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{Bis[2-(dicyclohexylphosphino)phenyl]-methylsilyl- $\kappa^3 P, Si, P'$]chloridoplatinum(II)}

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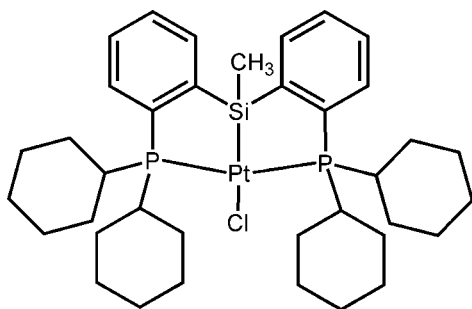
Received 26 August 2008; accepted 9 September 2008

Key indicators: single-crystal X-ray study; $T = 153$ K; mean $\sigma(C-C) = 0.004$ Å;
R factor = 0.020; wR factor = 0.048; data-to-parameter ratio = 22.0.

In the title compound, $[Pt(C_{37}H_{55}P_2Si)Cl]$, prepared from $MeSiH[(cy)_2PC_6H_4]_2$ and $[Pt(cod)Cl_2]$ (cy = cyclohexyl; cod = cycloocta-1,5-diene), the Pt^{II} atom is coordinated by two P atoms, one Si atom and one Cl atom in a distorted square-planar geometry. The two P atoms are in a *trans* arrangement and the four cyclohexane rings adopt a chair conformation.

Related literature

For related literature, see: van der Boom & Milstein (2003); Brost *et al.* (1997); Moulton & Shaw (1976).



Experimental

Crystal data

$[Pt(C_{37}H_{55}P_2Si)Cl]$
 $M_r = 820.38$
Monoclinic, $P2_1/c$
 $a = 13.104$ (3) Å

$b = 16.579$ (3) Å
 $c = 17.770$ (4) Å
 $\beta = 108.97$ (3)°
 $V = 3650.9$ (15) Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 4.06$ mm⁻¹

$T = 153$ (2) K
 $0.48 \times 0.40 \times 0.40$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{min} = 0.120$, $T_{max} = 0.200$

36373 measured reflections
8374 independent reflections
7059 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.035$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.020$
 $wR(F^2) = 0.047$
 $S = 0.97$
8374 reflections

380 parameters
H-atom parameters constrained
 $\Delta\rho_{max} = 1.00$ e Å⁻³
 $\Delta\rho_{min} = -0.55$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

| | | | |
|------------|------------|-------------|------------|
| Pt1—Si1 | 2.2790 (7) | Pt1—P2 | 2.2929 (7) |
| Pt1—P1 | 2.2925 (8) | Pt1—Cl1 | 2.4597 (7) |
| Si1—Pt1—P1 | 84.89 (3) | Si1—Pt1—Cl1 | 178.03 (2) |
| Si1—Pt1—P2 | 84.57 (3) | P1—Pt1—Cl1 | 93.68 (3) |
| P1—Pt1—P2 | 162.15 (2) | P2—Pt1—Cl1 | 97.15 (3) |

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINTE* (Bruker, 2007); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the Starter Fund of Southeast University for financial support to buy a CCD X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2153).

References

- Boom, M. E. van der & Milstein, D. (2003). *Chem. Rev.* **103**, 1759–1792.
Brost, R. D., Bruce, G. C., Joslin, F. L. & Stobart, S. R. (1997). *Organometallics*, **16**, 5669–5680.
Bruker (2007). *SMART* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
Moulton, C. J. & Shaw, B. L. (1976). *J. Chem. Soc. Dalton Trans.* pp. 1020–1024.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

supplementary materials

Acta Cryst. (2008). E64, m1272 [doi:10.1107/S1600536808028857]

{Bis[2-(dicyclohexylphosphino)phenyl]methylsilyl- κ^3P,Si,P' }chloridoplatinum(II)

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Comment

Pincers ligands incorporating two phosphine arms and a central donor site have attracted a substantial amount of interest since the initial investigations of "PCP" ligands by Moulton & Shaw (1976). Several variations of the central donor atom have been explored (Boom & Milstein, 2003). However, the "PSiP" pincers-like transition metal complexes have rarely been reported. We report here the synthesis and structure of a new Pt(η^3 -PSiP) complex. The molecular structure of the title compound is shown in Fig. 1.

The pincers-like title compound contains two stable five-membered cyclometalated rings with the P—Pt—Si angles of 84.89 (3) and 84.57 (3) ° (Table 1). The Pt atom is coordinated by two P atoms, one Si atom and one Cl atom in a distorted square-planar geometry. The bond distances of Pt—Si and Pt—Cl are 2.2790 (7) and 2.4597 (7) Å, respectively, which are similar to the other Pt analogue with pincers-like tridentate PSiP ligand, Pt[SiMe(CH₂CH₂CH₂PPh₂)₂]Cl (Brost *et al.*, 1997). The two P donor atoms are in a *trans* arrangement with a P—Pt—P angle of 162.15 (2)°. The four cyclohexane rings adopt the chair conformation.

Experimental

Dropwise addition of a solution of MeSiH[(cy)₂PC₆H₄]₂ (0.124 g, 0.21 mmol) (cy = cyclohexyl) in dry THF (5 ml) to a solution of [Pt(cod)Cl₂] (0.079 g, 0.21 mmol) (cod = cycloocta-1,5-diene) in a mixture of THF (7 ml) and NEt₃ (1 ml) resulted in rapid formation of a white precipitate. Removal of the volatiles left solid material, which gave the product after thorough washing (yield 78%, 0.134 g). Colorless crystals suitable for X-ray diffraction were obtained by slow evaporation of a benzene solution (5 ml) of the compound (0.028 g) after 2 d.

Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 (aromatic), 0.98 (CH), 0.97 (CH₂), 0.96 (CH₃) Å and $U_{\text{iso}}(\text{H}) = 1.2(\text{or } 1.5 \text{ for methyl})U_{\text{eq}}(\text{C})$.

Figures

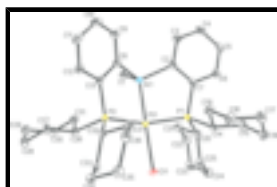


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

supplementary materials

{Bis[2-(dicyclohexylphosphino)phenyl]methylsilyl- $\kappa^3 P, Si, P'$]chloridoplatinum(II)}

Crystal data

| | |
|---|---|
| [Pt(C ₃₇ H ₅₅ P ₂ Si)Cl] | $F_{000} = 1664$ |
| $M_r = 820.38$ | $D_x = 1.493 \text{ Mg m}^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| Hall symbol: -P 2ybc | $\lambda = 0.71073 \text{ \AA}$ |
| $a = 13.104 (3) \text{ \AA}$ | Cell parameters from 8404 reflections |
| $b = 16.579 (3) \text{ \AA}$ | $\theta = 3.0\text{--}27.5^\circ$ |
| $c = 17.770 (4) \text{ \AA}$ | $\mu = 4.06 \text{ mm}^{-1}$ |
| $\beta = 108.97 (3)^\circ$ | $T = 153 (2) \text{ K}$ |
| $V = 3650.9 (15) \text{ \AA}^3$ | Block, colorless |
| $Z = 4$ | $0.48 \times 0.40 \times 0.40 \text{ mm}$ |

Data collection

| | |
|---|--|
| Bruker SMART APEX CCD area-detector diffractometer | 8374 independent reflections |
| Radiation source: fine-focus sealed tube | 7059 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{\text{int}} = 0.035$ |
| $T = 153(2) \text{ K}$ | $\theta_{\text{max}} = 27.5^\circ$ |
| φ and ω scans | $\theta_{\text{min}} = 1.6^\circ$ |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h = -16 \rightarrow 17$ |
| $T_{\text{min}} = 0.120$, $T_{\text{max}} = 0.200$ | $k = -21 \rightarrow 21$ |
| 36373 measured reflections | $l = -23 \rightarrow 23$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.020$ | H-atom parameters constrained |
| $wR(F^2) = 0.047$ | $w = 1/[\sigma^2(F_o^2) + (0.0241P)^2]$ |
| $S = 0.97$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 8374 reflections | $(\Delta/\sigma)_{\text{max}} = 0.003$ |
| 380 parameters | $\Delta\rho_{\text{max}} = 1.00 \text{ e \AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\text{min}} = -0.55 \text{ e \AA}^{-3}$ |
| | Extinction correction: none |

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

| | | | |
|-----|-----|-----|----------------------------------|
| x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-----|-----|----------------------------------|

| | | | | |
|-----|--------------|--------------|--------------|--------------|
| Si1 | 0.79709 (6) | 0.29114 (4) | 0.75245 (4) | 0.02238 (15) |
| C1 | 0.8794 (2) | 0.38510 (15) | 0.79101 (16) | 0.0312 (6) |
| H9 | 0.9530 | 0.3703 | 0.8182 | 0.047* |
| H10 | 0.8507 | 0.4127 | 0.8272 | 0.047* |
| H11 | 0.8762 | 0.4200 | 0.7472 | 0.047* |
| C2 | 0.6609 (2) | 0.33576 (15) | 0.69588 (15) | 0.0258 (6) |
| C3 | 0.6388 (2) | 0.38438 (17) | 0.62824 (16) | 0.0383 (7) |
| H1 | 0.6903 | 0.3894 | 0.6028 | 0.046* |
| C4 | 0.5422 (3) | 0.42510 (19) | 0.59835 (18) | 0.0459 (8) |
| H2 | 0.5281 | 0.4550 | 0.5518 | 0.055* |
| C5 | 0.4668 (2) | 0.42180 (17) | 0.63697 (16) | 0.0371 (7) |
| H3 | 0.4031 | 0.4511 | 0.6178 | 0.045* |
| C6 | 0.4859 (2) | 0.37465 (15) | 0.70450 (15) | 0.0291 (6) |
| H4 | 0.4351 | 0.3724 | 0.7307 | 0.035* |
| C7 | 0.5818 (2) | 0.33037 (15) | 0.73334 (14) | 0.0236 (5) |
| C8 | 0.8674 (2) | 0.23542 (15) | 0.69018 (14) | 0.0242 (5) |
| C9 | 0.8662 (2) | 0.25752 (16) | 0.61413 (15) | 0.0284 (6) |
| H5 | 0.8272 | 0.3027 | 0.5900 | 0.034* |
| C10 | 0.9217 (2) | 0.21384 (17) | 0.57387 (16) | 0.0341 (7) |
| H6 | 0.9181 | 0.2288 | 0.5226 | 0.041* |
| C11 | 0.9826 (2) | 0.14780 (19) | 0.60967 (16) | 0.0367 (7) |
| H7 | 1.0214 | 0.1190 | 0.5831 | 0.044* |
| C12 | 0.9855 (2) | 0.12458 (17) | 0.68555 (16) | 0.0313 (6) |
| H8 | 1.0269 | 0.0804 | 0.7098 | 0.038* |
| C13 | 0.92692 (19) | 0.16711 (16) | 0.72559 (14) | 0.0236 (5) |
| P1 | 0.61006 (5) | 0.26215 (4) | 0.81899 (4) | 0.01969 (13) |
| P2 | 0.91721 (5) | 0.13477 (4) | 0.82203 (4) | 0.02147 (14) |
| Pt1 | 0.773705 (7) | 0.200163 (5) | 0.841596 (5) | 0.01795 (3) |
| Cl1 | 0.74599 (5) | 0.10572 (4) | 0.93994 (3) | 0.02439 (13) |
| C14 | 0.50326 (19) | 0.18463 (14) | 0.78938 (14) | 0.0217 (5) |
| H52 | 0.5189 | 0.1456 | 0.8331 | 0.026* |
| C15 | 0.3878 (2) | 0.21183 (16) | 0.77279 (18) | 0.0338 (6) |
| H12 | 0.3691 | 0.2507 | 0.7297 | 0.041* |
| H13 | 0.3810 | 0.2382 | 0.8197 | 0.041* |
| C16 | 0.3096 (2) | 0.14051 (18) | 0.75032 (18) | 0.0387 (7) |
| H14 | 0.3256 | 0.1030 | 0.7945 | 0.046* |
| H15 | 0.2363 | 0.1597 | 0.7395 | 0.046* |
| C17 | 0.3191 (2) | 0.09773 (18) | 0.67749 (17) | 0.0400 (7) |
| H16 | 0.2704 | 0.0519 | 0.6648 | 0.048* |
| H17 | 0.2984 | 0.1343 | 0.6324 | 0.048* |
| C18 | 0.4322 (2) | 0.06942 (18) | 0.69221 (19) | 0.0434 (8) |
| H18 | 0.4378 | 0.0447 | 0.6442 | 0.052* |
| H19 | 0.4502 | 0.0290 | 0.7339 | 0.052* |
| C19 | 0.5119 (2) | 0.13911 (17) | 0.71671 (16) | 0.0317 (6) |
| H20 | 0.4987 | 0.1764 | 0.6725 | 0.038* |
| H21 | 0.5846 | 0.1183 | 0.7287 | 0.038* |
| C20 | 0.5814 (2) | 0.32223 (15) | 0.89640 (15) | 0.0262 (6) |
| H53 | 0.5119 | 0.3491 | 0.8720 | 0.031* |
| C21 | 0.6675 (2) | 0.38825 (16) | 0.92785 (16) | 0.0315 (6) |

supplementary materials

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|-----|--------------|---------------|--------------|------------|
| H22 | 0.6709 | 0.4219 | 0.8841 | 0.038* |
| H23 | 0.7376 | 0.3635 | 0.9519 | 0.038* |
| C22 | 0.6391 (3) | 0.44040 (17) | 0.99003 (17) | 0.0410 (7) |
| H24 | 0.6953 | 0.4803 | 1.0112 | 0.049* |
| H25 | 0.5720 | 0.4688 | 0.9645 | 0.049* |
| C23 | 0.6275 (2) | 0.39036 (18) | 1.05693 (16) | 0.0388 (7) |
| H26 | 0.6051 | 0.4245 | 1.0930 | 0.047* |
| H27 | 0.6969 | 0.3670 | 1.0864 | 0.047* |
| C24 | 0.5450 (3) | 0.32308 (18) | 1.02620 (17) | 0.0395 (7) |
| H28 | 0.4740 | 0.3466 | 1.0025 | 0.047* |
| H29 | 0.5431 | 0.2897 | 1.0705 | 0.047* |
| C25 | 0.5719 (2) | 0.27061 (17) | 0.96458 (16) | 0.0335 (6) |
| H30 | 0.6394 | 0.2425 | 0.9895 | 0.040* |
| H31 | 0.5157 | 0.2306 | 0.9441 | 0.040* |
| C26 | 1.0505 (2) | 0.14993 (17) | 0.89855 (15) | 0.0288 (6) |
| H54 | 1.0436 | 0.1302 | 0.9486 | 0.035* |
| C27 | 1.1442 (2) | 0.1034 (2) | 0.88627 (16) | 0.0391 (7) |
| H32 | 1.1545 | 0.1208 | 0.8371 | 0.047* |
| H33 | 1.1272 | 0.0463 | 0.8817 | 0.047* |
| C28 | 1.2483 (2) | 0.1173 (2) | 0.95581 (19) | 0.0495 (9) |
| H34 | 1.2405 | 0.0942 | 1.0038 | 0.059* |
| H35 | 1.3074 | 0.0897 | 0.9450 | 0.059* |
| C29 | 1.2751 (2) | 0.2056 (2) | 0.96936 (19) | 0.0505 (9) |
| H36 | 1.2933 | 0.2268 | 0.9245 | 0.061* |
| H37 | 1.3378 | 0.2118 | 1.0166 | 0.061* |
| C30 | 1.1819 (2) | 0.2537 (2) | 0.97950 (17) | 0.0452 (8) |
| H38 | 1.1999 | 0.3106 | 0.9826 | 0.054* |
| H39 | 1.1713 | 0.2383 | 1.0291 | 0.054* |
| C31 | 1.0772 (2) | 0.24003 (18) | 0.91103 (15) | 0.0327 (6) |
| H40 | 1.0840 | 0.2627 | 0.8626 | 0.039* |
| H41 | 1.0186 | 0.2677 | 0.9224 | 0.039* |
| C32 | 0.90420 (19) | 0.02456 (15) | 0.80991 (14) | 0.0239 (5) |
| H55 | 0.9576 | 0.0076 | 0.7852 | 0.029* |
| C33 | 0.9287 (2) | -0.02323 (15) | 0.88762 (15) | 0.0285 (6) |
| H42 | 0.9990 | -0.0082 | 0.9239 | 0.034* |
| H43 | 0.8750 | -0.0113 | 0.9129 | 0.034* |
| C34 | 0.9270 (2) | -0.11266 (17) | 0.86878 (17) | 0.0351 (7) |
| H44 | 0.9416 | -0.1433 | 0.9177 | 0.042* |
| H45 | 0.9835 | -0.1245 | 0.8463 | 0.042* |
| C35 | 0.8189 (2) | -0.13878 (17) | 0.81058 (18) | 0.0391 (7) |
| H46 | 0.7635 | -0.1328 | 0.8354 | 0.047* |
| H47 | 0.8225 | -0.1953 | 0.7976 | 0.047* |
| C36 | 0.7884 (2) | -0.08889 (16) | 0.73421 (17) | 0.0365 (7) |
| H48 | 0.8372 | -0.1015 | 0.7050 | 0.044* |
| H49 | 0.7159 | -0.1031 | 0.7010 | 0.044* |
| C37 | 0.7934 (2) | 0.00123 (15) | 0.75192 (15) | 0.0275 (6) |
| H50 | 0.7379 | 0.0153 | 0.7748 | 0.033* |
| H51 | 0.7797 | 0.0312 | 0.7028 | 0.033* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| Si1 | 0.0229 (4) | 0.0234 (4) | 0.0197 (3) | -0.0075 (3) | 0.0055 (3) | 0.0016 (3) |
| C1 | 0.0347 (16) | 0.0268 (14) | 0.0318 (14) | -0.0124 (12) | 0.0105 (12) | -0.0021 (12) |
| C2 | 0.0263 (14) | 0.0236 (13) | 0.0234 (13) | -0.0072 (11) | 0.0025 (11) | 0.0038 (11) |
| C3 | 0.0382 (17) | 0.0409 (17) | 0.0336 (15) | -0.0076 (14) | 0.0087 (13) | 0.0117 (13) |
| C4 | 0.0450 (19) | 0.0461 (19) | 0.0362 (17) | -0.0073 (15) | -0.0012 (15) | 0.0230 (14) |
| C5 | 0.0279 (16) | 0.0321 (16) | 0.0380 (16) | -0.0043 (12) | -0.0076 (13) | 0.0108 (13) |
| C6 | 0.0250 (14) | 0.0227 (14) | 0.0325 (14) | -0.0067 (11) | -0.0005 (12) | 0.0021 (11) |
| C7 | 0.0269 (14) | 0.0192 (12) | 0.0198 (12) | -0.0066 (11) | 0.0008 (11) | 0.0014 (10) |
| C8 | 0.0218 (13) | 0.0264 (13) | 0.0233 (13) | -0.0145 (11) | 0.0057 (11) | -0.0043 (11) |
| C9 | 0.0298 (15) | 0.0296 (15) | 0.0245 (13) | -0.0153 (12) | 0.0068 (12) | -0.0017 (11) |
| C10 | 0.0440 (18) | 0.0397 (17) | 0.0207 (13) | -0.0213 (14) | 0.0135 (13) | -0.0062 (12) |
| C11 | 0.0377 (17) | 0.0468 (18) | 0.0320 (15) | -0.0157 (14) | 0.0200 (14) | -0.0129 (14) |
| C12 | 0.0265 (15) | 0.0388 (16) | 0.0294 (14) | -0.0083 (12) | 0.0101 (12) | -0.0049 (12) |
| C13 | 0.0180 (13) | 0.0298 (14) | 0.0222 (12) | -0.0105 (11) | 0.0054 (10) | -0.0036 (11) |
| P1 | 0.0205 (3) | 0.0193 (3) | 0.0179 (3) | -0.0017 (3) | 0.0045 (3) | 0.0005 (2) |
| P2 | 0.0151 (3) | 0.0279 (3) | 0.0203 (3) | -0.0040 (3) | 0.0043 (3) | 0.0009 (3) |
| Pt1 | 0.01686 (5) | 0.02063 (5) | 0.01516 (5) | -0.00361 (4) | 0.00354 (3) | 0.00086 (4) |
| Cl1 | 0.0328 (3) | 0.0227 (3) | 0.0213 (3) | 0.0015 (3) | 0.0137 (3) | 0.0035 (2) |
| C14 | 0.0198 (13) | 0.0233 (13) | 0.0198 (12) | -0.0034 (10) | 0.0033 (10) | 0.0037 (10) |
| C15 | 0.0257 (15) | 0.0345 (16) | 0.0399 (16) | -0.0010 (12) | 0.0086 (13) | -0.0012 (13) |
| C16 | 0.0266 (15) | 0.0383 (17) | 0.0513 (18) | -0.0048 (13) | 0.0128 (14) | 0.0040 (14) |
| C17 | 0.0362 (17) | 0.0354 (16) | 0.0436 (17) | -0.0076 (14) | 0.0063 (14) | -0.0053 (14) |
| C18 | 0.0410 (19) | 0.0401 (18) | 0.0491 (19) | -0.0130 (14) | 0.0148 (15) | -0.0134 (15) |
| C19 | 0.0322 (16) | 0.0340 (15) | 0.0297 (14) | -0.0127 (12) | 0.0113 (12) | -0.0088 (12) |
| C20 | 0.0276 (14) | 0.0246 (13) | 0.0255 (13) | 0.0013 (11) | 0.0077 (11) | -0.0014 (11) |
| C21 | 0.0408 (17) | 0.0240 (14) | 0.0288 (14) | -0.0044 (12) | 0.0100 (13) | -0.0043 (11) |
| C22 | 0.048 (2) | 0.0273 (15) | 0.0414 (17) | -0.0023 (14) | 0.0053 (15) | -0.0083 (13) |
| C23 | 0.0417 (18) | 0.0408 (17) | 0.0291 (15) | 0.0085 (14) | 0.0050 (13) | -0.0085 (13) |
| C24 | 0.0437 (19) | 0.0451 (18) | 0.0312 (15) | 0.0015 (14) | 0.0141 (14) | -0.0079 (13) |
| C25 | 0.0352 (16) | 0.0336 (15) | 0.0303 (14) | -0.0012 (13) | 0.0089 (13) | -0.0041 (12) |
| C26 | 0.0182 (13) | 0.0439 (17) | 0.0217 (13) | -0.0082 (12) | 0.0031 (11) | 0.0022 (12) |
| C27 | 0.0186 (14) | 0.061 (2) | 0.0355 (16) | -0.0029 (14) | 0.0061 (12) | 0.0026 (15) |
| C28 | 0.0167 (14) | 0.078 (3) | 0.0464 (19) | -0.0048 (16) | 0.0004 (14) | 0.0082 (17) |
| C29 | 0.0211 (15) | 0.084 (3) | 0.0388 (17) | -0.0208 (16) | -0.0005 (13) | 0.0099 (17) |
| C30 | 0.0386 (18) | 0.059 (2) | 0.0303 (15) | -0.0290 (16) | 0.0009 (14) | 0.0019 (15) |
| C31 | 0.0265 (15) | 0.0449 (17) | 0.0237 (13) | -0.0166 (13) | 0.0043 (12) | 0.0004 (12) |
| C32 | 0.0157 (12) | 0.0263 (13) | 0.0288 (13) | 0.0015 (10) | 0.0059 (11) | 0.0013 (11) |
| C33 | 0.0208 (14) | 0.0318 (15) | 0.0330 (14) | 0.0051 (11) | 0.0087 (12) | 0.0073 (12) |
| C34 | 0.0310 (16) | 0.0359 (16) | 0.0424 (16) | 0.0111 (13) | 0.0174 (13) | 0.0140 (13) |
| C35 | 0.0387 (18) | 0.0237 (15) | 0.058 (2) | 0.0011 (13) | 0.0205 (16) | 0.0021 (14) |
| C36 | 0.0301 (16) | 0.0315 (16) | 0.0474 (18) | -0.0021 (13) | 0.0118 (14) | -0.0067 (13) |
| C37 | 0.0195 (13) | 0.0262 (14) | 0.0327 (14) | -0.0001 (11) | 0.0030 (11) | 0.0009 (12) |

supplementary materials

Geometric parameters (Å, °)

| | | | |
|---------|------------|---------|-----------|
| Si1—C2 | 1.891 (3) | C19—H21 | 0.9700 |
| Si1—C1 | 1.892 (3) | C20—C25 | 1.521 (4) |
| Si1—C8 | 1.894 (3) | C20—C21 | 1.540 (4) |
| Pt1—Si1 | 2.2790 (7) | C20—H53 | 0.9800 |
| C1—H9 | 0.9600 | C21—C22 | 1.541 (4) |
| C1—H10 | 0.9600 | C21—H22 | 0.9700 |
| C1—H11 | 0.9600 | C21—H23 | 0.9700 |
| C2—C3 | 1.397 (4) | C22—C23 | 1.497 (4) |
| C2—C7 | 1.405 (4) | C22—H24 | 0.9700 |
| C3—C4 | 1.379 (4) | C22—H25 | 0.9700 |
| C3—H1 | 0.9300 | C23—C24 | 1.526 (4) |
| C4—C5 | 1.376 (4) | C23—H26 | 0.9700 |
| C4—H2 | 0.9300 | C23—H27 | 0.9700 |
| C5—C6 | 1.385 (4) | C24—C25 | 1.527 (4) |
| C5—H3 | 0.9300 | C24—H28 | 0.9700 |
| C6—C7 | 1.401 (4) | C24—H29 | 0.9700 |
| C6—H4 | 0.9300 | C25—H30 | 0.9700 |
| C7—P1 | 1.835 (2) | C25—H31 | 0.9700 |
| C8—C9 | 1.396 (3) | C26—C27 | 1.524 (4) |
| C8—C13 | 1.403 (4) | C26—C31 | 1.534 (4) |
| C9—C10 | 1.379 (4) | C26—H54 | 0.9800 |
| C9—H5 | 0.9300 | C27—C28 | 1.532 (4) |
| C10—C11 | 1.382 (4) | C27—H32 | 0.9700 |
| C10—H6 | 0.9300 | C27—H33 | 0.9700 |
| C11—C12 | 1.391 (4) | C28—C29 | 1.507 (4) |
| C11—H7 | 0.9300 | C28—H34 | 0.9700 |
| C12—C13 | 1.396 (4) | C28—H35 | 0.9700 |
| C12—H8 | 0.9300 | C29—C30 | 1.518 (5) |
| C13—P2 | 1.839 (2) | C29—H36 | 0.9700 |
| P1—C20 | 1.833 (3) | C29—H37 | 0.9700 |
| P1—C14 | 1.846 (2) | C30—C31 | 1.526 (4) |
| Pt1—P1 | 2.2925 (8) | C30—H38 | 0.9700 |
| P2—C32 | 1.841 (3) | C30—H39 | 0.9700 |
| P2—C26 | 1.849 (3) | C31—H40 | 0.9700 |
| Pt1—P2 | 2.2929 (7) | C31—H41 | 0.9700 |
| Pt1—C11 | 2.4597 (7) | C32—C37 | 1.532 (3) |
| C14—C15 | 1.513 (4) | C32—C33 | 1.533 (3) |
| C14—C19 | 1.531 (3) | C32—H55 | 0.9800 |
| C14—H52 | 0.9800 | C33—C34 | 1.519 (4) |
| C15—C16 | 1.530 (4) | C33—H42 | 0.9700 |
| C15—H12 | 0.9700 | C33—H43 | 0.9700 |
| C15—H13 | 0.9700 | C34—C35 | 1.520 (4) |
| C16—C17 | 1.516 (4) | C34—H44 | 0.9700 |
| C16—H14 | 0.9700 | C34—H45 | 0.9700 |
| C16—H15 | 0.9700 | C35—C36 | 1.527 (4) |
| C17—C18 | 1.495 (4) | C35—H46 | 0.9700 |

| | | | |
|-------------|-------------|-------------|-------------|
| C17—H16 | 0.9700 | C35—H47 | 0.9700 |
| C17—H17 | 0.9700 | C36—C37 | 1.524 (4) |
| C18—C19 | 1.523 (4) | C36—H48 | 0.9700 |
| C18—H18 | 0.9700 | C36—H49 | 0.9700 |
| C18—H19 | 0.9700 | C37—H50 | 0.9700 |
| C19—H20 | 0.9700 | C37—H51 | 0.9700 |
| C2—Si1—C1 | 101.47 (12) | C25—C20—H53 | 107.6 |
| C2—Si1—C8 | 115.74 (12) | C21—C20—H53 | 107.6 |
| C1—Si1—C8 | 106.56 (12) | P1—C20—H53 | 107.6 |
| C2—Si1—Pt1 | 108.15 (8) | C20—C21—C22 | 109.9 (2) |
| C1—Si1—Pt1 | 118.87 (9) | C20—C21—H22 | 109.7 |
| C8—Si1—Pt1 | 106.50 (8) | C22—C21—H22 | 109.7 |
| Si1—C1—H9 | 109.5 | C20—C21—H23 | 109.7 |
| Si1—C1—H10 | 109.5 | C22—C21—H23 | 109.7 |
| H9—C1—H10 | 109.5 | H22—C21—H23 | 108.2 |
| Si1—C1—H11 | 109.5 | C23—C22—C21 | 111.6 (2) |
| H9—C1—H11 | 109.5 | C23—C22—H24 | 109.3 |
| H10—C1—H11 | 109.5 | C21—C22—H24 | 109.3 |
| C3—C2—C7 | 117.8 (3) | C23—C22—H25 | 109.3 |
| C3—C2—Si1 | 125.4 (2) | C21—C22—H25 | 109.3 |
| C7—C2—Si1 | 115.93 (18) | H24—C22—H25 | 108.0 |
| C4—C3—C2 | 121.4 (3) | C22—C23—C24 | 111.3 (2) |
| C4—C3—H1 | 119.3 | C22—C23—H26 | 109.4 |
| C2—C3—H1 | 119.3 | C24—C23—H26 | 109.4 |
| C5—C4—C3 | 120.4 (3) | C22—C23—H27 | 109.4 |
| C5—C4—H2 | 119.8 | C24—C23—H27 | 109.4 |
| C3—C4—H2 | 119.8 | H26—C23—H27 | 108.0 |
| C4—C5—C6 | 119.8 (3) | C23—C24—C25 | 111.8 (3) |
| C4—C5—H3 | 120.1 | C23—C24—H28 | 109.3 |
| C6—C5—H3 | 120.1 | C25—C24—H28 | 109.3 |
| C5—C6—C7 | 120.1 (3) | C23—C24—H29 | 109.3 |
| C5—C6—H4 | 120.0 | C25—C24—H29 | 109.3 |
| C7—C6—H4 | 120.0 | H28—C24—H29 | 107.9 |
| C6—C7—C2 | 120.4 (2) | C20—C25—C24 | 110.4 (2) |
| C6—C7—P1 | 122.8 (2) | C20—C25—H30 | 109.6 |
| C2—C7—P1 | 116.83 (19) | C24—C25—H30 | 109.6 |
| C9—C8—C13 | 118.4 (2) | C20—C25—H31 | 109.6 |
| C9—C8—Si1 | 125.7 (2) | C24—C25—H31 | 109.6 |
| C13—C8—Si1 | 115.90 (18) | H30—C25—H31 | 108.1 |
| C10—C9—C8 | 121.5 (3) | C27—C26—C31 | 110.9 (2) |
| C10—C9—H5 | 119.2 | C27—C26—P2 | 115.99 (19) |
| C8—C9—H5 | 119.2 | C31—C26—P2 | 110.80 (18) |
| C9—C10—C11 | 120.0 (2) | C27—C26—H54 | 106.1 |
| C9—C10—H6 | 120.0 | C31—C26—H54 | 106.1 |
| C11—C10—H6 | 120.0 | P2—C26—H54 | 106.1 |
| C10—C11—C12 | 119.7 (3) | C26—C27—C28 | 110.9 (2) |
| C10—C11—H7 | 120.2 | C26—C27—H32 | 109.5 |
| C12—C11—H7 | 120.2 | C28—C27—H32 | 109.5 |
| C11—C12—C13 | 120.5 (3) | C26—C27—H33 | 109.5 |

supplementary materials

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|-------------|-------------|-------------|-------------|
| C11—C12—H8 | 119.7 | C28—C27—H33 | 109.5 |
| C13—C12—H8 | 119.7 | H32—C27—H33 | 108.0 |
| C12—C13—C8 | 119.8 (2) | C29—C28—C27 | 112.0 (3) |
| C12—C13—P2 | 122.9 (2) | C29—C28—H34 | 109.2 |
| C8—C13—P2 | 117.15 (19) | C27—C28—H34 | 109.2 |
| C20—P1—C7 | 104.61 (12) | C29—C28—H35 | 109.2 |
| C20—P1—C14 | 105.71 (12) | C27—C28—H35 | 109.2 |
| C7—P1—C14 | 105.24 (11) | H34—C28—H35 | 107.9 |
| C20—P1—Pt1 | 121.34 (9) | C28—C29—C30 | 112.0 (2) |
| C7—P1—Pt1 | 110.28 (9) | C28—C29—H36 | 109.2 |
| C14—P1—Pt1 | 108.49 (8) | C30—C29—H36 | 109.2 |
| C13—P2—C32 | 102.25 (12) | C28—C29—H37 | 109.2 |
| C13—P2—C26 | 108.10 (11) | C30—C29—H37 | 109.2 |
| C32—P2—C26 | 104.49 (12) | H36—C29—H37 | 107.9 |
| C13—P2—Pt1 | 108.18 (9) | C29—C30—C31 | 112.2 (3) |
| C32—P2—Pt1 | 115.95 (8) | C29—C30—H38 | 109.2 |
| C26—P2—Pt1 | 116.71 (9) | C31—C30—H38 | 109.2 |
| Si1—Pt1—P1 | 84.89 (3) | C29—C30—H39 | 109.2 |
| Si1—Pt1—P2 | 84.57 (3) | C31—C30—H39 | 109.2 |
| P1—Pt1—P2 | 162.15 (2) | H38—C30—H39 | 107.9 |
| Si1—Pt1—Cl1 | 178.03 (2) | C30—C31—C26 | 111.3 (2) |
| P1—Pt1—Cl1 | 93.68 (3) | C30—C31—H40 | 109.4 |
| P2—Pt1—Cl1 | 97.15 (3) | C26—C31—H40 | 109.4 |
| C15—C14—C19 | 109.0 (2) | C30—C31—H41 | 109.4 |
| C15—C14—P1 | 117.74 (18) | C26—C31—H41 | 109.4 |
| C19—C14—P1 | 109.06 (17) | H40—C31—H41 | 108.0 |
| C15—C14—H52 | 106.8 | C37—C32—C33 | 110.5 (2) |
| C19—C14—H52 | 106.8 | C37—C32—P2 | 111.14 (17) |
| P1—C14—H52 | 106.8 | C33—C32—P2 | 115.04 (17) |
| C14—C15—C16 | 111.3 (2) | C37—C32—H55 | 106.5 |
| C14—C15—H12 | 109.4 | C33—C32—H55 | 106.5 |
| C16—C15—H12 | 109.4 | P2—C32—H55 | 106.5 |
| C14—C15—H13 | 109.4 | C34—C33—C32 | 108.8 (2) |
| C16—C15—H13 | 109.4 | C34—C33—H42 | 109.9 |
| H12—C15—H13 | 108.0 | C32—C33—H42 | 109.9 |
| C17—C16—C15 | 110.5 (2) | C34—C33—H43 | 109.9 |
| C17—C16—H14 | 109.5 | C32—C33—H43 | 109.9 |
| C15—C16—H14 | 109.5 | H42—C33—H43 | 108.3 |
| C17—C16—H15 | 109.5 | C33—C34—C35 | 111.8 (2) |
| C15—C16—H15 | 109.5 | C33—C34—H44 | 109.2 |
| H14—C16—H15 | 108.1 | C35—C34—H44 | 109.2 |
| C18—C17—C16 | 110.5 (2) | C33—C34—H45 | 109.2 |
| C18—C17—H16 | 109.6 | C35—C34—H45 | 109.2 |
| C16—C17—H16 | 109.6 | H44—C34—H45 | 107.9 |
| C18—C17—H17 | 109.6 | C34—C35—C36 | 111.6 (2) |
| C16—C17—H17 | 109.6 | C34—C35—H46 | 109.3 |
| H16—C17—H17 | 108.1 | C36—C35—H46 | 109.3 |
| C17—C18—C19 | 111.1 (3) | C34—C35—H47 | 109.3 |
| C17—C18—H18 | 109.4 | C36—C35—H47 | 109.3 |

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|-----------------|--------------|-----------------|--------------|
| C19—C18—H18 | 109.4 | H46—C35—H47 | 108.0 |
| C17—C18—H19 | 109.4 | C37—C36—C35 | 111.5 (2) |
| C19—C18—H19 | 109.4 | C37—C36—H48 | 109.3 |
| H18—C18—H19 | 108.0 | C35—C36—H48 | 109.3 |
| C18—C19—C14 | 112.5 (2) | C37—C36—H49 | 109.3 |
| C18—C19—H20 | 109.1 | C35—C36—H49 | 109.3 |
| C14—C19—H20 | 109.1 | H48—C36—H49 | 108.0 |
| C18—C19—H21 | 109.1 | C36—C37—C32 | 110.7 (2) |
| C14—C19—H21 | 109.1 | C36—C37—H50 | 109.5 |
| H20—C19—H21 | 107.8 | C32—C37—H50 | 109.5 |
| C25—C20—C21 | 110.5 (2) | C36—C37—H51 | 109.5 |
| C25—C20—P1 | 112.44 (18) | C32—C37—H51 | 109.5 |
| C21—C20—P1 | 110.72 (18) | H50—C37—H51 | 108.1 |
| C1—Si1—C2—C3 | 64.5 (3) | C26—P2—Pt1—Si1 | 100.07 (10) |
| C8—Si1—C2—C3 | -50.4 (3) | C13—P2—Pt1—P1 | 32.02 (12) |
| Pt1—Si1—C2—C3 | -169.7 (2) | C32—P2—Pt1—P1 | -82.07 (12) |
| C1—Si1—C2—C7 | -104.1 (2) | C26—P2—Pt1—P1 | 154.11 (11) |
| C8—Si1—C2—C7 | 140.99 (19) | C13—P2—Pt1—C11 | 158.94 (8) |
| Pt1—Si1—C2—C7 | 21.7 (2) | C32—P2—Pt1—C11 | 44.85 (9) |
| C7—C2—C3—C4 | -0.8 (4) | C26—P2—Pt1—C11 | -78.97 (10) |
| Si1—C2—C3—C4 | -169.2 (2) | C20—P1—C14—C15 | 47.3 (2) |
| C2—C3—C4—C5 | 3.1 (5) | C7—P1—C14—C15 | -63.1 (2) |
| C3—C4—C5—C6 | -2.6 (5) | Pt1—P1—C14—C15 | 178.91 (17) |
| C4—C5—C6—C7 | -0.1 (4) | C20—P1—C14—C19 | 172.15 (18) |
| C5—C6—C7—C2 | 2.4 (4) | C7—P1—C14—C19 | 61.8 (2) |
| C5—C6—C7—P1 | -176.5 (2) | Pt1—P1—C14—C19 | -56.25 (18) |
| C3—C2—C7—C6 | -2.0 (4) | C19—C14—C15—C16 | 56.0 (3) |
| Si1—C2—C7—C6 | 167.58 (19) | P1—C14—C15—C16 | -179.13 (19) |
| C3—C2—C7—P1 | 177.00 (19) | C14—C15—C16—C17 | -58.6 (3) |
| Si1—C2—C7—P1 | -13.5 (3) | C15—C16—C17—C18 | 57.8 (3) |
| C2—Si1—C8—C9 | 37.3 (2) | C16—C17—C18—C19 | -56.2 (3) |
| C1—Si1—C8—C9 | -74.6 (2) | C17—C18—C19—C14 | 55.6 (3) |
| Pt1—Si1—C8—C9 | 157.52 (19) | C15—C14—C19—C18 | -54.8 (3) |
| C2—Si1—C8—C13 | -144.02 (18) | P1—C14—C19—C18 | 175.4 (2) |
| C1—Si1—C8—C13 | 104.1 (2) | C7—P1—C20—C25 | 165.15 (19) |
| Pt1—Si1—C8—C13 | -23.8 (2) | C14—P1—C20—C25 | 54.3 (2) |
| C13—C8—C9—C10 | 0.1 (4) | Pt1—P1—C20—C25 | -69.5 (2) |
| Si1—C8—C9—C10 | 178.77 (19) | C7—P1—C20—C21 | -70.7 (2) |
| C8—C9—C10—C11 | -1.8 (4) | C14—P1—C20—C21 | 178.52 (17) |
| C9—C10—C11—C12 | 1.5 (4) | Pt1—P1—C20—C21 | 54.7 (2) |
| C10—C11—C12—C13 | 0.4 (4) | C25—C20—C21—C22 | -57.3 (3) |
| C11—C12—C13—C8 | -2.1 (4) | P1—C20—C21—C22 | 177.45 (18) |
| C11—C12—C13—P2 | 174.4 (2) | C20—C21—C22—C23 | 56.5 (3) |
| C9—C8—C13—C12 | 1.8 (4) | C21—C22—C23—C24 | -55.3 (3) |
| Si1—C8—C13—C12 | -176.97 (19) | C22—C23—C24—C25 | 55.1 (3) |
| C9—C8—C13—P2 | -174.89 (18) | C21—C20—C25—C24 | 57.2 (3) |
| Si1—C8—C13—P2 | 6.3 (3) | P1—C20—C25—C24 | -178.5 (2) |
| C6—C7—P1—C20 | -49.8 (2) | C23—C24—C25—C20 | -55.9 (3) |
| C2—C7—P1—C20 | 131.3 (2) | C13—P2—C26—C27 | -60.2 (2) |

supplementary materials

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| C6—C7—P1—C14 | 61.4 (2) | C32—P2—C26—C27 | 48.2 (2) |
| C2—C7—P1—C14 | -117.6 (2) | Pt1—P2—C26—C27 | 177.69 (17) |
| C6—C7—P1—Pt1 | 178.19 (18) | C13—P2—C26—C31 | 67.4 (2) |
| C2—C7—P1—Pt1 | -0.7 (2) | C32—P2—C26—C31 | 175.79 (17) |
| C12—C13—P2—C32 | -39.7 (2) | Pt1—P2—C26—C31 | -54.71 (19) |
| C8—C13—P2—C32 | 136.91 (19) | C31—C26—C27—C28 | 55.7 (3) |
| C12—C13—P2—C26 | 70.2 (2) | P2—C26—C27—C28 | -176.7 (2) |
| C8—C13—P2—C26 | -113.2 (2) | C26—C27—C28—C29 | -55.5 (3) |
| C12—C13—P2—Pt1 | -162.57 (19) | C27—C28—C29—C30 | 53.9 (4) |
| C8—C13—P2—Pt1 | 14.0 (2) | C28—C29—C30—C31 | -53.1 (3) |
| C2—Si1—Pt1—P1 | -16.37 (9) | C29—C30—C31—C26 | 53.7 (3) |
| C1—Si1—Pt1—P1 | 98.44 (11) | C27—C26—C31—C30 | -55.1 (3) |
| C8—Si1—Pt1—P1 | -141.38 (8) | P2—C26—C31—C30 | 174.6 (2) |
| C2—Si1—Pt1—P2 | 149.20 (9) | C13—P2—C32—C37 | -71.31 (19) |
| C1—Si1—Pt1—P2 | -95.99 (11) | C26—P2—C32—C37 | 176.08 (18) |
| C8—Si1—Pt1—P2 | 24.19 (8) | Pt1—P2—C32—C37 | 46.13 (19) |
| C20—P1—Pt1—Si1 | -111.73 (10) | C13—P2—C32—C33 | 162.15 (18) |
| C7—P1—Pt1—Si1 | 10.95 (9) | C26—P2—C32—C33 | 49.5 (2) |
| C14—P1—Pt1—Si1 | 125.73 (9) | Pt1—P2—C32—C33 | -80.41 (18) |
| C20—P1—Pt1—P2 | -165.73 (11) | C37—C32—C33—C34 | 59.5 (3) |
| C7—P1—Pt1—P2 | -43.05 (12) | P2—C32—C33—C34 | -173.69 (17) |
| C14—P1—Pt1—P2 | 71.72 (11) | C32—C33—C34—C35 | -58.3 (3) |
| C20—P1—Pt1—C11 | 66.92 (10) | C33—C34—C35—C36 | 55.5 (3) |
| C7—P1—Pt1—C11 | -170.41 (8) | C34—C35—C36—C37 | -52.8 (3) |
| C14—P1—Pt1—C11 | -55.63 (8) | C35—C36—C37—C32 | 54.3 (3) |
| C13—P2—Pt1—Si1 | -22.03 (8) | C33—C32—C37—C36 | -58.1 (3) |
| C32—P2—Pt1—Si1 | -136.12 (9) | P2—C32—C37—C36 | 172.88 (18) |

Fig. 1

