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# *trans*-Bis(*tert*-butylisocyanido-*C*)bis(triphenylphosphine-*P*)rhodium(I) *nido*-7,8-dicarbaundecarboranide

**G. Ferguson, P. A. McEneaney and T. R. Spalding**


## Abstract

In the crystal structure of $[Rh(t\text{-}BuNC)_2(PPh_3)_2]^+[7,8\text{-}nido\text{-}C_2H_{12}B_9]^-$ the Rh atom lies on an inversion centre and has a square-planar geometry with Rh—P 2.3217 (6), Rh—C 1.954 (2) Å, P—Rh—C 86.74 (7)°. The carborane anion lies about a twofold axis and has disordered C and B atoms.


## Comment

Disorder of the atoms in both cation and anion precludes any meaningful discussion of the geometry of this complex.

## Experimental

The title compound was synthesized in 33% yield from the reaction of a $CH_2Cl_2$ solution of [3,3-bis(triphenylphosphine)-3-hydrido-1,2-dicarba-3- rhodadodecaborane] with *tert*-BuNC at reflux temperature for 8 h followed by stirring at 293 K for a further 18 h. Crystals suitable for X-ray analysis were grown by evaporation of a $CH_2Cl_2$ solution of the compound.

## Refinement

The compound crystallized in the monoclinic system; space group *C*2/*c* or *Cc* from the systematic absences. Both options were tried and *C*2/*c* chosen.

The $[C_2H_{12}B_9]^-$ anion lies about a two fold axis and is disordered with the two C and nine B atoms distributed unequally over 12 sites; as a result of the imposed twofold symmetry, only six of these atom sites are unique. Allowing for these six sites as B atoms (labelled as B1 - B6) and allowing the occupancies to refine, indicated that four of the sites (B3 - B6) were consistent with their being unit occupancy B atoms and that the carbon-boron disorder was limited to sites labelled as B1 and B2. To keep the electron count approximately correct, and noting that there should be 28.5 non-H electrons in half of a $C_2B_9$ cage, we allowed for the B1, B2 sites as B atoms but with occupancies linked so that their occupancy sum was 1.70 (occupancies refined to B1 0.846 (11), B2 0.854 (11)); *i.e.* each of the B1 and B2 sites is effectively shared by (0.50 C and 0.25B). In this way we effectively allowed for the required 28.5 electrons in the half of the $C_2B_9$ cage (4 *x* 5.0 + 1.70 *x* 5.0 = 28.5).

In the $[C_2H_{12}B_9]^-$ cage, each of the C and B atoms should have one terminal H atom and one of the B sites should have an additional H atom bonded to it; because of the disorder noted above, we were not able to decide the location of the twelfth H atom. Difference maps of the asymmetric unit showed six maxima (one per B or C/B site of the cage) consistent with the H atoms of terminal B—H or C—H groups and we allowed for these as riding atoms (B(or C)—H 1.10 Å) with unit occupancy. Changing the H atom occupancies on the C/B sites B1 and B2 had no significant effect on the dimensions or *R*-factors.

The Rh atom of the $[(Ph_3P)_2(CNBu^t)_2Rh]^+$ cation lies on an inversion centre and the methyl groups of the unique *tert*-butyl group are disordered unequally over two sites (0.669 (6)/0.331 (6)); the minor site C atoms were refined with isotropic vibration parameters. Cation H atoms were treated as riding atoms (C—H 0.93 and 0.96 Å)

Structure solution and refinement in space group *Cc* was also considered. With $Z = 4$, this choice of space group requires no crystallographic symmetry for either cation or anion. As all attempts consistently yielded a scrambled anion cage as found for the *C*2/*c* solution and refinements always yielded non- sensible anisotropic vibration parameters; this approach was abandoned.

### Computing details

Data collection: *CAD-4-PC* Software (Enraf-Nonius, 1992); cell refinement: *SET4* & *CELDIM* in *CAD-4-PC* Software (Enraf-Nonius, 1992); data reduction: *DATRD2* in *NRCVAX96* (Gabe *et al.*, 1989); program(s) used to solve structure: *NRCVAX96* via Patterson heavy-atom method; program(s) used to refine structure: *NRCVAX96* and *SHELXL97* (Sheldrick, 1997); software used to prepare material for publication: *NRCVAX96*, *SHELXL97* and *WORDPERFECT* macro PREP8 (Ferguson, 1998).

### *trans*-Bis(triphenylphosphine)bis(*tert*-butylisocyanide)rhodium(I) *nido*-7,8-dicarbaundecaborane.

*Crystal data*

| | |
|---|---|
| $[Rh(C_5H_9N_1)_2(C_{18}H_{15}P_1)_2](C_2H_{12}B_9)$ | $V = 4931.8\ (9)$ Å$^3$ |
| $M_r = 927.12$ | $Z = 4$ |
| Monoclinic, *C*2/*c* | Mo *K*α |
| $a = 23.7306\ (14)$ Å | $\mu = 0.45$ mm$^{-1}$ |
| $b = 11.9542\ (12)$ Å | $T = 294\ (1)$ K |
| $c = 17.468\ (3)$ Å | 0.49 × 0.48 × 0.21 mm |
| $\beta = 95.597\ (19)^o$ | |

*Data collection*

| | |
|---|---|
| Enraf-Nonius CAD-4 diffractometer | 4206 reflections with $I > 2\sigma(I)$ |
| Absorption correction: Gaussian (ABSO in NRCVAX; Gabe et al., 1989) | $R_{int} = 0.010$ |
| $T_{min} = 0.822$, $T_{max} = 0.918$ | 3 standard reflections |
| 5506 measured reflections | every 120 min |
| 5339 independent reflections | intensity decay: no decay, variation 1.1% |

*Refinement*

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.034$ | 37 restraints |
| $wR(F^2) = 0.090$ | H-atom parameters constrained |
| $S = 1.19$ | $\Delta\rho_{max} = 0.65$ e Å$^{-3}$ |
| 5339 reflections | $\Delta\rho_{min} = -0.40$ e Å$^{-3}$ |
| 303 parameters | |

**Acknowledgements**

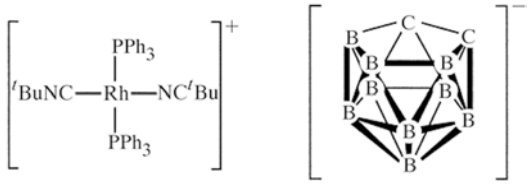
We thank Dr J. F. Gallagher and Dublin City University for the funds to purchase the X-ray tube used in the data collections.

**References**

Enraf-Nonius (1992). *CAD-4-PC* Software. Version 1.1. Enraf-Nonius, Delft, Holland.
Ferguson, G. (1998). PREP8. A *WORDPERFECT5*.1 macro to merge and polish CIF format files from *NRCVAX* and *SHELXL97* programs. University of Guelph, Canada.
Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* **22**, 384–387.
Sheldrick, G. M. (1997). *SHELXL97*. Program for the refinement of crystal structures. University of Göttingen, Germany.

# CIF access

**Scheme 1**



# supplementary materials

**_trans_-Bis(triphenylphosphine)bis(_tert_-butylisocyanide)rhodium(I) _nido_-7,8-dicarbaundecaborane.**

*Crystal data*

| | |
|---|---|
| $[Rh(C_5H_9N_1)_2(C_{18}H_{15}P_1)_2](C_2H_{12}B_9)$ | ? #Insert any comments here. |
| $M_r = 927.12$ | $D_x = 1.249$ Mg m$^{-3}$ |
| Monoclinic, $C2/c$ | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $a = 23.7306$ (14) Å | Cell parameters from 25 reflections |
| $b = 11.9542$ (12) Å | $\theta = 16.7$–$23.6$º |
| $c = 17.468$ (3) Å | $\mu = 0.45$ mm$^{-1}$ |
| $\beta = 95.597$ (19)º | $T = 294$ (1) K |
| $V = 4931.8$ (9) Å$^3$ | Plate, colourless |
| $Z = 4$ | 0.49 × 0.48 × 0.21 mm |
| $F_{000} = 1928$ | |

*Data collection*

| | |
|---|---|
| Enraf-Nonius CAD-4 diffractometer | $R_{int} = 0.010$ |
| Radiation source: X-ray tube | $\theta_{max} = 26.9$º |
| Monochromator: graphite | $\theta_{min} = 2.2$º |
| $T = 294$(1) K | $h = -30 \rightarrow 30$ |
| θ/2θ scans | $k = 0 \rightarrow 15$ |
| Absorption correction: Gaussian<br>(ABSO in NRCVAX; Gabe et al., 1989) | $l = 0 \rightarrow 22$ |
| $T_{min} = 0.822$, $T_{max} = 0.918$ | 3 standard reflections |
| 5506 measured reflections | every 120 min |
| 5339 independent reflections | intensity decay: no decay, variation 1.1% |
| 4206 reflections with $I > 2\sigma(I)$ | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.034$ | H-atom parameters constrained |
| $wR(F^2) = 0.090$ | $w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 1.2748P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.19$ | $(\Delta/\sigma)_{max} = <0.001$ |
| 5339 reflections | $\Delta\rho_{max} = 0.65$ e Å$^{-3}$ |
| 303 parameters | $\Delta\rho_{min} = -0.40$ e Å$^{-3}$ |
| 37 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Rh1 | 0.2500 | 0.2500 | 0.0000 | 0.03055 (9) | |
| P1 | 0.18349 (2) | 0.14578 (5) | 0.05820 (3) | 0.03089 (14) | |
| C1 | 0.29472 (10) | 0.1128 (2) | −0.00029 (14) | 0.0364 (5) | |
| N1 | 0.31841 (9) | 0.02938 (19) | 0.00239 (13) | 0.0457 (5) | |
| C2 | 0.34491 (12) | −0.0798 (2) | 0.01578 (16) | 0.0528 (7) | |
| C3 | 0.3033 (2) | −0.1518 (5) | 0.0549 (4) | 0.101 (3) | 0.670 (6) |
| C4 | 0.3957 (2) | −0.0628 (5) | 0.0749 (3) | 0.085 (2) | 0.670 (6) |
| C5 | 0.3603 (4) | −0.1271 (6) | −0.0560 (3) | 0.149 (4) | 0.670 (6) |
| C3A | 0.3567 (6) | −0.1092 (13) | 0.0981 (4) | 0.128 (7)* | 0.330 (6) |
| C4A | 0.3994 (3) | −0.0802 (11) | −0.0239 (6) | 0.090 (4)* | 0.330 (6) |
| C5A | 0.3045 (4) | −0.1616 (9) | −0.0265 (6) | 0.084 (4)* | 0.330 (6) |
| C11 | 0.21589 (10) | 0.0677 (2) | 0.14148 (13) | 0.0364 (5) | |
| C12 | 0.26577 (11) | 0.1092 (3) | 0.17886 (15) | 0.0484 (6) | |
| C13 | 0.29145 (14) | 0.0560 (3) | 0.24343 (17) | 0.0654 (9) | |
| C14 | 0.26790 (15) | −0.0392 (3) | 0.27079 (18) | 0.0706 (10) | |
| C15 | 0.21840 (16) | −0.0808 (3) | 0.23442 (19) | 0.0702 (10) | |
| C16 | 0.19229 (13) | −0.0280 (3) | 0.16924 (17) | 0.0550 (7) | |
| C21 | 0.12641 (10) | 0.22363 (19) | 0.09724 (14) | 0.0342 (5) | |
| C22 | 0.08396 (11) | 0.2691 (2) | 0.04636 (16) | 0.0464 (7) | |
| C23 | 0.04132 (12) | 0.3326 (3) | 0.07307 (18) | 0.0579 (8) | |
| C24 | 0.04082 (13) | 0.3523 (3) | 0.15060 (19) | 0.0611 (8) | |
| C25 | 0.08306 (15) | 0.3085 (3) | 0.20129 (18) | 0.0655 (9) | |
| C26 | 0.12559 (13) | 0.2436 (2) | 0.17534 (16) | 0.0507 (7) | |
| C31 | 0.14397 (10) | 0.0437 (2) | −0.00381 (13) | 0.0362 (5) | |
| C32 | 0.16246 (12) | 0.0170 (2) | −0.07455 (15) | 0.0473 (6) | |
| C33 | 0.13192 (15) | −0.0576 (3) | −0.12333 (18) | 0.0633 (9) | |
| C34 | 0.08302 (15) | −0.1056 (3) | −0.1027 (2) | 0.0644 (9) | |
| C35 | 0.06472 (13) | −0.0808 (3) | −0.0327 (2) | 0.0607 (8) | |
| C36 | 0.09423 (11) | −0.0053 (2) | 0.01628 (17) | 0.0495 (6) | |
| B1 | 0.4978 (3) | 0.3319 (4) | 0.1726 (3) | 0.079 (2) | 0.846 (11) |
| B2 | 0.4685 (2) | 0.3694 (4) | 0.2515 (4) | 0.085 (2) | 0.855 (11) |
| B3 | 0.4417 (2) | 0.2630 (4) | 0.2961 (3) | 0.0756 (13) | |
| B4 | 0.46244 (15) | 0.1435 (3) | 0.2468 (2) | 0.0598 (9) | |
| B5 | 0.49753 (18) | 0.1882 (4) | 0.1673 (2) | 0.0650 (10) | |
| B6 | 0.43758 (19) | 0.2620 (4) | 0.1945 (3) | 0.0724 (12) | |
| H3A | 0.2942 | −0.1157 | 0.1012 | 0.151* | 0.670 (6) |
| H3B | 0.3200 | −0.2234 | 0.0673 | 0.151* | 0.670 (6) |
| H3C | 0.2694 | −0.1617 | 0.0208 | 0.151* | 0.670 (6) |
| H4A | 0.3832 | −0.0322 | 0.1212 | 0.128* | 0.670 (6) |
| H4B | 0.4219 | −0.0121 | 0.0548 | 0.128* | 0.670 (6) |
| H4C | 0.4140 | −0.1334 | 0.0862 | 0.128* | 0.670 (6) |
| H5A | 0.3870 | −0.0787 | −0.0774 | 0.223* | 0.670 (6) |
| H5B | 0.3271 | −0.1343 | −0.0916 | 0.223* | 0.670 (6) |
| H5C | 0.3771 | −0.1994 | −0.0463 | 0.223* | 0.670 (6) |
| H3A1 | 0.3830 | −0.0565 | 0.1227 | 0.192* | 0.330 (6) |

| | | | | | |
|---|---|---|---|---|---|
| H3A2 | 0.3725 | −0.1830 | 0.1026 | 0.192* | 0.330 (6) |
| H3A3 | 0.3220 | −0.1070 | 0.1223 | 0.192* | 0.330 (6) |
| H4A1 | 0.3904 | −0.0702 | −0.0783 | 0.135* | 0.330 (6) |
| H4A2 | 0.4186 | −0.1503 | −0.0145 | 0.135* | 0.330 (6) |
| H4A3 | 0.4235 | −0.0203 | −0.0040 | 0.135* | 0.330 (6) |
| H5A1 | 0.2969 | −0.1386 | −0.0791 | 0.126* | 0.330 (6) |
| H5A2 | 0.2697 | −0.1633 | −0.0026 | 0.126* | 0.330 (6) |
| H5A3 | 0.3212 | −0.2348 | −0.0245 | 0.126* | 0.330 (6) |
| H12 | 0.2821 | 0.1732 | 0.1604 | 0.058* | |
| H13 | 0.3247 | 0.0847 | 0.2684 | 0.079* | |
| H14 | 0.2854 | −0.0753 | 0.3139 | 0.085* | |
| H15 | 0.2022 | −0.1446 | 0.2534 | 0.084* | |
| H16 | 0.1590 | −0.0572 | 0.1444 | 0.066* | |
| H22 | 0.0842 | 0.2568 | −0.0062 | 0.056* | |
| H23 | 0.0129 | 0.3621 | 0.0385 | 0.070* | |
| H24 | 0.0121 | 0.3949 | 0.1686 | 0.073* | |
| H25 | 0.0830 | 0.3226 | 0.2537 | 0.079* | |
| H26 | 0.1536 | 0.2135 | 0.2102 | 0.061* | |
| H32 | 0.1954 | 0.0491 | −0.0893 | 0.057* | |
| H33 | 0.1447 | −0.0752 | −0.1705 | 0.076* | |
| H34 | 0.0625 | −0.1546 | −0.1361 | 0.077* | |
| H35 | 0.0323 | −0.1149 | −0.0179 | 0.073* | |
| H36 | 0.0807 | 0.0128 | 0.0629 | 0.059* | |
| H1 | 0.4957 | 0.3821 | 0.1196 | 0.094* | |
| H2 | 0.4464 | 0.4499 | 0.2543 | 0.102* | |
| H3 | 0.4029 | 0.2653 | 0.3258 | 0.091* | |
| H4 | 0.4378 | 0.0654 | 0.2447 | 0.072* | |
| H5 | 0.4961 | 0.1405 | 0.1133 | 0.078* | |
| H6 | 0.3970 | 0.2645 | 0.1581 | 0.087* | |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Rh1 | 0.02694 (13) | 0.02842 (13) | 0.03716 (14) | 0.00416 (11) | 0.00767 (9) | 0.00550 (11) |
| P1 | 0.0280 (3) | 0.0321 (3) | 0.0330 (3) | 0.0007 (2) | 0.0053 (2) | 0.0034 (2) |
| C1 | 0.0305 (12) | 0.0356 (13) | 0.0443 (13) | 0.0039 (10) | 0.0090 (10) | 0.0056 (10) |
| N1 | 0.0390 (12) | 0.0400 (13) | 0.0583 (14) | 0.0098 (10) | 0.0053 (10) | 0.0034 (10) |
| C2 | 0.0532 (17) | 0.0373 (15) | 0.0674 (19) | 0.0183 (13) | 0.0033 (14) | 0.0027 (13) |
| C3 | 0.070 (4) | 0.051 (3) | 0.184 (7) | 0.008 (3) | 0.027 (4) | 0.032 (4) |
| C4 | 0.070 (4) | 0.068 (3) | 0.110 (5) | 0.016 (3) | −0.034 (3) | 0.011 (3) |
| C5 | 0.270 (9) | 0.113 (5) | 0.064 (4) | 0.122 (6) | 0.023 (5) | −0.007 (4) |
| C11 | 0.0350 (13) | 0.0398 (13) | 0.0349 (12) | 0.0043 (10) | 0.0061 (9) | 0.0055 (10) |
| C12 | 0.0448 (15) | 0.0586 (17) | 0.0416 (14) | −0.0016 (13) | 0.0029 (11) | 0.0022 (12) |
| C13 | 0.0515 (18) | 0.104 (3) | 0.0390 (15) | 0.0086 (18) | −0.0044 (13) | 0.0016 (16) |
| C14 | 0.073 (2) | 0.095 (3) | 0.0434 (16) | 0.029 (2) | 0.0011 (15) | 0.0208 (17) |
| C15 | 0.090 (3) | 0.063 (2) | 0.059 (2) | 0.0075 (19) | 0.0123 (18) | 0.0288 (16) |
| C16 | 0.0568 (18) | 0.0507 (17) | 0.0566 (17) | −0.0015 (14) | 0.0011 (13) | 0.0183 (13) |
| C21 | 0.0294 (11) | 0.0348 (13) | 0.0392 (12) | −0.0018 (9) | 0.0085 (9) | −0.0005 (9) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C22 | 0.0380 (14) | 0.0580 (19) | 0.0435 (14) | 0.0107 (12) | 0.0048 (11) | −0.0014 (12) |
| C23 | 0.0378 (15) | 0.071 (2) | 0.0642 (18) | 0.0156 (14) | 0.0024 (13) | −0.0028 (15) |
| C24 | 0.0456 (17) | 0.065 (2) | 0.075 (2) | 0.0121 (15) | 0.0179 (15) | −0.0147 (16) |
| C25 | 0.069 (2) | 0.082 (2) | 0.0478 (17) | 0.0153 (19) | 0.0162 (15) | −0.0172 (16) |
| C26 | 0.0505 (16) | 0.0603 (18) | 0.0417 (14) | 0.0107 (14) | 0.0060 (11) | 0.0008 (13) |
| C31 | 0.0359 (13) | 0.0340 (12) | 0.0380 (12) | 0.0030 (10) | −0.0004 (9) | 0.0008 (10) |
| C32 | 0.0523 (16) | 0.0488 (16) | 0.0411 (14) | 0.0014 (13) | 0.0061 (11) | −0.0046 (12) |
| C33 | 0.078 (2) | 0.059 (2) | 0.0519 (17) | 0.0047 (17) | 0.0003 (15) | −0.0172 (14) |
| C34 | 0.072 (2) | 0.0434 (17) | 0.073 (2) | −0.0020 (16) | −0.0176 (17) | −0.0139 (15) |
| C35 | 0.0456 (17) | 0.0500 (18) | 0.084 (2) | −0.0098 (14) | −0.0045 (15) | −0.0048 (16) |
| C36 | 0.0424 (15) | 0.0483 (16) | 0.0577 (17) | −0.0072 (13) | 0.0052 (12) | −0.0029 (13) |
| B1 | 0.103 (4) | 0.065 (3) | 0.073 (3) | 0.011 (3) | 0.034 (3) | 0.027 (3) |
| B2 | 0.106 (4) | 0.052 (3) | 0.102 (5) | 0.020 (3) | 0.035 (4) | 0.017 (3) |
| B3 | 0.076 (3) | 0.083 (3) | 0.072 (3) | 0.018 (2) | 0.032 (2) | 0.013 (2) |
| B4 | 0.052 (2) | 0.057 (2) | 0.069 (2) | −0.0087 (17) | −0.0017 (16) | 0.0113 (18) |
| B5 | 0.064 (2) | 0.077 (3) | 0.053 (2) | 0.005 (2) | 0.0061 (17) | −0.0049 (19) |
| B6 | 0.064 (2) | 0.082 (3) | 0.071 (2) | 0.020 (2) | 0.0062 (19) | 0.022 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Rh1—C1 | 1.954 (2) | C31—C32 | 1.388 (3) |
| Rh1—C1$^{i}$ | 1.954 (2) | C31—C36 | 1.393 (4) |
| Rh1—P1$^{i}$ | 2.3217 (6) | C32—C33 | 1.387 (4) |
| Rh1—P1 | 2.3217 (6) | C33—C34 | 1.374 (5) |
| P1—C31 | 1.829 (2) | C34—C35 | 1.370 (5) |
| P1—C21 | 1.829 (2) | C35—C36 | 1.386 (4) |
| P1—C11 | 1.833 (2) | B1—B2$^{ii}$ | 1.546 (8) |
| C1—N1 | 1.143 (3) | B1—B2 | 1.664 (8) |
| N1—C2 | 1.458 (3) | B1—B3$^{ii}$ | 1.700 (8) |
| C2—C5 | 1.454 (4) | B1—B5 | 1.721 (7) |
| C2—C3A | 1.480 (6) | B1—B6 | 1.730 (7) |
| C2—C5A | 1.511 (5) | B2—B2$^{ii}$ | 1.500 (11) |
| C2—C3 | 1.521 (5) | B2—B1$^{ii}$ | 1.546 (8) |
| C2—C4 | 1.523 (4) | B2—B3 | 1.651 (7) |
| C2—C4A | 1.526 (6) | B2—B6 | 1.743 (8) |
| C11—C16 | 1.383 (4) | B3—B1$^{ii}$ | 1.700 (8) |
| C11—C12 | 1.387 (4) | B3—B5$^{ii}$ | 1.763 (6) |
| C12—C13 | 1.384 (4) | B3—B4 | 1.763 (6) |
| C13—C14 | 1.373 (5) | B3—B6 | 1.769 (6) |
| C14—C15 | 1.373 (5) | B4—B6 | 1.757 (5) |
| C15—C16 | 1.393 (4) | B4—B5 | 1.770 (6) |
| C21—C26 | 1.387 (4) | B4—B4$^{ii}$ | 1.775 (7) |
| C21—C22 | 1.388 (4) | B4—B5$^{ii}$ | 1.778 (5) |
| C22—C23 | 1.382 (4) | B5—B3$^{ii}$ | 1.763 (6) |
| C23—C24 | 1.376 (4) | B5—B6 | 1.777 (6) |
| C24—C25 | 1.375 (5) | B5—B4$^{ii}$ | 1.778 (5) |
| C25—C26 | 1.383 (4) | | |

| | | | |
|---|---|---|---|
| C1—Rh1—C1$^{i}$ | 180.0 | B2$^{ii}$—B1—B3$^{ii}$ | 61.0 (3) |
| C1—Rh1—P1$^{i}$ | 93.25 (7) | B2—B1—B3$^{ii}$ | 105.8 (4) |
| C1$^{i}$—Rh1—P1$^{i}$ | 86.75 (7) | B2$^{ii}$—B1—B5 | 109.5 (4) |
| C1—Rh1—P1 | 86.74 (7) | B2—B1—B5 | 108.3 (3) |
| C1$^{i}$—Rh1—P1 | 93.25 (7) | B3$^{ii}$—B1—B5 | 62.0 (3) |
| P1$^{i}$—Rh1—P1 | 180.00 (2) | B2$^{ii}$—B1—B6 | 108.7 (4) |
| C31—P1—C21 | 101.81 (11) | B2—B1—B6 | 61.8 (3) |
| C31—P1—C11 | 106.35 (11) | B3$^{ii}$—B1—B6 | 112.6 (3) |
| C21—P1—C11 | 103.40 (11) | B5—B1—B6 | 62.0 (3) |
| C31—P1—Rh1 | 115.47 (8) | B2$^{ii}$—B2—B1$^{ii}$ | 66.2 (5) |
| C21—P1—Rh1 | 116.74 (8) | B2$^{ii}$—B2—B3 | 116.6 (4) |
| C11—P1—Rh1 | 111.74 (8) | B1$^{ii}$—B2—B3 | 64.1 (3) |
| N1—C1—Rh1 | 175.6 (2) | B2$^{ii}$—B2—B1 | 58.2 (4) |
| C1—N1—C2 | 171.9 (3) | B1$^{ii}$—B2—B1 | 114.2 (4) |
| C5—C2—N1 | 110.5 (3) | B3—B2—B1 | 113.3 (4) |
| C5—C2—C3A | 134.9 (7) | B2$^{ii}$—B2—B6 | 110.2 (4) |
| N1—C2—C3A | 113.9 (7) | B1$^{ii}$—B2—B6 | 115.5 (4) |
| C5—C2—C5A | 61.9 (4) | B3—B2—B6 | 62.8 (3) |
| N1—C2—C5A | 104.9 (5) | B1—B2—B6 | 61.0 (3) |
| C3A—C2—C5A | 111.8 (4) | B2—B3—B1$^{ii}$ | 54.9 (3) |
| C5—C2—C3 | 113.3 (3) | B2—B3—B5$^{ii}$ | 102.8 (4) |
| N1—C2—C3 | 106.9 (3) | B1$^{ii}$—B3—B5$^{ii}$ | 59.6 (3) |
| C3A—C2—C3 | 59.9 (5) | B2—B3—B4 | 104.7 (3) |
| C5A—C2—C3 | 56.2 (4) | B1$^{ii}$—B3—B4 | 106.4 (3) |
| C5—C2—C4 | 112.8 (3) | B5$^{ii}$—B3—B4 | 60.6 (2) |
| N1—C2—C4 | 106.9 (3) | B2—B3—B6 | 61.1 (3) |
| C3A—C2—C4 | 46.4 (5) | B1$^{ii}$—B3—B6 | 106.7 (3) |
| C5A—C2—C4 | 147.2 (5) | B5$^{ii}$—B3—B6 | 108.9 (3) |
| C3—C2—C4 | 106.0 (3) | B4—B3—B6 | 59.7 (2) |
| C5—C2—C4A | 46.5 (4) | B6—B4—B3 | 60.4 (2) |
| N1—C2—C4A | 107.5 (5) | B6—B4—B5 | 60.5 (2) |
| C3A—C2—C4A | 110.7 (4) | B3—B4—B5 | 108.3 (3) |
| C5A—C2—C4A | 107.6 (4) | B6—B4—B4$^{ii}$ | 108.5 (2) |
| C3—C2—C4A | 144.9 (6) | B3—B4—B4$^{ii}$ | 107.2 (3) |
| C4—C2—C4A | 70.1 (4) | B5—B4—B4$^{ii}$ | 60.2 (3) |
| C16—C11—C12 | 119.2 (2) | B6—B4—B5$^{ii}$ | 108.7 (3) |
| C16—C11—P1 | 123.2 (2) | B3—B4—B5$^{ii}$ | 59.7 (3) |
| C12—C11—P1 | 117.66 (19) | B5—B4—B5$^{ii}$ | 108.5 (3) |
| C13—C12—C11 | 120.5 (3) | B4$^{ii}$—B4—B5$^{ii}$ | 59.8 (2) |
| C14—C13—C12 | 120.2 (3) | B1—B5—B3$^{ii}$ | 58.4 (3) |
| C15—C14—C13 | 119.9 (3) | B1—B5—B4 | 105.0 (3) |
| C14—C15—C16 | 120.4 (3) | B3$^{ii}$—B5—B4 | 107.4 (3) |
| C11—C16—C15 | 119.9 (3) | B1—B5—B6 | 59.2 (3) |

| | | | |
|---|---|---|---|
| C26—C21—C22 | 118.9 (2) | B3$^{ii}$—B5—B6 | 107.4 (3) |
| C26—C21—P1 | 122.43 (19) | B4—B5—B6 | 59.4 (2) |
| C22—C21—P1 | 118.56 (19) | B1—B5—B4$^{ii}$ | 104.9 (3) |
| C23—C22—C21 | 120.6 (3) | B3$^{ii}$—B5—B4$^{ii}$ | 59.7 (2) |
| C24—C23—C22 | 120.2 (3) | B4—B5—B4$^{ii}$ | 60.0 (2) |
| C25—C24—C23 | 119.5 (3) | B6—B5—B4$^{ii}$ | 107.5 (3) |
| C24—C25—C26 | 120.8 (3) | B1—B6—B2 | 57.3 (3) |
| C25—C26—C21 | 120.0 (3) | B1—B6—B4 | 105.2 (3) |
| C32—C31—C36 | 118.5 (2) | B2—B6—B4 | 101.2 (3) |
| C32—C31—P1 | 119.5 (2) | B1—B6—B3 | 104.6 (4) |
| C36—C31—P1 | 122.0 (2) | B2—B6—B3 | 56.1 (3) |
| C33—C32—C31 | 120.2 (3) | B4—B6—B3 | 60.0 (2) |
| C34—C33—C32 | 120.8 (3) | B1—B6—B5 | 58.8 (3) |
| C35—C34—C33 | 119.6 (3) | B2—B6—B5 | 102.4 (3) |
| C34—C35—C36 | 120.5 (3) | B4—B6—B5 | 60.1 (2) |
| C35—C36—C31 | 120.5 (3) | B3—B6—B5 | 107.7 (3) |
| B2$^{ii}$—B1—B2 | 55.6 (4) | | |

Symmetry codes: (i) −*x*+1/2, −*y*+1/2, −*z*; (ii) −*x*+1, *y*, −*z*+1/2.