.0183 (19) | -0.0018 (17) | 0.0045 (16) | -0.0010 (15) |
| C223 | 0.043 (3) | 0.019 (2) | 0.023 (2) | -0.0067 (19) | 0.0062 (19) | -0.0041 (17) |
| C224 | 0.044 (3) | 0.021 (2) | 0.034 (2) | 0.0035 (19) | 0.013 (2) | 0.0047 (18) |
| C225 | 0.031 (2) | 0.025 (2) | 0.028 (2) | 0.0032 (18) | 0.0067 (19) | 0.0045 (18) |
| C226 | 0.022 (2) | 0.0241 (19) | 0.0208 (18) | 0.0051 (16) | 0.0055 (16) | 0.0034 (15) |
| C227 | 0.018 (2) | 0.035 (2) | 0.026 (2) | 0.0108 (17) | -0.0017 (16) | 0.0066 (18) |
| C228 | 0.017 (2) | 0.031 (2) | 0.0246 (19) | 0.0002 (18) | -0.0050 (17) | 0.0008 (17) |
| C229 | 0.021 (2) | 0.0189 (18) | 0.0227 (19) | 0.0014 (15) | 0.0002 (16) | 0.0017 (15) |
| C230 | 0.0181 (19) | 0.0148 (17) | 0.0235 (19) | -0.0066 (14) | -0.0036 (15) | 0.0018 (15) |
| C231 | 0.0162 (18) | 0.0153 (18) | 0.0250 (19) | -0.0024 (14) | -0.0051 (15) | 0.0021 (15) |
| C232 | 0.024 (2) | 0.0176 (18) | 0.027 (2) | 0.0002 (16) | -0.0050 (16) | -0.0024 (15) |
| C233 | 0.022 (2) | 0.027 (2) | 0.030 (2) | 0.0028 (17) | -0.0033 (17) | -0.0062 (17) |
| C234 | 0.027 (2) | 0.026 (2) | 0.042 (3) | 0.0020 (18) | -0.007 (2) | -0.0115 (19) |
| C235 | 0.027 (2) | 0.017 (2) | 0.043 (3) | 0.0008 (17) | -0.013 (2) | 0.0022 (18) |
| C236 | 0.023 (2) | 0.0159 (19) | 0.031 (2) | -0.0036 (16) | -0.0065 (17) | 0.0035 (16) |
| C237 | 0.027 (2) | 0.025 (2) | 0.039 (2) | -0.0059 (17) | -0.0077 (19) | 0.0128 (19) |
| C238 | 0.028 (2) | 0.027 (2) | 0.026 (2) | -0.0101 (17) | -0.0012 (17) | 0.0049 (17) |
| C239 | 0.020 (2) | 0.024 (2) | 0.027 (2) | 0.0009 (16) | -0.0014 (17) | 0.0075 (16) |
| O1 | 0.0229 (16) | 0.0266 (16) | 0.0404 (18) | -0.0012 (13) | -0.0051 (13) | -0.0105 (13) |
| O2 | 0.073 (3) | 0.040 (2) | 0.045 (2) | -0.0016 (19) | -0.0150 (19) | -0.0119 (17) |
| O3 | 0.060 (3) | 0.0357 (19) | 0.056 (2) | 0.0065 (18) | 0.0086 (19) | 0.0126 (17) |
| C43 | 0.074 (4) | 0.043 (3) | 0.049 (3) | 0.020 (3) | 0.009 (3) | -0.006 (3) |
| P1 | 0.0155 (5) | 0.0155 (5) | 0.0166 (4) | -0.0012 (4) | -0.0002 (4) | 0.0012 (4) |
| P2 | 0.0162 (5) | 0.0146 (4) | 0.0164 (4) | -0.0008 (4) | -0.0010 (4) | -0.0006 (4) |
| Cl1 | 0.0168 (5) | 0.0252 (5) | 0.0266 (5) | -0.0027 (4) | -0.0001 (4) | -0.0049 (4) |
| Rh1 | 0.01477 (13) | 0.01523 (12) | 0.01692 (11) | -0.00188 (14) | -0.00049 (9) | -0.00096 (13) |

Geometric parameters (Å, °)

| | | | |
|----------|-----------|-----------|-----------|
| C1—O1 | 1.136 (5) | C132—H132 | 0.93 |
| C1—Rh1 | 1.823 (4) | C133—C134 | 1.400 (5) |
| C10—C210 | 1.384 (5) | C133—H133 | 0.93 |
| C10—C219 | 1.391 (5) | C134—C135 | 1.357 (6) |
| C10—H10 | 0.93 | C134—H134 | 0.93 |
| C21—C22 | 1.488 (7) | C135—C136 | 1.416 (5) |
| C21—H21A | 0.96 | C135—H135 | 0.93 |
| C21—H21B | 0.96 | C136—C137 | 1.411 (6) |
| C21—H21C | 0.96 | C137—C138 | 1.357 (5) |
| C22—O2 | 1.204 (5) | C137—H137 | 0.93 |
| C22—C23 | 1.482 (7) | C138—C139 | 1.396 (5) |
| C23—H23A | 0.96 | C138—H138 | 0.93 |
| C23—H23B | 0.96 | C139—H139 | 0.93 |
| C23—H23C | 0.96 | C210—C211 | 1.428 (5) |
| C31—C33 | 1.500 (6) | C210—P2 | 1.827 (4) |
| C31—H31A | 0.96 | C211—C217 | 1.422 (5) |
| C31—H31B | 0.96 | C211—C213 | 1.430 (5) |

supplementary materials

| | | | |
|-----------|-----------|-----------|-----------|
| C31—H31C | 0.96 | C213—C214 | 1.358 (5) |
| C32—C33 | 1.506 (6) | C213—H213 | 0.93 |
| C32—H32A | 0.96 | C214—C215 | 1.410 (6) |
| C32—H32B | 0.96 | C214—H214 | 0.93 |
| C32—H32C | 0.96 | C215—C216 | 1.361 (6) |
| C33—O3 | 1.202 (5) | C215—H215 | 0.93 |
| C41—C42 | 1.479 (9) | C216—C217 | 1.415 (5) |
| C41—H41A | 0.96 | C216—H216 | 0.93 |
| C41—H41B | 0.96 | C217—C218 | 1.417 (5) |
| C41—H41C | 0.96 | C218—C219 | 1.364 (5) |
| C42—O4 | 1.225 (7) | C218—H218 | 0.93 |
| C42—C43 | 1.483 (7) | C219—H219 | 0.93 |
| C110—C119 | 1.375 (5) | C220—C229 | 1.370 (5) |
| C110—C111 | 1.437 (5) | C220—C221 | 1.446 (5) |
| C110—P1 | 1.827 (4) | C220—P2 | 1.830 (4) |
| C111—C116 | 1.416 (5) | C221—C222 | 1.413 (6) |
| C111—C112 | 1.429 (5) | C221—C226 | 1.421 (5) |
| C112—C113 | 1.357 (5) | C222—C223 | 1.363 (5) |
| C112—H112 | 0.93 | C222—H222 | 0.93 |
| C113—C114 | 1.403 (6) | C223—C224 | 1.418 (6) |
| C113—H113 | 0.93 | C223—H223 | 0.93 |
| C114—C115 | 1.356 (6) | C224—C225 | 1.361 (6) |
| C114—H114 | 0.93 | C224—H224 | 0.93 |
| C115—C116 | 1.424 (5) | C225—C226 | 1.413 (6) |
| C115—H115 | 0.93 | C225—H225 | 0.93 |
| C116—C117 | 1.416 (5) | C226—C227 | 1.411 (6) |
| C117—C118 | 1.366 (6) | C227—C228 | 1.354 (6) |
| C117—H117 | 0.93 | C227—H227 | 0.93 |
| C118—C119 | 1.402 (5) | C228—C229 | 1.400 (5) |
| C118—H118 | 0.93 | C228—H228 | 0.93 |
| C119—H119 | 0.93 | C229—H229 | 0.93 |
| C120—C129 | 1.378 (5) | C230—C239 | 1.372 (5) |
| C120—C121 | 1.445 (5) | C230—C231 | 1.426 (5) |
| C120—P1 | 1.834 (4) | C230—P2 | 1.837 (4) |
| C121—C126 | 1.412 (5) | C231—C232 | 1.417 (5) |
| C121—C122 | 1.415 (5) | C231—C236 | 1.442 (5) |
| C122—C123 | 1.364 (5) | C232—C233 | 1.365 (5) |
| C122—H122 | 0.93 | C232—H232 | 0.93 |
| C123—C124 | 1.411 (6) | C233—C234 | 1.402 (6) |
| C123—H123 | 0.93 | C233—H233 | 0.93 |
| C124—C125 | 1.352 (6) | C234—C235 | 1.363 (6) |
| C124—H124 | 0.93 | C234—H234 | 0.93 |
| C125—C126 | 1.421 (6) | C235—C236 | 1.410 (6) |
| C125—H125 | 0.93 | C235—H235 | 0.93 |
| C126—C127 | 1.425 (6) | C236—C237 | 1.414 (6) |
| C127—C128 | 1.353 (6) | C237—C238 | 1.360 (6) |
| C127—H127 | 0.93 | C237—H237 | 0.93 |
| C128—C129 | 1.401 (5) | C238—C239 | 1.402 (5) |
| C128—H128 | 0.93 | C238—H238 | 0.93 |

| | | | |
|---------------|-----------|----------------|-------------|
| C129—H129 | 0.93 | C239—H239 | 0.93 |
| C130—C139 | 1.377 (5) | C43—H43A | 0.96 |
| C130—C131 | 1.423 (5) | C43—H43B | 0.96 |
| C130—P1 | 1.834 (4) | C43—H43C | 0.96 |
| C131—C132 | 1.416 (5) | P1—Rh1 | 2.3360 (10) |
| C131—C136 | 1.428 (5) | P2—Rh1 | 2.3258 (10) |
| C132—C133 | 1.372 (5) | Cl1—Rh1 | 2.3525 (11) |
| O1—C1—Rh1 | 177.9 (4) | C137—C136—C131 | 119.1 (3) |
| C210—C10—C219 | 121.9 (4) | C135—C136—C131 | 119.9 (4) |
| C210—C10—H10 | 119.1 | C138—C137—C136 | 120.8 (4) |
| C219—C10—H10 | 119.1 | C138—C137—H137 | 119.6 |
| C22—C21—H21A | 109.5 | C136—C137—H137 | 119.6 |
| C22—C21—H21B | 109.5 | C137—C138—C139 | 120.4 (4) |
| H21A—C21—H21B | 109.5 | C137—C138—H138 | 119.8 |
| C22—C21—H21C | 109.5 | C139—C138—H138 | 119.8 |
| H21A—C21—H21C | 109.5 | C130—C139—C138 | 121.6 (4) |
| H21B—C21—H21C | 109.5 | C130—C139—H139 | 119.2 |
| O2—C22—C23 | 121.2 (5) | C138—C139—H139 | 119.2 |
| O2—C22—C21 | 121.1 (5) | C10—C210—C211 | 118.8 (3) |
| C23—C22—C21 | 117.7 (5) | C10—C210—P2 | 119.7 (3) |
| C22—C23—H23A | 109.5 | C211—C210—P2 | 121.5 (3) |
| C22—C23—H23B | 109.5 | C217—C211—C210 | 119.0 (3) |
| H23A—C23—H23B | 109.5 | C217—C211—C213 | 117.5 (3) |
| C22—C23—H23C | 109.5 | C210—C211—C213 | 123.5 (3) |
| H23A—C23—H23C | 109.5 | C214—C213—C211 | 120.9 (4) |
| H23B—C23—H23C | 109.5 | C214—C213—H213 | 119.5 |
| C33—C31—H31A | 109.5 | C211—C213—H213 | 119.5 |
| C33—C31—H31B | 109.5 | C213—C214—C215 | 121.2 (4) |
| H31A—C31—H31B | 109.5 | C213—C214—H214 | 119.4 |
| C33—C31—H31C | 109.5 | C215—C214—H214 | 119.4 |
| H31A—C31—H31C | 109.5 | C216—C215—C214 | 119.5 (4) |
| H31B—C31—H31C | 109.5 | C216—C215—H215 | 120.3 |
| C33—C32—H32A | 109.5 | C214—C215—H215 | 120.3 |
| C33—C32—H32B | 109.5 | C215—C216—C217 | 121.2 (4) |
| H32A—C32—H32B | 109.5 | C215—C216—H216 | 119.4 |
| C33—C32—H32C | 109.5 | C217—C216—H216 | 119.4 |
| H32A—C32—H32C | 109.5 | C216—C217—C218 | 120.9 (4) |
| H32B—C32—H32C | 109.5 | C216—C217—C211 | 119.6 (3) |
| O3—C33—C31 | 121.9 (4) | C218—C217—C211 | 119.5 (3) |
| O3—C33—C32 | 122.4 (4) | C219—C218—C217 | 120.4 (4) |
| C31—C33—C32 | 115.7 (4) | C219—C218—H218 | 119.8 |
| C42—C41—H41A | 109.5 | C217—C218—H218 | 119.8 |
| C42—C41—H41B | 109.5 | C218—C219—C10 | 120.4 (4) |
| H41A—C41—H41B | 109.5 | C218—C219—H219 | 119.8 |
| C42—C41—H41C | 109.5 | C10—C219—H219 | 119.8 |
| H41A—C41—H41C | 109.5 | C229—C220—C221 | 119.0 (3) |
| H41B—C41—H41C | 109.5 | C229—C220—P2 | 120.4 (3) |
| O4—C42—C41 | 121.9 (6) | C221—C220—P2 | 119.1 (3) |
| O4—C42—C43 | 118.3 (7) | C222—C221—C226 | 118.4 (4) |

supplementary materials

| | | | |
|----------------|-----------|----------------|-----------|
| C41—C42—C43 | 119.8 (5) | C222—C221—C220 | 123.2 (4) |
| C119—C110—C111 | 119.3 (3) | C226—C221—C220 | 118.3 (4) |
| C119—C110—P1 | 120.8 (3) | C223—C222—C221 | 121.1 (4) |
| C111—C110—P1 | 119.8 (3) | C223—C222—H222 | 119.4 |
| C116—C111—C112 | 117.8 (3) | C221—C222—H222 | 119.4 |
| C116—C111—C110 | 118.7 (3) | C222—C223—C224 | 120.6 (4) |
| C112—C111—C110 | 123.4 (4) | C222—C223—H223 | 119.7 |
| C113—C112—C111 | 121.0 (4) | C224—C223—H223 | 119.7 |
| C113—C112—H112 | 119.5 | C225—C224—C223 | 119.4 (4) |
| C111—C112—H112 | 119.5 | C225—C224—H224 | 120.3 |
| C112—C113—C114 | 121.1 (4) | C223—C224—H224 | 120.3 |
| C112—C113—H113 | 119.5 | C224—C225—C226 | 121.5 (4) |
| C114—C113—H113 | 119.5 | C224—C225—H225 | 119.3 |
| C115—C114—C113 | 119.7 (4) | C226—C225—H225 | 119.3 |
| C115—C114—H114 | 120.2 | C227—C226—C225 | 121.3 (4) |
| C113—C114—H114 | 120.2 | C227—C226—C221 | 119.7 (3) |
| C114—C115—C116 | 121.4 (4) | C225—C226—C221 | 119.0 (4) |
| C114—C115—H115 | 119.3 | C228—C227—C226 | 120.8 (4) |
| C116—C115—H115 | 119.3 | C228—C227—H227 | 119.6 |
| C111—C116—C117 | 119.9 (3) | C226—C227—H227 | 119.6 |
| C111—C116—C115 | 119.0 (4) | C227—C228—C229 | 120.4 (4) |
| C117—C116—C115 | 121.1 (4) | C227—C228—H228 | 119.8 |
| C118—C117—C116 | 120.1 (4) | C229—C228—H228 | 119.8 |
| C118—C117—H117 | 120 | C220—C229—C228 | 121.7 (4) |
| C116—C117—H117 | 120 | C220—C229—H229 | 119.1 |
| C117—C118—C119 | 120.8 (4) | C228—C229—H229 | 119.1 |
| C117—C118—H118 | 119.6 | C239—C230—C231 | 120.2 (3) |
| C119—C118—H118 | 119.6 | C239—C230—P2 | 114.9 (3) |
| C110—C119—C118 | 121.2 (4) | C231—C230—P2 | 124.7 (3) |
| C110—C119—H119 | 119.4 | C232—C231—C230 | 124.7 (3) |
| C118—C119—H119 | 119.4 | C232—C231—C236 | 117.1 (3) |
| C129—C120—C121 | 119.1 (3) | C230—C231—C236 | 118.2 (3) |
| C129—C120—P1 | 115.4 (3) | C233—C232—C231 | 121.8 (4) |
| C121—C120—P1 | 125.5 (3) | C233—C232—H232 | 119.1 |
| C126—C121—C122 | 117.4 (3) | C231—C232—H232 | 119.1 |
| C126—C121—C120 | 118.2 (3) | C232—C233—C234 | 120.7 (4) |
| C122—C121—C120 | 124.4 (3) | C232—C233—H233 | 119.6 |
| C123—C122—C121 | 122.0 (4) | C234—C233—H233 | 119.6 |
| C123—C122—H122 | 119 | C235—C234—C233 | 119.7 (4) |
| C121—C122—H122 | 119 | C235—C234—H234 | 120.2 |
| C122—C123—C124 | 119.7 (4) | C233—C234—H234 | 120.2 |
| C122—C123—H123 | 120.1 | C234—C235—C236 | 121.5 (4) |
| C124—C123—H123 | 120.1 | C234—C235—H235 | 119.2 |
| C125—C124—C123 | 120.3 (4) | C236—C235—H235 | 119.2 |
| C125—C124—H124 | 119.8 | C235—C236—C237 | 122.1 (4) |
| C123—C124—H124 | 119.8 | C235—C236—C231 | 119.2 (4) |
| C124—C125—C126 | 120.7 (4) | C237—C236—C231 | 118.7 (4) |
| C124—C125—H125 | 119.6 | C238—C237—C236 | 121.4 (4) |
| C126—C125—H125 | 119.6 | C238—C237—H237 | 119.3 |

| | | | |
|---------------------|------------|---------------------|-------------|
| C121—C126—C125 | 119.8 (4) | C236—C237—H237 | 119.3 |
| C121—C126—C127 | 120.1 (4) | C237—C238—C239 | 120.0 (4) |
| C125—C126—C127 | 120.2 (4) | C237—C238—H238 | 120 |
| C128—C127—C126 | 120.6 (4) | C239—C238—H238 | 120 |
| C128—C127—H127 | 119.7 | C230—C239—C238 | 121.3 (4) |
| C126—C127—H127 | 119.7 | C230—C239—H239 | 119.3 |
| C127—C128—C129 | 120.1 (4) | C238—C239—H239 | 119.3 |
| C127—C128—H128 | 120 | C42—C43—H43A | 109.5 |
| C129—C128—H128 | 120 | C42—C43—H43B | 109.5 |
| C120—C129—C128 | 121.9 (4) | H43A—C43—H43B | 109.5 |
| C120—C129—H129 | 119 | C42—C43—H43C | 109.5 |
| C128—C129—H129 | 119 | H43A—C43—H43C | 109.5 |
| C139—C130—C131 | 119.2 (3) | H43B—C43—H43C | 109.5 |
| C139—C130—P1 | 119.8 (3) | C110—P1—C120 | 104.45 (17) |
| C131—C130—P1 | 120.4 (3) | C110—P1—C130 | 106.37 (17) |
| C132—C131—C130 | 123.9 (3) | C120—P1—C130 | 106.86 (17) |
| C132—C131—C136 | 117.1 (3) | C110—P1—Rh1 | 116.05 (12) |
| C130—C131—C136 | 118.9 (3) | C120—P1—Rh1 | 114.49 (12) |
| C133—C132—C131 | 121.4 (4) | C130—P1—Rh1 | 108.00 (12) |
| C133—C132—H132 | 119.3 | C210—P2—C220 | 107.01 (16) |
| C131—C132—H132 | 119.3 | C210—P2—C230 | 104.38 (17) |
| C132—C133—C134 | 120.8 (4) | C220—P2—C230 | 106.60 (17) |
| C132—C133—H133 | 119.6 | C210—P2—Rh1 | 117.67 (12) |
| C134—C133—H133 | 119.6 | C220—P2—Rh1 | 105.81 (12) |
| C135—C134—C133 | 119.9 (4) | C230—P2—Rh1 | 114.70 (12) |
| C135—C134—H134 | 120 | C1—Rh1—P2 | 93.94 (11) |
| C133—C134—H134 | 120 | C1—Rh1—P1 | 92.46 (11) |
| C134—C135—C136 | 120.9 (4) | P2—Rh1—P1 | 173.41 (4) |
| C134—C135—H135 | 119.5 | C1—Rh1—Cl1 | 176.51 (13) |
| C136—C135—H135 | 119.5 | P2—Rh1—Cl1 | 87.04 (3) |
| C137—C136—C135 | 121.0 (4) | P1—Rh1—Cl1 | 86.67 (3) |
| C119—C110—C111—C116 | -1.2 (5) | P2—C220—C221—C226 | 166.3 (3) |
| P1—C110—C111—C116 | 175.7 (3) | C226—C221—C222—C223 | -1.5 (5) |
| C119—C110—C111—C112 | 178.0 (3) | C220—C221—C222—C223 | 177.8 (4) |
| P1—C110—C111—C112 | -5.1 (5) | C221—C222—C223—C224 | -0.6 (6) |
| C116—C111—C112—C113 | -1.2 (5) | C222—C223—C224—C225 | 2.2 (6) |
| C110—C111—C112—C113 | 179.5 (3) | C223—C224—C225—C226 | -1.7 (6) |
| C111—C112—C113—C114 | -0.1 (6) | C224—C225—C226—C227 | -179.1 (4) |
| C112—C113—C114—C115 | 1.0 (6) | C224—C225—C226—C221 | -0.4 (6) |
| C113—C114—C115—C116 | -0.5 (6) | C222—C221—C226—C227 | -179.3 (3) |
| C112—C111—C116—C117 | -177.2 (3) | C220—C221—C226—C227 | 1.4 (5) |
| C110—C111—C116—C117 | 2.1 (5) | C222—C221—C226—C225 | 2.0 (5) |
| C112—C111—C116—C115 | 1.7 (5) | C220—C221—C226—C225 | -177.3 (3) |
| C110—C111—C116—C115 | -179.1 (3) | C225—C226—C227—C228 | 178.1 (4) |
| C114—C115—C116—C111 | -0.9 (6) | C221—C226—C227—C228 | -0.5 (5) |
| C114—C115—C116—C117 | 178.0 (4) | C226—C227—C228—C229 | -1.5 (6) |
| C111—C116—C117—C118 | -1.7 (6) | C221—C220—C229—C228 | -1.8 (5) |
| C115—C116—C117—C118 | 179.5 (4) | P2—C220—C229—C228 | -168.1 (3) |
| C116—C117—C118—C119 | 0.4 (6) | C227—C228—C229—C220 | 2.7 (6) |

supplementary materials

| | | | |
|---------------------|------------|---------------------|------------|
| C111—C110—C119—C118 | 0.0 (5) | C239—C230—C231—C232 | -177.9 (4) |
| P1—C110—C119—C118 | -176.9 (3) | P2—C230—C231—C232 | 7.2 (6) |
| C117—C118—C119—C110 | 0.5 (6) | C239—C230—C231—C236 | 1.8 (5) |
| C129—C120—C121—C126 | -0.8 (5) | P2—C230—C231—C236 | -173.0 (3) |
| P1—C120—C121—C126 | -179.3 (3) | C230—C231—C232—C233 | -178.6 (4) |
| C129—C120—C121—C122 | 180.0 (4) | C236—C231—C232—C233 | 1.6 (6) |
| P1—C120—C121—C122 | 1.5 (6) | C231—C232—C233—C234 | -0.9 (6) |
| C126—C121—C122—C123 | -0.9 (6) | C232—C233—C234—C235 | -0.6 (6) |
| C120—C121—C122—C123 | 178.4 (4) | C233—C234—C235—C236 | 1.4 (6) |
| C121—C122—C123—C124 | -0.5 (6) | C234—C235—C236—C237 | 177.8 (4) |
| C122—C123—C124—C125 | 2.2 (7) | C234—C235—C236—C231 | -0.7 (6) |
| C123—C124—C125—C126 | -2.4 (7) | C232—C231—C236—C235 | -0.8 (6) |
| C122—C121—C126—C125 | 0.7 (6) | C230—C231—C236—C235 | 179.4 (4) |
| C120—C121—C126—C125 | -178.6 (4) | C232—C231—C236—C237 | -179.3 (4) |
| C122—C121—C126—C127 | -179.4 (4) | C230—C231—C236—C237 | 0.9 (6) |
| C120—C121—C126—C127 | 1.3 (6) | C235—C236—C237—C238 | 178.5 (4) |
| C124—C125—C126—C121 | 1.0 (7) | C231—C236—C237—C238 | -2.9 (6) |
| C124—C125—C126—C127 | -179.0 (4) | C236—C237—C238—C239 | 2.3 (7) |
| C121—C126—C127—C128 | -0.4 (6) | C231—C230—C239—C238 | -2.6 (6) |
| C125—C126—C127—C128 | 179.6 (4) | P2—C230—C239—C238 | 172.7 (3) |
| C126—C127—C128—C129 | -1.1 (6) | C237—C238—C239—C230 | 0.5 (6) |
| C121—C120—C129—C128 | -0.7 (6) | C119—C110—P1—C120 | -120.0 (3) |
| P1—C120—C129—C128 | 178.0 (3) | C111—C110—P1—C120 | 63.2 (3) |
| C127—C128—C129—C120 | 1.7 (6) | C119—C110—P1—C130 | -7.1 (3) |
| C139—C130—C131—C132 | -178.4 (3) | C111—C110—P1—C130 | 176.0 (3) |
| P1—C130—C131—C132 | -7.7 (5) | C119—C110—P1—Rh1 | 113.0 (3) |
| C139—C130—C131—C136 | -1.3 (5) | C111—C110—P1—Rh1 | -63.9 (3) |
| P1—C130—C131—C136 | 169.4 (3) | C129—C120—P1—C110 | -132.0 (3) |
| C130—C131—C132—C133 | 176.5 (3) | C121—C120—P1—C110 | 46.5 (4) |
| C136—C131—C132—C133 | -0.6 (5) | C129—C120—P1—C130 | 115.6 (3) |
| C131—C132—C133—C134 | 0.6 (6) | C121—C120—P1—C130 | -65.9 (4) |
| C132—C133—C134—C135 | 0.3 (6) | C129—C120—P1—Rh1 | -4.0 (3) |
| C133—C134—C135—C136 | -1.1 (6) | C121—C120—P1—Rh1 | 174.6 (3) |
| C134—C135—C136—C137 | -178.5 (4) | C139—C130—P1—C110 | -110.0 (3) |
| C134—C135—C136—C131 | 1.0 (6) | C131—C130—P1—C110 | 79.4 (3) |
| C132—C131—C136—C137 | 179.4 (3) | C139—C130—P1—C120 | 1.1 (3) |
| C130—C131—C136—C137 | 2.1 (5) | C131—C130—P1—C120 | -169.5 (3) |
| C132—C131—C136—C135 | -0.1 (5) | C139—C130—P1—Rh1 | 124.8 (3) |
| C130—C131—C136—C135 | -177.4 (3) | C131—C130—P1—Rh1 | -45.8 (3) |
| C135—C136—C137—C138 | 178.4 (4) | C10—C210—P2—C220 | -7.8 (3) |
| C131—C136—C137—C138 | -1.1 (6) | C211—C210—P2—C220 | 174.4 (3) |
| C136—C137—C138—C139 | -0.7 (6) | C10—C210—P2—C230 | -120.5 (3) |
| C131—C130—C139—C138 | -0.5 (5) | C211—C210—P2—C230 | 61.7 (3) |
| P1—C130—C139—C138 | -171.2 (3) | C10—C210—P2—Rh1 | 111.0 (3) |
| C137—C138—C139—C130 | 1.5 (6) | C211—C210—P2—Rh1 | -66.7 (3) |
| C219—C10—C210—C211 | 1.8 (6) | C229—C220—P2—C210 | -116.3 (3) |
| C219—C10—C210—P2 | -176.0 (3) | C221—C220—P2—C210 | 77.5 (3) |
| C10—C210—C211—C217 | -3.9 (5) | C229—C220—P2—C230 | -5.0 (3) |
| P2—C210—C211—C217 | 173.8 (3) | C221—C220—P2—C230 | -171.3 (3) |

| | | | |
|---------------------|------------|-------------------|--------------|
| C10—C210—C211—C213 | 175.5 (3) | C229—C220—P2—Rh1 | 117.5 (3) |
| P2—C210—C211—C213 | -6.7 (5) | C221—C220—P2—Rh1 | -48.8 (3) |
| C217—C211—C213—C214 | 0.1 (5) | C239—C230—P2—C210 | -129.5 (3) |
| C210—C211—C213—C214 | -179.4 (4) | C231—C230—P2—C210 | 45.5 (4) |
| C211—C213—C214—C215 | -1.6 (6) | C239—C230—P2—C220 | 117.4 (3) |
| C213—C214—C215—C216 | 1.1 (6) | C231—C230—P2—C220 | -67.5 (4) |
| C214—C215—C216—C217 | 1.0 (6) | C239—C230—P2—Rh1 | 0.7 (3) |
| C215—C216—C217—C218 | 176.4 (4) | C231—C230—P2—Rh1 | 175.7 (3) |
| C215—C216—C217—C211 | -2.6 (5) | C210—P2—Rh1—C1 | 14.29 (18) |
| C210—C211—C217—C216 | -178.5 (3) | C220—P2—Rh1—C1 | 133.75 (17) |
| C213—C211—C217—C216 | 2.0 (5) | C230—P2—Rh1—C1 | -109.06 (18) |
| C210—C211—C217—C218 | 2.5 (5) | C210—P2—Rh1—Cl1 | -169.07 (14) |
| C213—C211—C217—C218 | -177.0 (3) | C220—P2—Rh1—Cl1 | -49.61 (13) |
| C216—C217—C218—C219 | -177.8 (4) | C230—P2—Rh1—Cl1 | 67.58 (14) |
| C211—C217—C218—C219 | 1.1 (5) | C110—P1—Rh1—C1 | 5.02 (18) |
| C217—C218—C219—C10 | -3.4 (6) | C120—P1—Rh1—C1 | -116.85 (18) |
| C210—C10—C219—C218 | 1.9 (6) | C130—P1—Rh1—C1 | 124.26 (18) |
| C229—C220—C221—C222 | -179.5 (3) | C110—P1—Rh1—Cl1 | -171.60 (13) |
| P2—C220—C221—C222 | -13.0 (5) | C120—P1—Rh1—Cl1 | 66.54 (13) |
| C229—C220—C221—C226 | -0.2 (5) | C130—P1—Rh1—Cl1 | -52.35 (13) |

Fig. 1

