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## Structure Reports

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**{*N,N*-Bis[2-(diphenylphosphanyl)ethyl]-aniline}( $\eta^2$ -dibenzylideneacetone)-palladium(0)**

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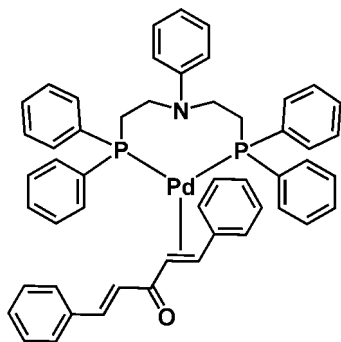
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Key indicators: single-crystal X-ray study;  $T = 153$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.041;  $wR$  factor = 0.089; data-to-parameter ratio = 18.5.

In the title complex,  $[\text{Pd}(\text{C}_{34}\text{H}_{33}\text{NP}_2)(\text{C}_{17}\text{H}_{14}\text{O})]$ , the Pd<sup>0</sup> atom is coordinated in a trigonal planar geometry formed by two P atoms of a bis[(diphenylphosphino)ethyl]aniline ligand and a C=C ( $\eta^2$ ) bond involving the C atoms that are in the  $\alpha,\beta$  positions relative to the central ketone of the dibenzylideneacetone ligand.

## Related literature

For general background and the potential applications of palladium complexes incorporating multidentate ligands, see: Blower *et al.* (1997); Michos *et al.* (1992); Kostas (2001); Lee *et al.* (2006); Hii *et al.* (1999). For similar structures, see: Retbøll *et al.* (2002); Goddard *et al.* (1995).



## Experimental

## Crystal data

 $[\text{Pd}(\text{C}_{34}\text{H}_{33}\text{NP}_2)(\text{C}_{17}\text{H}_{14}\text{O})]$  $M_r = 858.24$ Triclinic,  $P\bar{1}$  $a = 10.087$  (2) Å $b = 11.974$  (2) Å $c = 17.473$  (4) Å $\alpha = 86.34$  (3)° $\beta = 81.27$  (2)° $\gamma = 83.15$  (3)° $V = 2068.8$  (7) Å<sup>3</sup> $Z = 2$ Mo  $K\alpha$  radiation $\mu = 0.57$  mm<sup>-1</sup>  
 $T = 153$  K

0.27 × 0.14 × 0.12 mm

## Data collection

Nonius Kappa CCD diffractometer  
Absorption correction: multi-scan  
(*DENZO* and *SCALEPACK*;  
Otwinowski & Minor, 1997)  
 $T_{\min} = 0.837$ ,  $T_{\max} = 1.000$ 15976 measured reflections  
9324 independent reflections  
7745 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.031$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.041$   
 $wR(F^2) = 0.089$   
 $S = 1.58$   
9324 reflections505 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 1.56$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.67$  e Å<sup>-3</sup>

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *COLLECT*; data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999) within *WinGX* (Farrugia, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5314).

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**supplementary materials**

*Acta Cryst.* (2011). E67, m1327 [ doi:10.1107/S1600536811033800 ]

## {*N,N*-Bis[2-(diphenylphosphanyl)ethyl]aniline}(η<sup>2</sup>-dibenzylideneacetone)palladium(0)

S. G. Keskin, J. M. Stanley, M. L. Mejía and B. J. Holliday

### Comment

Palladium complexes which incorporate multidentate ligands have been used in a variety of applications, such as catalysis, biotechnology and materials science (Blower *et al.*, 1997; Michos *et al.*, 1992; Kostas, 2001; Lee *et al.*, 2006). These multidentate ligands may contain donor atoms of the same type or be comprised of mixed donor atoms such as oxygen, carbon, phosphorous, sulfur and nitrogen (*i.e.*, NNN, PNP, SPS). Advantages of mixed donor systems include flexible coordination modes and complex stability, both of which have the potential to increase performance in catalytic applications (Hii *et al.*, 1999), including coupling, hydrogenation and dehydrogenation reactions. Many examples of PNP-type (phosphorous/nitrogen/phosphorous) ligands have been studied because the hemilabile property of the nitrogen atom gives different coordination geometries, including tridentate monomeric (PNP), bidentate monomeric (PP) and bidentate dimeric (PP) modes, which can be controlled by substitution of the nitrogen atom, thereby affecting the nitrogen donor strength.

The molecular structure of the title compound is shown in Fig. 1. The geometry around the palladium atom is trigonal planar with the angle between the Pd—P1—P2 and Pd—C41—C42 planes being 1.40°. The *N,N*-bis[(diphenylphosphino)ethyl]aniline ligand is in a monomeric (PP) binding mode in which the nitrogen atom of the ligand is not bound to the metal center (distance between N1 and Pd1 is 3.405 Å). The average Pd1—P bond length is 2.326 Å, which is consistent with similar structures reported in the literature (Retbøll *et al.*, 2002; Goddard *et al.*, 1995). Dibenzylideneacetone (dba) is bound to Pd1 *via* one of the carbon-carbon double bonds in an η<sup>2</sup> fashion, with the C41=C42 bond (1.411 (3) Å) slightly elongated due to complexation when compared to C44=C45 (1.327 (3) Å) and the C41=C42 centroid-Pd1 distance is 2.044 Å. Similar Pd(0) coordination environments have been previously reported with chelating diphosphine and dba ligands which also display the elongated carbon-carbon double bond (1.417 (3) Å) (Retbøll *et al.*, 2002). This coordination mode is not surprising since Pd<sub>2</sub>dba<sub>3</sub> is the metal precursor used in the synthesis of the title complex and includes two palladium atoms with each metal bound η<sup>2</sup> to the three dba ligands.

### Experimental

To 0.202 g of *N,N*-bis[(diphenylphosphino)ethyl]aniline under nitrogen in 5 ml anhydrous THF was added 0.179 g Pd<sub>2</sub>dba<sub>3</sub>. The reaction mixture was stirred at room temperature for 15 h, followed by filtration and removal of the solvent. Pure product was obtained by recrystallization from methylene chloride and hexanes yielding orange crystals suitable for diffraction. Purity and composition were confirmed by comparing <sup>1</sup>H and <sup>31</sup>P{<sup>1</sup>H} NMR spectroscopy and mass spectrometry data to literature values (Hii *et al.*, 1999). Yield = 54%.

### Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95–0.99 Å and with *U*<sub>iso</sub>(H) = 1.2 times *U*<sub>eq</sub>(C).

## Figures

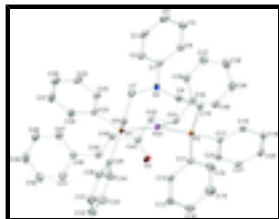


Fig. 1. The molecular structure of dibenzylideneacetone  $\{N,N$ -bis[(diphenylphosphino)ethyl]aniline}palladium(0) showing ellipsoids at the 30% probability level. Hydrogen atoms are omitted for clarity.

## $\{N,N$ -Bis[2-(diphenylphosphanyl)ethyl]aniline} $\}(\eta^2$ -dibenzylideneacetone)palladium(0)

### Crystal data

[Pd(C<sub>34</sub>H<sub>33</sub>NP<sub>2</sub>)(C<sub>17</sub>H<sub>14</sub>O)]

$M_r = 858.24$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 10.087$  (2) Å

$b = 11.974$  (2) Å

$c = 17.473$  (4) Å

$\alpha = 86.34$  (3)°

$\beta = 81.27$  (2)°

$\gamma = 83.15$  (3)°

$V = 2068.8$  (7) Å<sup>3</sup>

$Z = 2$

$F(000) = 888$

$D_x = 1.378$  Mg m<sup>-3</sup>

Melting point: 420 K

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 27945 reflections

$\theta = 1.0$ – $27.5$ °

$\mu = 0.57$  mm<sup>-1</sup>

$T = 153$  K

Prism, orange

$0.27 \times 0.14 \times 0.12$  mm

### Data collection

Nonius Kappa CCD  
diffractometer

Radiation source: fine-focus sealed tube  
graphite

$\omega$ -scans

Absorption correction: multi-scan

(*DENZO* and *SCALEPACK*; Otwinowski & Minor, 1997)

$T_{\min} = 0.837$ ,  $T_{\max} = 1.000$

15976 measured reflections

9324 independent reflections

7745 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\max} = 27.5$ °,  $\theta_{\min} = 1.7$ °

$h = -12 \rightarrow 13$

$k = -14 \rightarrow 15$

$l = -22 \rightarrow 22$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.089$

$S = 1.58$

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

$w = 1/[\sigma^2(F_o^2) + (0.020P)^2]$

9324 reflections  
505 parameters  
0 restraints

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.002$$

$$\Delta\rho_{\max} = 1.56 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.67 \text{ e } \text{\AA}^{-3}$$

*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 ( $\text{\AA}^2$ )*

|      | <i>x</i>      | <i>y</i>      | <i>z</i>      | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|---------------|---------------|---------------|----------------------------------|
| Pd1  | 0.699379 (17) | 0.165949 (14) | 0.714724 (10) | 0.02103 (7)                      |
| P1   | 0.76258 (6)   | 0.26802 (5)   | 0.60129 (3)   | 0.02080 (14)                     |
| P2   | 0.88250 (6)   | 0.14942 (5)   | 0.78434 (3)   | 0.02179 (14)                     |
| O1   | 0.60286 (17)  | -0.08845 (14) | 0.71914 (10)  | 0.0329 (4)                       |
| N1   | 0.80565 (19)  | 0.41621 (16)  | 0.74653 (11)  | 0.0243 (5)                       |
| C29  | 1.0050 (2)    | 0.0255 (2)    | 0.76262 (13)  | 0.0231 (5)                       |
| C17  | 0.6584 (2)    | 0.26165 (19)  | 0.52443 (12)  | 0.0213 (5)                       |
| C45  | 0.6737 (2)    | -0.1747 (2)   | 0.86247 (14)  | 0.0283 (6)                       |
| H45  | 0.6959        | -0.2166       | 0.8170        | 0.034*                           |
| C10  | 0.7601 (2)    | 0.42025 (19)  | 0.61030 (14)  | 0.0247 (5)                       |
| H10A | 0.7884        | 0.4555        | 0.5585        | 0.030*                           |
| H10B | 0.6665        | 0.4526        | 0.6285        | 0.030*                           |
| C21  | 0.5339 (2)    | 0.3398 (2)    | 0.42294 (14)  | 0.0288 (6)                       |
| H21  | 0.5012        | 0.4036        | 0.3933        | 0.035*                           |
| C44  | 0.6082 (2)    | -0.0729 (2)   | 0.85348 (14)  | 0.0267 (6)                       |
| H44  | 0.5801        | -0.0282       | 0.8973        | 0.032*                           |
| C36  | 0.3912 (2)    | 0.3359 (2)    | 0.73626 (15)  | 0.0312 (6)                       |
| H36  | 0.4375        | 0.3298        | 0.7801        | 0.037*                           |
| C22  | 0.6075 (2)    | 0.3537 (2)    | 0.48183 (13)  | 0.0246 (5)                       |
| H22  | 0.6231        | 0.4272        | 0.4930        | 0.030*                           |
| C11  | 0.9295 (2)    | 0.22565 (19)  | 0.54657 (13)  | 0.0223 (5)                       |
| C24  | 0.7150 (3)    | 0.1589 (2)    | 0.92741 (14)  | 0.0278 (6)                       |
| H24  | 0.6434        | 0.1666        | 0.8972        | 0.033*                           |
| C12  | 1.0002 (2)    | 0.1268 (2)    | 0.57025 (14)  | 0.0278 (6)                       |
| H12  | 0.9654        | 0.0868        | 0.6162        | 0.033*                           |
| C19  | 0.5585 (2)    | 0.1407 (2)    | 0.44922 (14)  | 0.0270 (6)                       |
| H19  | 0.5423        | 0.0673        | 0.4380        | 0.032*                           |
| C35  | 0.4079 (2)    | 0.2461 (2)    | 0.68703 (13)  | 0.0254 (6)                       |

## supplementary materials

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|     |            |              |              |            |
|-----|------------|--------------|--------------|------------|
| C6  | 0.6271 (2) | 0.5772 (2)   | 0.75423 (14) | 0.0273 (6) |
| H6  | 0.6659     | 0.6085       | 0.7059       | 0.033*     |
| C46 | 0.7162 (2) | -0.2308 (2)  | 0.93276 (14) | 0.0295 (6) |
| C23 | 0.8463 (2) | 0.14303 (19) | 0.89111 (13) | 0.0251 (5) |
| C40 | 0.3364 (2) | 0.2593 (2)   | 0.62354 (14) | 0.0315 (6) |
| H40 | 0.3455     | 0.1998       | 0.5890       | 0.038*     |
| C20 | 0.5078 (2) | 0.2336 (2)   | 0.40700 (14) | 0.0291 (6) |
| H20 | 0.4556     | 0.2245       | 0.3674       | 0.035*     |
| C47 | 0.6983 (3) | -0.1807 (2)  | 1.00444 (15) | 0.0356 (6) |
| H47 | 0.6571     | -0.1054      | 1.0088       | 0.043*     |
| C14 | 1.1723 (3) | 0.1405 (2)   | 0.46096 (16) | 0.0351 (6) |
| H14 | 1.2544     | 0.1109       | 0.4314       | 0.042*     |
| C30 | 1.1453 (2) | 0.0263 (2)   | 0.75161 (14) | 0.0297 (6) |
| H30 | 1.1826     | 0.0938       | 0.7577       | 0.036*     |
| C32 | 1.1778 (3) | -0.1687 (2)  | 0.72396 (16) | 0.0374 (7) |
| H32 | 1.2361     | -0.2351      | 0.7107       | 0.045*     |
| C31 | 1.2304 (3) | -0.0709 (2)  | 0.73177 (14) | 0.0337 (6) |
| H31 | 1.3254     | -0.0691      | 0.7236       | 0.040*     |
| C38 | 0.2385 (3) | 0.4442 (2)   | 0.65952 (16) | 0.0386 (7) |
| H38 | 0.1811     | 0.5111       | 0.6505       | 0.046*     |
| C18 | 0.6324 (2) | 0.1547 (2)   | 0.50759 (13) | 0.0238 (5) |
| H18 | 0.6660     | 0.0907       | 0.5367       | 0.029*     |
| C51 | 0.7793 (3) | -0.3413 (2)  | 0.92972 (17) | 0.0410 (7) |
| H51 | 0.7931     | -0.3775      | 0.8819       | 0.049*     |
| C9  | 0.8522 (2) | 0.4495 (2)   | 0.66621 (13) | 0.0266 (6) |
| H9A | 0.9442     | 0.4115       | 0.6507       | 0.032*     |
| H9B | 0.8575     | 0.5317       | 0.6621       | 0.032*     |
| C5  | 0.5092 (3) | 0.6314 (2)   | 0.79378 (16) | 0.0368 (7) |
| H5  | 0.4683     | 0.6992       | 0.7720       | 0.044*     |
| C48 | 0.7397 (3) | -0.2391 (3)  | 1.06887 (16) | 0.0418 (7) |
| H48 | 0.7252     | -0.2040      | 1.1171       | 0.050*     |
| C2  | 0.6271 (3) | 0.4334 (2)   | 0.85650 (14) | 0.0297 (6) |
| H2  | 0.6669     | 0.3653       | 0.8785       | 0.036*     |
| C42 | 0.5221 (2) | 0.0900 (2)   | 0.76997 (14) | 0.0253 (5) |
| H42 | 0.5020     | 0.1320       | 0.8154       | 0.030*     |
| C16 | 0.9820 (3) | 0.2829 (2)   | 0.47930 (16) | 0.0403 (7) |
| H16 | 0.9353     | 0.3513       | 0.4622       | 0.048*     |
| C43 | 0.5779 (2) | -0.0273 (2)  | 0.77551 (14) | 0.0257 (5) |
| C39 | 0.2532 (2) | 0.3565 (2)   | 0.61000 (15) | 0.0372 (7) |
| H39 | 0.2059     | 0.3631       | 0.5666       | 0.045*     |
| C13 | 1.1214 (3) | 0.0854 (2)   | 0.52758 (15) | 0.0342 (6) |
| H13 | 1.1696     | 0.0179       | 0.5450       | 0.041*     |
| C33 | 1.0403 (3) | -0.1711 (2)  | 0.7353 (2)   | 0.0509 (8) |
| H33 | 1.0038     | -0.2396      | 0.7312       | 0.061*     |
| C1  | 0.6888 (2) | 0.4776 (2)   | 0.78474 (13) | 0.0251 (5) |
| C41 | 0.4974 (2) | 0.1423 (2)   | 0.69805 (13) | 0.0249 (5) |
| H41 | 0.5428     | 0.1071       | 0.6527       | 0.030*     |
| C25 | 0.6851 (3) | 0.1638 (2)   | 1.00788 (15) | 0.0369 (7) |
| H25 | 0.5939     | 0.1750       | 1.0321       | 0.044*     |

|     |            |              |              |            |
|-----|------------|--------------|--------------|------------|
| C37 | 0.3084 (3) | 0.4333 (2)   | 0.72226 (16) | 0.0376 (7) |
| H37 | 0.2995     | 0.4935       | 0.7562       | 0.045*     |
| C34 | 0.9547 (3) | -0.0739 (2)  | 0.75257 (17) | 0.0391 (7) |
| H34 | 0.8599     | -0.0757      | 0.7576       | 0.047*     |
| C3  | 0.5102 (3) | 0.4874 (2)   | 0.89517 (16) | 0.0384 (7) |
| H3  | 0.4697     | 0.4561       | 0.9431       | 0.046*     |
| C8  | 0.9909 (2) | 0.26442 (19) | 0.76920 (14) | 0.0257 (5) |
| H8A | 1.0655     | 0.2465       | 0.8004       | 0.031*     |
| H8B | 1.0313     | 0.2691       | 0.7140       | 0.031*     |
| C28 | 0.9503 (3) | 0.1305 (2)   | 0.93644 (15) | 0.0374 (7) |
| H28 | 1.0414     | 0.1181       | 0.9123       | 0.045*     |
| C15 | 1.1036 (3) | 0.2395 (2)   | 0.43694 (17) | 0.0458 (7) |
| H15 | 1.1394     | 0.2789       | 0.3909       | 0.055*     |
| C26 | 0.7889 (3) | 0.1523 (2)   | 1.05210 (15) | 0.0429 (7) |
| H26 | 0.7691     | 0.1555       | 1.1069       | 0.052*     |
| C4  | 0.4513 (3) | 0.5879 (3)   | 0.86398 (17) | 0.0418 (7) |
| H4  | 0.3716     | 0.6261       | 0.8910       | 0.050*     |
| C49 | 0.8019 (3) | -0.3480 (3)  | 1.06404 (17) | 0.0470 (8) |
| H49 | 0.8306     | -0.3875      | 1.1086       | 0.056*     |
| C27 | 0.9215 (3) | 0.1361 (3)   | 1.01663 (16) | 0.0466 (8) |
| H27 | 0.9928     | 0.1288       | 1.0470       | 0.056*     |
| C7  | 0.9154 (2) | 0.3793 (2)   | 0.79127 (14) | 0.0278 (6) |
| H7A | 0.8779     | 0.3754       | 0.8470       | 0.033*     |
| H7B | 0.9804     | 0.4362       | 0.7835       | 0.033*     |
| C50 | 0.8220 (3) | -0.3990 (3)  | 0.99378 (18) | 0.0480 (8) |
| H50 | 0.8652     | -0.4738      | 0.9898       | 0.058*     |

Atomic displacement parameters ( $\text{\AA}^2$ )

|     | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$     | $U^{13}$     | $U^{23}$     |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Pd1 | 0.02037 (11) | 0.02645 (12) | 0.01626 (11) | -0.00308 (7) | -0.00279 (7) | 0.00024 (8)  |
| P1  | 0.0207 (3)   | 0.0243 (3)   | 0.0169 (3)   | -0.0005 (3)  | -0.0029 (3)  | -0.0006 (3)  |
| P2  | 0.0220 (3)   | 0.0262 (3)   | 0.0169 (3)   | -0.0021 (3)  | -0.0027 (3)  | 0.0001 (3)   |
| O1  | 0.0411 (11)  | 0.0346 (10)  | 0.0253 (9)   | -0.0077 (8)  | -0.0074 (8)  | -0.0081 (8)  |
| N1  | 0.0286 (11)  | 0.0254 (11)  | 0.0192 (10)  | -0.0001 (9)  | -0.0063 (9)  | -0.0012 (9)  |
| C29 | 0.0251 (13)  | 0.0285 (13)  | 0.0142 (11)  | 0.0001 (10)  | -0.0012 (10) | 0.0011 (10)  |
| C17 | 0.0196 (12)  | 0.0300 (13)  | 0.0130 (11)  | -0.0008 (10) | 0.0011 (9)   | -0.0024 (10) |
| C45 | 0.0286 (14)  | 0.0335 (14)  | 0.0238 (13)  | -0.0092 (11) | -0.0025 (11) | -0.0020 (12) |
| C10 | 0.0297 (13)  | 0.0235 (12)  | 0.0207 (12)  | -0.0010 (10) | -0.0043 (11) | -0.0012 (11) |
| C21 | 0.0321 (14)  | 0.0298 (14)  | 0.0247 (13)  | 0.0024 (11)  | -0.0105 (11) | 0.0009 (11)  |
| C44 | 0.0264 (13)  | 0.0326 (14)  | 0.0218 (13)  | -0.0089 (11) | -0.0008 (11) | -0.0017 (11) |
| C36 | 0.0304 (14)  | 0.0399 (15)  | 0.0263 (14)  | -0.0104 (12) | -0.0100 (11) | 0.0015 (12)  |
| C22 | 0.0255 (13)  | 0.0255 (13)  | 0.0224 (13)  | -0.0009 (10) | -0.0038 (10) | -0.0010 (11) |
| C11 | 0.0207 (12)  | 0.0262 (13)  | 0.0199 (12)  | -0.0024 (10) | -0.0024 (10) | -0.0020 (11) |
| C24 | 0.0321 (14)  | 0.0278 (14)  | 0.0238 (13)  | -0.0062 (11) | -0.0028 (11) | -0.0026 (11) |
| C12 | 0.0330 (14)  | 0.0323 (14)  | 0.0167 (12)  | 0.0013 (11)  | -0.0039 (11) | 0.0004 (11)  |
| C19 | 0.0296 (14)  | 0.0285 (14)  | 0.0233 (13)  | -0.0056 (11) | -0.0001 (11) | -0.0077 (11) |
| C35 | 0.0184 (12)  | 0.0373 (15)  | 0.0212 (13)  | -0.0088 (11) | -0.0010 (10) | -0.0003 (11) |

## supplementary materials

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|     |             |             |             |              |              |              |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C6  | 0.0307 (14) | 0.0266 (13) | 0.0268 (13) | -0.0025 (11) | -0.0099 (11) | -0.0061 (11) |
| C46 | 0.0264 (14) | 0.0333 (15) | 0.0304 (14) | -0.0056 (11) | -0.0074 (11) | -0.0009 (12) |
| C23 | 0.0320 (14) | 0.0230 (13) | 0.0200 (12) | -0.0022 (10) | -0.0032 (11) | -0.0011 (10) |
| C40 | 0.0218 (13) | 0.0491 (17) | 0.0231 (13) | -0.0031 (12) | -0.0015 (11) | -0.0046 (12) |
| C20 | 0.0271 (14) | 0.0418 (16) | 0.0191 (13) | -0.0054 (12) | -0.0041 (11) | -0.0029 (12) |
| C47 | 0.0289 (15) | 0.0452 (16) | 0.0321 (15) | 0.0001 (12)  | -0.0044 (12) | -0.0042 (13) |
| C14 | 0.0276 (14) | 0.0355 (15) | 0.0393 (16) | 0.0011 (12)  | 0.0033 (12)  | -0.0079 (14) |
| C30 | 0.0267 (14) | 0.0354 (14) | 0.0282 (14) | -0.0022 (11) | -0.0069 (11) | -0.0056 (12) |
| C32 | 0.0350 (16) | 0.0336 (15) | 0.0400 (16) | 0.0063 (12)  | -0.0005 (13) | -0.0055 (13) |
| C31 | 0.0224 (13) | 0.0487 (17) | 0.0292 (14) | 0.0012 (12)  | -0.0045 (11) | -0.0033 (13) |
| C38 | 0.0275 (15) | 0.0439 (17) | 0.0426 (17) | -0.0050 (12) | -0.0043 (13) | 0.0129 (14)  |
| C18 | 0.0252 (13) | 0.0255 (13) | 0.0185 (12) | 0.0020 (10)  | 0.0004 (10)  | -0.0014 (11) |
| C51 | 0.0532 (18) | 0.0347 (16) | 0.0390 (17) | -0.0075 (13) | -0.0161 (14) | -0.0035 (14) |
| C9  | 0.0298 (14) | 0.0262 (13) | 0.0242 (13) | -0.0014 (11) | -0.0063 (11) | -0.0009 (11) |
| C5  | 0.0410 (17) | 0.0329 (15) | 0.0388 (17) | 0.0034 (12)  | -0.0155 (14) | -0.0110 (13) |
| C48 | 0.0334 (16) | 0.064 (2)   | 0.0289 (15) | -0.0039 (14) | -0.0077 (13) | -0.0063 (15) |
| C2  | 0.0357 (15) | 0.0301 (14) | 0.0251 (14) | -0.0070 (12) | -0.0060 (12) | -0.0045 (12) |
| C42 | 0.0239 (13) | 0.0326 (14) | 0.0216 (13) | -0.0094 (11) | -0.0050 (10) | -0.0032 (11) |
| C16 | 0.0399 (16) | 0.0346 (15) | 0.0378 (16) | 0.0046 (13)  | 0.0091 (13)  | 0.0122 (13)  |
| C43 | 0.0196 (12) | 0.0339 (14) | 0.0249 (13) | -0.0117 (11) | -0.0011 (10) | 0.0004 (12)  |
| C39 | 0.0235 (14) | 0.0583 (19) | 0.0297 (15) | -0.0045 (13) | -0.0076 (12) | 0.0069 (14)  |
| C13 | 0.0311 (15) | 0.0373 (15) | 0.0305 (15) | 0.0088 (12)  | -0.0027 (12) | -0.0010 (13) |
| C33 | 0.0401 (18) | 0.0304 (16) | 0.080 (2)   | -0.0066 (13) | 0.0052 (16)  | -0.0119 (16) |
| C1  | 0.0273 (13) | 0.0290 (13) | 0.0206 (13) | -0.0033 (11) | -0.0064 (11) | -0.0066 (11) |
| C41 | 0.0189 (12) | 0.0381 (15) | 0.0179 (12) | -0.0067 (11) | -0.0003 (10) | -0.0032 (11) |
| C25 | 0.0453 (17) | 0.0372 (16) | 0.0255 (14) | -0.0087 (13) | 0.0082 (13)  | -0.0058 (13) |
| C37 | 0.0371 (16) | 0.0351 (15) | 0.0427 (17) | -0.0079 (13) | -0.0086 (13) | -0.0027 (13) |
| C34 | 0.0234 (14) | 0.0345 (15) | 0.0563 (19) | -0.0042 (12) | 0.0062 (13)  | -0.0050 (14) |
| C3  | 0.0414 (17) | 0.0514 (18) | 0.0252 (14) | -0.0131 (14) | -0.0038 (13) | -0.0112 (14) |
| C8  | 0.0250 (13) | 0.0283 (13) | 0.0246 (13) | -0.0048 (10) | -0.0067 (11) | 0.0018 (11)  |
| C28 | 0.0375 (16) | 0.0485 (17) | 0.0255 (14) | 0.0040 (13)  | -0.0094 (12) | -0.0016 (13) |
| C15 | 0.0420 (18) | 0.0453 (18) | 0.0413 (17) | -0.0059 (14) | 0.0175 (14)  | 0.0097 (15)  |
| C26 | 0.063 (2)   | 0.0445 (17) | 0.0183 (14) | 0.0002 (15)  | 0.0008 (14)  | -0.0026 (13) |
| C4  | 0.0363 (16) | 0.0512 (19) | 0.0389 (17) | 0.0008 (14)  | -0.0047 (14) | -0.0221 (16) |
| C49 | 0.0449 (18) | 0.062 (2)   | 0.0375 (17) | -0.0124 (16) | -0.0170 (14) | 0.0135 (16)  |
| C27 | 0.058 (2)   | 0.0569 (19) | 0.0270 (15) | 0.0048 (16)  | -0.0193 (15) | -0.0033 (14) |
| C7  | 0.0324 (14) | 0.0273 (13) | 0.0262 (13) | -0.0066 (11) | -0.0091 (11) | -0.0023 (11) |
| C50 | 0.057 (2)   | 0.0389 (17) | 0.052 (2)   | -0.0024 (14) | -0.0248 (16) | 0.0026 (15)  |

### *Geometric parameters (Å, °)*

|         |             |         |           |
|---------|-------------|---------|-----------|
| Pd1—C41 | 2.155 (2)   | C14—C13 | 1.362 (4) |
| Pd1—C42 | 2.170 (2)   | C14—C15 | 1.375 (4) |
| Pd1—P1  | 2.3068 (10) | C14—H14 | 0.9500    |
| Pd1—P2  | 2.3441 (9)  | C30—C31 | 1.390 (3) |
| P1—C10  | 1.836 (2)   | C30—H30 | 0.9500    |
| P1—C17  | 1.837 (2)   | C32—C31 | 1.366 (4) |
| P1—C11  | 1.837 (2)   | C32—C33 | 1.374 (4) |
| P2—C29  | 1.835 (2)   | C32—H32 | 0.9500    |



|             |           |             |           |
|-------------|-----------|-------------|-----------|
| P2—C8       | 1.840 (2) | C31—H31     | 0.9500    |
| P2—C23      | 1.844 (2) | C38—C37     | 1.382 (4) |
| O1—C43      | 1.242 (3) | C38—C39     | 1.384 (4) |
| N1—C1       | 1.411 (3) | C38—H38     | 0.9500    |
| N1—C9       | 1.457 (3) | C18—H18     | 0.9500    |
| N1—C7       | 1.460 (3) | C51—C50     | 1.376 (4) |
| C29—C34     | 1.379 (3) | C51—H51     | 0.9500    |
| C29—C30     | 1.399 (3) | C9—H9A      | 0.9900    |
| C17—C22     | 1.381 (3) | C9—H9B      | 0.9900    |
| C17—C18     | 1.395 (3) | C5—C4       | 1.375 (4) |
| C45—C44     | 1.327 (3) | C5—H5       | 0.9500    |
| C45—C46     | 1.459 (3) | C48—C49     | 1.379 (4) |
| C45—H45     | 0.9500    | C48—H48     | 0.9500    |
| C10—C9      | 1.529 (3) | C2—C3       | 1.377 (4) |
| C10—H10A    | 0.9900    | C2—C1       | 1.413 (4) |
| C10—H10B    | 0.9900    | C2—H2       | 0.9500    |
| C21—C20     | 1.382 (3) | C42—C41     | 1.411 (3) |
| C21—C22     | 1.386 (3) | C42—C43     | 1.453 (3) |
| C21—H21     | 0.9500    | C42—H42     | 0.9500    |
| C44—C43     | 1.496 (3) | C16—C15     | 1.394 (4) |
| C44—H44     | 0.9500    | C16—H16     | 0.9500    |
| C36—C37     | 1.382 (4) | C39—H39     | 0.9500    |
| C36—C35     | 1.398 (3) | C13—H13     | 0.9500    |
| C36—H36     | 0.9500    | C33—C34     | 1.384 (4) |
| C22—H22     | 0.9500    | C33—H33     | 0.9500    |
| C11—C12     | 1.380 (3) | C41—H41     | 0.9500    |
| C11—C16     | 1.388 (4) | C25—C26     | 1.382 (4) |
| C24—C23     | 1.376 (3) | C25—H25     | 0.9500    |
| C24—C25     | 1.396 (3) | C37—H37     | 0.9500    |
| C24—H24     | 0.9500    | C34—H34     | 0.9500    |
| C12—C13     | 1.387 (3) | C3—C4       | 1.394 (4) |
| C12—H12     | 0.9500    | C3—H3       | 0.9500    |
| C19—C18     | 1.381 (3) | C8—C7       | 1.533 (3) |
| C19—C20     | 1.384 (3) | C8—H8A      | 0.9900    |
| C19—H19     | 0.9500    | C8—H8B      | 0.9900    |
| C35—C40     | 1.403 (3) | C28—C27     | 1.391 (4) |
| C35—C41     | 1.467 (3) | C28—H28     | 0.9500    |
| C6—C1       | 1.392 (3) | C15—H15     | 0.9500    |
| C6—C5       | 1.392 (3) | C26—C27     | 1.383 (4) |
| C6—H6       | 0.9500    | C26—H26     | 0.9500    |
| C46—C51     | 1.399 (4) | C4—H4       | 0.9500    |
| C46—C47     | 1.401 (3) | C49—C50     | 1.383 (4) |
| C23—C28     | 1.396 (3) | C49—H49     | 0.9500    |
| C40—C39     | 1.380 (4) | C27—H27     | 0.9500    |
| C40—H40     | 0.9500    | C7—H7A      | 0.9900    |
| C20—H20     | 0.9500    | C7—H7B      | 0.9900    |
| C47—C48     | 1.379 (4) | C50—H50     | 0.9500    |
| C47—H47     | 0.9500    |             |           |
| C41—Pd1—C42 | 38.09 (9) | C19—C18—C17 | 120.9 (2) |

## supplementary materials

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|               |             |             |             |
|---------------|-------------|-------------|-------------|
| C41—Pd1—P1    | 99.11 (7)   | C19—C18—H18 | 119.5       |
| C42—Pd1—P1    | 137.21 (7)  | C17—C18—H18 | 119.5       |
| C41—Pd1—P2    | 154.31 (7)  | C50—C51—C46 | 122.1 (3)   |
| C42—Pd1—P2    | 116.24 (7)  | C50—C51—H51 | 119.0       |
| P1—Pd1—P2     | 106.54 (3)  | C46—C51—H51 | 119.0       |
| C10—P1—C17    | 102.49 (11) | N1—C9—C10   | 112.9 (2)   |
| C10—P1—C11    | 104.10 (11) | N1—C9—H9A   | 109.0       |
| C17—P1—C11    | 99.22 (10)  | C10—C9—H9A  | 109.0       |
| C10—P1—Pd1    | 115.73 (8)  | N1—C9—H9B   | 109.0       |
| C17—P1—Pd1    | 115.60 (8)  | C10—C9—H9B  | 109.0       |
| C11—P1—Pd1    | 117.32 (8)  | H9A—C9—H9B  | 107.8       |
| C29—P2—C8     | 102.03 (11) | C4—C5—C6    | 120.8 (3)   |
| C29—P2—C23    | 103.60 (11) | C4—C5—H5    | 119.6       |
| C8—P2—C23     | 99.81 (11)  | C6—C5—H5    | 119.6       |
| C29—P2—Pd1    | 114.30 (8)  | C49—C48—C47 | 120.8 (3)   |
| C8—P2—Pd1     | 116.74 (8)  | C49—C48—H48 | 119.6       |
| C23—P2—Pd1    | 117.99 (8)  | C47—C48—H48 | 119.6       |
| C1—N1—C9      | 117.92 (19) | C3—C2—C1    | 121.2 (3)   |
| C1—N1—C7      | 117.68 (18) | C3—C2—H2    | 119.4       |
| C9—N1—C7      | 113.44 (19) | C1—C2—H2    | 119.4       |
| C34—C29—C30   | 117.9 (2)   | C41—C42—C43 | 120.9 (2)   |
| C34—C29—P2    | 117.35 (18) | C41—C42—Pd1 | 70.40 (14)  |
| C30—C29—P2    | 124.61 (18) | C43—C42—Pd1 | 100.38 (15) |
| C22—C17—C18   | 118.5 (2)   | C41—C42—H42 | 119.5       |
| C22—C17—P1    | 124.97 (17) | C43—C42—H42 | 119.5       |
| C18—C17—P1    | 116.49 (17) | Pd1—C42—H42 | 99.1        |
| C44—C45—C46   | 128.7 (2)   | C11—C16—C15 | 119.8 (3)   |
| C44—C45—H45   | 115.7       | C11—C16—H16 | 120.1       |
| C46—C45—H45   | 115.7       | C15—C16—H16 | 120.1       |
| C9—C10—P1     | 113.19 (17) | O1—C43—C42  | 123.2 (2)   |
| C9—C10—H10A   | 108.9       | O1—C43—C44  | 120.1 (2)   |
| P1—C10—H10A   | 108.9       | C42—C43—C44 | 116.7 (2)   |
| C9—C10—H10B   | 108.9       | C40—C39—C38 | 120.2 (2)   |
| P1—C10—H10B   | 108.9       | C40—C39—H39 | 119.9       |
| H10A—C10—H10B | 107.8       | C38—C39—H39 | 119.9       |
| C20—C21—C22   | 120.4 (2)   | C14—C13—C12 | 120.7 (2)   |
| C20—C21—H21   | 119.8       | C14—C13—H13 | 119.6       |
| C22—C21—H21   | 119.8       | C12—C13—H13 | 119.6       |
| C45—C44—C43   | 121.1 (2)   | C32—C33—C34 | 120.3 (3)   |
| C45—C44—H44   | 119.5       | C32—C33—H33 | 119.9       |
| C43—C44—H44   | 119.5       | C34—C33—H33 | 119.9       |
| C37—C36—C35   | 121.1 (2)   | C6—C1—N1    | 123.7 (2)   |
| C37—C36—H36   | 119.5       | C6—C1—C2    | 117.7 (2)   |
| C35—C36—H36   | 119.5       | N1—C1—C2    | 118.5 (2)   |
| C17—C22—C21   | 120.6 (2)   | C42—C41—C35 | 125.9 (2)   |
| C17—C22—H22   | 119.7       | C42—C41—Pd1 | 71.51 (13)  |
| C21—C22—H22   | 119.7       | C35—C41—Pd1 | 115.32 (16) |
| C12—C11—C16   | 118.8 (2)   | C42—C41—H41 | 117.0       |
| C12—C11—P1    | 117.87 (19) | C35—C41—H41 | 117.0       |

|                |             |                 |             |
|----------------|-------------|-----------------|-------------|
| C16—C11—P1     | 123.10 (19) | Pd1—C41—H41     | 83.0        |
| C23—C24—C25    | 121.2 (2)   | C26—C25—C24     | 119.6 (3)   |
| C23—C24—H24    | 119.4       | C26—C25—H25     | 120.2       |
| C25—C24—H24    | 119.4       | C24—C25—H25     | 120.2       |
| C11—C12—C13    | 120.6 (2)   | C36—C37—C38     | 120.9 (3)   |
| C11—C12—H12    | 119.7       | C36—C37—H37     | 119.6       |
| C13—C12—H12    | 119.7       | C38—C37—H37     | 119.6       |
| C18—C19—C20    | 120.0 (2)   | C29—C34—C33     | 121.0 (2)   |
| C18—C19—H19    | 120.0       | C29—C34—H34     | 119.5       |
| C20—C19—H19    | 120.0       | C33—C34—H34     | 119.5       |
| C36—C35—C40    | 117.1 (2)   | C2—C3—C4        | 120.1 (3)   |
| C36—C35—C41    | 123.2 (2)   | C2—C3—H3        | 120.0       |
| C40—C35—C41    | 119.7 (2)   | C4—C3—H3        | 120.0       |
| C1—C6—C5       | 120.8 (2)   | C7—C8—P2        | 113.37 (17) |
| C1—C6—H6       | 119.6       | C7—C8—H8A       | 108.9       |
| C5—C6—H6       | 119.6       | P2—C8—H8A       | 108.9       |
| C51—C46—C47    | 116.9 (2)   | C7—C8—H8B       | 108.9       |
| C51—C46—C45    | 119.1 (2)   | P2—C8—H8B       | 108.9       |
| C47—C46—C45    | 124.1 (2)   | H8A—C8—H8B      | 107.7       |
| C24—C23—C28    | 118.7 (2)   | C27—C28—C23     | 120.5 (3)   |
| C24—C23—P2     | 119.91 (18) | C27—C28—H28     | 119.7       |
| C28—C23—P2     | 121.23 (19) | C23—C28—H28     | 119.7       |
| C39—C40—C35    | 121.7 (2)   | C14—C15—C16     | 120.8 (3)   |
| C39—C40—H40    | 119.2       | C14—C15—H15     | 119.6       |
| C35—C40—H40    | 119.2       | C16—C15—H15     | 119.6       |
| C21—C20—C19    | 119.4 (2)   | C25—C26—C27     | 120.0 (2)   |
| C21—C20—H20    | 120.3       | C25—C26—H26     | 120.0       |
| C19—C20—H20    | 120.3       | C27—C26—H26     | 120.0       |
| C48—C47—C46    | 121.1 (2)   | C5—C4—C3        | 119.5 (3)   |
| C48—C47—H47    | 119.5       | C5—C4—H4        | 120.2       |
| C46—C47—H47    | 119.5       | C3—C4—H4        | 120.2       |
| C13—C14—C15    | 119.3 (2)   | C48—C49—C50     | 119.4 (3)   |
| C13—C14—H14    | 120.3       | C48—C49—H49     | 120.3       |
| C15—C14—H14    | 120.3       | C50—C49—H49     | 120.3       |
| C31—C30—C29    | 120.6 (2)   | C26—C27—C28     | 120.0 (3)   |
| C31—C30—H30    | 119.7       | C26—C27—H27     | 120.0       |
| C29—C30—H30    | 119.7       | C28—C27—H27     | 120.0       |
| C31—C32—C33    | 119.9 (2)   | N1—C7—C8        | 113.58 (18) |
| C31—C32—H32    | 120.0       | N1—C7—H7A       | 108.9       |
| C33—C32—H32    | 120.0       | C8—C7—H7A       | 108.9       |
| C32—C31—C30    | 120.2 (2)   | N1—C7—H7B       | 108.9       |
| C32—C31—H31    | 119.9       | C8—C7—H7B       | 108.9       |
| C30—C31—H31    | 119.9       | H7A—C7—H7B      | 107.7       |
| C37—C38—C39    | 119.1 (3)   | C51—C50—C49     | 119.8 (3)   |
| C37—C38—H38    | 120.4       | C51—C50—H50     | 120.1       |
| C39—C38—H38    | 120.4       | C49—C50—H50     | 120.1       |
| C41—Pd1—P1—C10 | 102.55 (11) | C47—C46—C51—C50 | 0.1 (4)     |
| C42—Pd1—P1—C10 | 102.35 (13) | C45—C46—C51—C50 | 179.9 (3)   |
| P2—Pd1—P1—C10  | -76.02 (9)  | C1—N1—C9—C10    | -71.2 (3)   |

## supplementary materials

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|                 |              |                 |              |
|-----------------|--------------|-----------------|--------------|
| C41—Pd1—P1—C17  | -17.26 (10)  | C7—N1—C9—C10    | 145.40 (19)  |
| C42—Pd1—P1—C17  | -17.46 (12)  | P1—C10—C9—N1    | -67.7 (2)    |
| P2—Pd1—P1—C17   | 164.17 (8)   | C1—C6—C5—C4     | 0.2 (4)      |
| C41—Pd1—P1—C11  | -133.85 (10) | C46—C47—C48—C49 | 1.1 (4)      |
| C42—Pd1—P1—C11  | -134.05 (12) | P1—Pd1—C42—C41  | 0.32 (18)    |
| P2—Pd1—P1—C11   | 47.59 (8)    | P2—Pd1—C42—C41  | 178.58 (11)  |
| C41—Pd1—P2—C29  | 93.86 (17)   | C41—Pd1—C42—C43 | 119.3 (2)    |
| C42—Pd1—P2—C29  | 91.83 (11)   | P1—Pd1—C42—C43  | 119.61 (14)  |
| P1—Pd1—P2—C29   | -89.40 (9)   | P2—Pd1—C42—C43  | -62.14 (15)  |
| C41—Pd1—P2—C8   | -147.22 (16) | C12—C11—C16—C15 | 0.4 (4)      |
| C42—Pd1—P2—C8   | -149.25 (11) | P1—C11—C16—C15  | -173.9 (2)   |
| P1—Pd1—P2—C8    | 29.51 (9)    | C41—C42—C43—O1  | -2.2 (4)     |
| C41—Pd1—P2—C23  | -28.29 (17)  | Pd1—C42—C43—O1  | -75.5 (2)    |
| C42—Pd1—P2—C23  | -30.32 (11)  | C41—C42—C43—C44 | 176.4 (2)    |
| P1—Pd1—P2—C23   | 148.44 (9)   | Pd1—C42—C43—C44 | 103.1 (2)    |
| C8—P2—C29—C34   | -166.8 (2)   | C45—C44—C43—O1  | 6.6 (4)      |
| C23—P2—C29—C34  | 89.9 (2)     | C45—C44—C43—C42 | -172.0 (2)   |
| Pd1—P2—C29—C34  | -39.8 (2)    | C35—C40—C39—C38 | 0.0 (4)      |
| C8—P2—C29—C30   | 9.7 (2)      | C37—C38—C39—C40 | 0.2 (4)      |
| C23—P2—C29—C30  | -93.6 (2)    | C15—C14—C13—C12 | 1.4 (4)      |
| Pd1—P2—C29—C30  | 136.65 (19)  | C11—C12—C13—C14 | -0.9 (4)     |
| C10—P1—C17—C22  | 6.0 (2)      | C31—C32—C33—C34 | 1.7 (5)      |
| C11—P1—C17—C22  | -100.8 (2)   | C5—C6—C1—N1     | 177.7 (2)    |
| Pd1—P1—C17—C22  | 132.78 (18)  | C5—C6—C1—C2     | 0.5 (3)      |
| C10—P1—C17—C18  | -175.49 (17) | C9—N1—C1—C6     | -9.6 (3)     |
| C11—P1—C17—C18  | 77.73 (19)   | C7—N1—C1—C6     | 132.3 (2)    |
| Pd1—P1—C17—C18  | -48.67 (19)  | C9—N1—C1—C2     | 167.6 (2)    |
| C17—P1—C10—C9   | -174.41 (17) | C7—N1—C1—C2     | -50.6 (3)    |
| C11—P1—C10—C9   | -71.42 (19)  | C3—C2—C1—C6     | -0.3 (3)     |
| Pd1—P1—C10—C9   | 58.86 (19)   | C3—C2—C1—N1     | -177.7 (2)   |
| C46—C45—C44—C43 | 177.5 (2)    | C43—C42—C41—C35 | 161.1 (2)    |
| C18—C17—C22—C21 | -0.9 (3)     | Pd1—C42—C41—C35 | -108.3 (2)   |
| P1—C17—C22—C21  | 177.59 (18)  | C43—C42—C41—Pd1 | -90.6 (2)    |
| C20—C21—C22—C17 | 1.4 (4)      | C36—C35—C41—C42 | 34.9 (4)     |
| C10—P1—C11—C12  | 137.82 (18)  | C40—C35—C41—C42 | -146.5 (2)   |
| C17—P1—C11—C12  | -116.71 (19) | C36—C35—C41—Pd1 | -49.9 (3)    |
| Pd1—P1—C11—C12  | 8.5 (2)      | C40—C35—C41—Pd1 | 128.7 (2)    |
| C10—P1—C11—C16  | -47.8 (2)    | P1—Pd1—C41—C42  | -179.78 (12) |
| C17—P1—C11—C16  | 57.6 (2)     | P2—Pd1—C41—C42  | -2.9 (2)     |
| Pd1—P1—C11—C16  | -177.17 (18) | C42—Pd1—C41—C35 | 121.7 (2)    |
| C16—C11—C12—C13 | 0.0 (3)      | P1—Pd1—C41—C35  | -58.05 (17)  |
| P1—C11—C12—C13  | 174.56 (18)  | P2—Pd1—C41—C35  | 118.79 (18)  |
| C37—C36—C35—C40 | -0.4 (4)     | C23—C24—C25—C26 | -0.2 (4)     |
| C37—C36—C35—C41 | 178.2 (2)    | C35—C36—C37—C38 | 0.7 (4)      |
| C44—C45—C46—C51 | 177.1 (3)    | C39—C38—C37—C36 | -0.6 (4)     |
| C44—C45—C46—C47 | -3.1 (4)     | C30—C29—C34—C33 | 2.6 (4)      |
| C25—C24—C23—C28 | 0.7 (4)      | P2—C29—C34—C33  | 179.3 (2)    |
| C25—C24—C23—P2  | -174.62 (19) | C32—C33—C34—C29 | -3.2 (5)     |
| C29—P2—C23—C24  | -133.7 (2)   | C1—C2—C3—C4     | -0.5 (4)     |

|                 |              |                 |              |
|-----------------|--------------|-----------------|--------------|
| C8—P2—C23—C24   | 121.2 (2)    | C29—P2—C8—C7    | -174.39 (16) |
| Pd1—P2—C23—C24  | -6.3 (2)     | C23—P2—C8—C7    | -68.07 (18)  |
| C29—P2—C23—C28  | 51.0 (2)     | Pd1—P2—C8—C7    | 60.27 (18)   |
| C8—P2—C23—C28   | -54.0 (2)    | C24—C23—C28—C27 | -1.2 (4)     |
| Pd1—P2—C23—C28  | 178.47 (18)  | P2—C23—C28—C27  | 174.1 (2)    |
| C36—C35—C40—C39 | 0.0 (4)      | C13—C14—C15—C16 | -1.0 (4)     |
| C41—C35—C40—C39 | -178.7 (2)   | C11—C16—C15—C14 | 0.1 (4)      |
| C22—C21—C20—C19 | -1.5 (4)     | C24—C25—C26—C27 | 0.1 (4)      |
| C18—C19—C20—C21 | 1.1 (4)      | C6—C5—C4—C3     | -1.1 (4)     |
| C51—C46—C47—C48 | -0.9 (4)     | C2—C3—C4—C5     | 1.3 (4)      |
| C45—C46—C47—C48 | 179.3 (2)    | C47—C48—C49—C50 | -0.4 (4)     |
| C34—C29—C30—C31 | -0.5 (4)     | C25—C26—C27—C28 | -0.5 (4)     |
| P2—C29—C30—C31  | -176.98 (19) | C23—C28—C27—C26 | 1.1 (4)      |
| C33—C32—C31—C30 | 0.4 (4)      | C1—N1—C7—C8     | 144.8 (2)    |
| C29—C30—C31—C32 | -1.0 (4)     | C9—N1—C7—C8     | -71.7 (3)    |
| C20—C19—C18—C17 | -0.7 (3)     | P2—C8—C7—N1     | -60.7 (2)    |
| C22—C17—C18—C19 | 0.6 (3)      | C46—C51—C50—C49 | 0.5 (5)      |
| P1—C17—C18—C19  | -178.07 (18) | C48—C49—C50—C51 | -0.4 (5)     |

Fig. 1

