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P,P-Diphenyl-*N*-(1,1,2,2-tetraphenyl-1 λ^5 -diphosphanlydene)phosphinous amide

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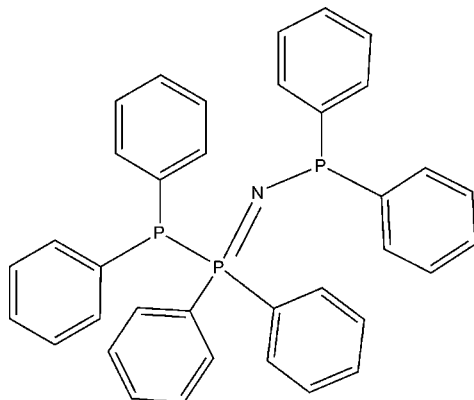
Received 23 June 2008; accepted 2 July 2008

 Key indicators: single-crystal X-ray study; $T = 228$ K; mean $\sigma(C-C) = 0.002$ Å; R factor = 0.042; wR factor = 0.118; data-to-parameter ratio = 23.9.

The title compound, $C_{36}H_{30}NP_3$, a structural isomer of tris(diphenylphosphino)amine, was unexpectedly isolated as the sole phosphorus-containing product from the reaction of $Mg[N(PPh_2)_2]_2(THF)_2$ (THF is tetrahydrofuran) with CO_2 . Its identity was confirmed by ^{31}P NMR spectroscopy and single-crystal X-ray diffraction. The geometry at the two P(III) atoms is trigonal pyramidal, while the P(V) atom adopts a distorted tetrahedral geometry.

Related literature

For the original synthesis and spectroscopic characterization of the title compound, see: Nöth & Meinel (1967); Meinel & Nöth (1970). For the crystallographic characterization of the structural isomer $N[P(C_6H_5)_2]_3$, see: Ellermann *et al.* (1987). For related literature, see: Bruno *et al.* (2004).



Experimental

Crystal data

| | |
|-----------------------|-----------------------------------|
| $C_{36}H_{30}NP_3$ | $V = 2960.0$ (7) Å ³ |
| $M_r = 569.52$ | $Z = 4$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation |
| $a = 9.3026$ (13) Å | $\mu = 0.23$ mm ⁻¹ |
| $b = 10.8167$ (15) Å | $T = 228$ (2) K |
| $c = 29.750$ (4) Å | $0.57 \times 0.51 \times 0.18$ mm |
| $\beta = 98.589$ (6)° | |

Data collection

| | |
|--|--|
| Bruker SMART CCD area-detector diffractometer | 76797 measured reflections |
| Absorption correction: multi-scan (SADABS; Bruker, 2001) | 11496 independent reflections |
| $T_{min} = 0.88$, $T_{max} = 0.96$ | 9167 reflections with $I > 2\sigma(I)$ |
| | $R_{int} = 0.029$ |

Refinement

| | |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.042$ | 481 parameters |
| $wR(F^2) = 0.118$ | All H-atom parameters refined |
| $S = 1.05$ | $\Delta\rho_{max} = 0.41$ e Å ⁻³ |
| 11496 reflections | $\Delta\rho_{min} = -0.29$ e Å ⁻³ |

Data collection: SMART (Bruker, 2003); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 1999); software used to prepare material for publication: publCIF (Westrip, 2008).

The authors thank Eileen Duesler (UNM) for the X-ray data collection. Funding was provided by the Natural Sciences and Engineering Research Council of Canada (NSERC PDF to DAD), the National Science Foundation (grant Nos. CHE-0213165 and CHE-0443580) and the Sandia LDRD Program (grant Nos. 105932 and 113486). Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract No. DE-AC04-94AL85000.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2581).

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supporting information

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***P,P*-Diphenyl-*N*-(1,1,2,2-tetraphenyl-1 λ^5 -diphosphanilidene)phosphinous amide**

Diane A. Dickie and Richard A. Kemp

S1. Comment

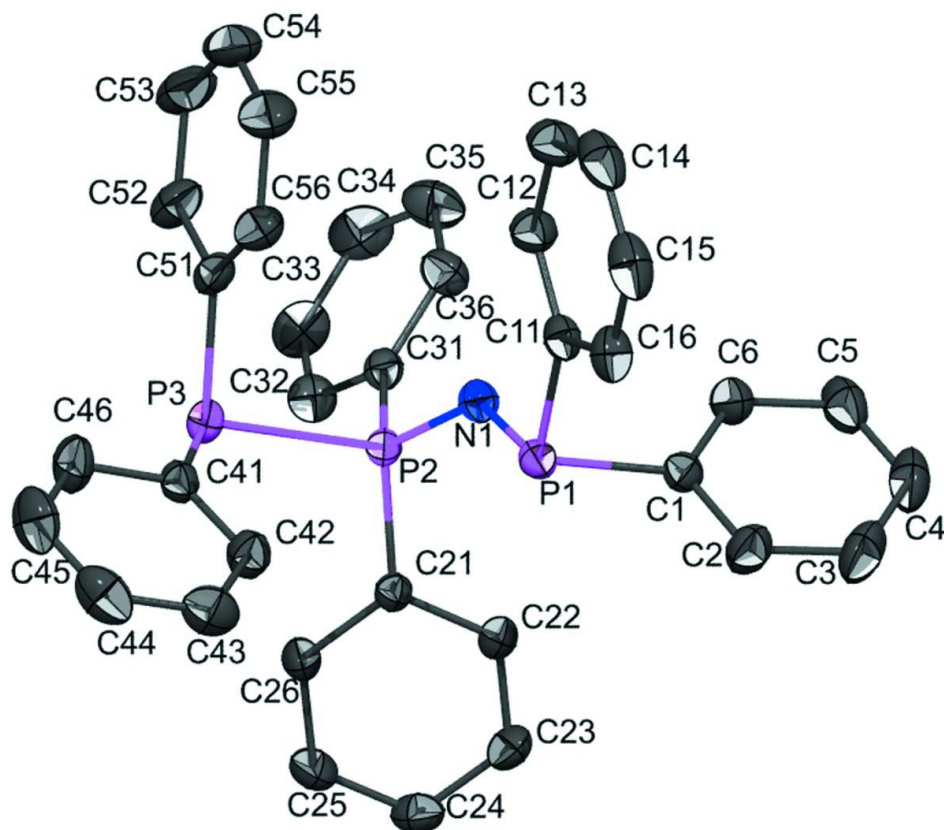
The molecular structure of the title compound, (I), is shown in Fig. 1. It was originally prepared by Nöth and Meinel [Nöth & Meinel (1967); and Meinel & Nöth (1970)] but its crystal structure was not determined at that time. We report herein the isolation of (I) as an unexpected product of the reaction of carbon dioxide with $\text{Mg}[\text{N}(\text{PPh}_2)_2](\text{THF})_2$. This compound was characterized by ^{31}P NMR spectroscopy and single-crystal X-ray diffraction. The $\text{P}=\text{N}$ double bond measures 1.5690 (10) Å, very close to the average value of similar bonds in a *Mogul* (Bruno *et al.*, 2004) search of the Cambridge structural database (mean $\text{P}=\text{N}$ 1.573 Å). The $\text{P}-\text{N}$ single bond of 1.6755 (11) Å is significantly shorter than those in the structural isomer $\text{N}(\text{PPh}_2)_3$ (Ellermann, *et al.* 1987) (mean $\text{P}-\text{N}$ = 1.740 Å), which is not surprising when the different hybridization of nitrogen (sp^2 versus sp^3) is considered. It is also, however, shorter than the average $\text{P}-\text{N}(sp^2)$ bond length of 1.706 Å. The geometry at each of the two P(III) atoms is trigonal pyramidal, due to the stereochemically active lone pair on each of these atoms. The P(V) atom adopts distorted tetrahedral geometry.

S2. Experimental

Under an inert argon atmosphere, $\text{Mg}[\text{N}(\text{PPh}_2)_2](\text{THF})_2$ (0.67 g, 0.72 mmol) was dissolved in 40 ml anhydrous THF. The solution was exposed to 2 eq. of carbon dioxide at 10 psig. After 16 h, the solution was purged with argon. Colourless crystals of the title compound crystallized from the solution over the course of two weeks. $^{31}\text{P}\{^1\text{H}\}$ NMR (101.255 MHz, THF) δ 41.5 (d, $^2J_{\text{PP}} = 97$ Hz, $\text{Ph}_2\text{P}-\text{N}$), 17.8 (d of d, $^2J_{\text{PP}} = 97$ Hz, $^1J_{\text{PP}} = 249$ Hz, $\text{N}=\text{PPh}_2$), -9.4 (d, $^1J_{\text{PP}} = 249$ Hz, $\text{P}-\text{PPh}_2$) p.p.m..

S3. Refinement

H atoms were located from a difference Fourier map and refined isotropically.

**Figure 1**

View of the title compound showing full numbering scheme. Ellipsoids are shown at 50% probability and hydrogen atoms have been removed for clarity.

P,P-Diphenyl-*N*-(1,1,2,2-tetraphenyl-1 λ^5 -diphosphanylidene)phosphinous amide

Crystal data

$C_{36}H_{30}NP_3$

$M_r = 569.52$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1/n$

$a = 9.3026$ (13) Å

$b = 10.8167$ (15) Å

$c = 29.750$ (4) Å

$\beta = 98.589$ (6)°

$V = 2960.0$ (7) Å³

$Z = 4$

$F(000) = 1192$

$D_x = 1.278$ Mg m⁻³

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

Cell parameters from 9384 reflections

$\theta = 2.3$ – 33.2 °

$\mu = 0.23$ mm⁻¹

$T = 228$ K

Square, colourless

$0.58 \times 0.51 \times 0.18$ mm

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2001)

$T_{\min} = 0.88$, $T_{\max} = 0.96$

76797 measured reflections

11496 independent reflections

9167 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 33.5$ °, $\theta_{\min} = 2.4$ °

$h = -14 \rightarrow 14$

$k = -16 \rightarrow 16$

$l = -45 \rightarrow 45$

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.042$ | All H-atom parameters refined |
| $wR(F^2) = 0.118$ | $w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 1.05P]$ |
| $S = 1.06$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 11496 reflections | $(\Delta/\sigma)_{\max} = 0.001$ |
| 481 parameters | $\Delta\rho_{\max} = 0.41 \text{ e } \text{\AA}^{-3}$ |
| 0 restraints | $\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | |

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)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|---------------|----------------------------------|
| N1 | 0.89827 (12) | 0.55872 (10) | 0.13502 (4) | 0.0285 (2) |
| P1 | 0.83490 (3) | 0.52397 (3) | 0.080793 (10) | 0.02539 (7) |
| P2 | 0.98888 (3) | 0.67406 (3) | 0.154676 (10) | 0.02169 (6) |
| P3 | 0.88674 (3) | 0.85071 (3) | 0.171889 (11) | 0.02562 (7) |
| C1 | 0.92572 (12) | 0.37613 (11) | 0.07254 (4) | 0.0265 (2) |
| C2 | 0.94010 (18) | 0.34039 (15) | 0.02865 (5) | 0.0398 (3) |
| H2 | 0.915 (2) | 0.396 (2) | 0.0046 (7) | 0.052 (5)* |
| C3 | 0.9911 (2) | 0.22253 (18) | 0.02040 (7) | 0.0533 (4) |
| H3 | 0.998 (3) | 0.200 (2) | -0.0104 (8) | 0.067 (7)* |
| C4 | 1.03047 (18) | 0.14200 (15) | 0.05566 (7) | 0.0494 (4) |
| H4 | 1.062 (2) | 0.061 (2) | 0.0493 (7) | 0.064 (6)* |
| C5 | 1.02013 (17) | 0.17767 (14) | 0.09955 (7) | 0.0433 (3) |
| H5 | 1.045 (2) | 0.120 (2) | 0.1238 (7) | 0.059 (6)* |
| C6 | 0.96912 (15) | 0.29430 (13) | 0.10817 (5) | 0.0344 (3) |
| H6 | 0.958 (2) | 0.3171 (19) | 0.1389 (7) | 0.053 (6)* |
| C11 | 0.65810 (12) | 0.45178 (11) | 0.08595 (4) | 0.0270 (2) |
| C12 | 0.60725 (15) | 0.43744 (13) | 0.12725 (5) | 0.0339 (3) |
| H12 | 0.661 (2) | 0.4670 (17) | 0.1541 (6) | 0.039 (5)* |
| C13 | 0.47230 (17) | 0.38278 (15) | 0.12874 (6) | 0.0444 (3) |
| H13 | 0.437 (2) | 0.380 (2) | 0.1578 (7) | 0.055 (6)* |
| C14 | 0.38678 (16) | 0.34312 (14) | 0.08938 (7) | 0.0468 (4) |
| H14 | 0.297 (2) | 0.306 (2) | 0.0912 (7) | 0.063 (6)* |
| C15 | 0.43625 (16) | 0.35656 (14) | 0.04816 (7) | 0.0439 (4) |
| H15 | 0.378 (2) | 0.332 (2) | 0.0199 (7) | 0.062 (6)* |
| C16 | 0.57122 (15) | 0.41024 (13) | 0.04646 (5) | 0.0349 (3) |

| | | | | |
|-----|--------------|--------------|-------------|--------------|
| H16 | 0.6072 (19) | 0.4179 (17) | 0.0181 (6) | 0.037 (4)* |
| C21 | 1.13511 (12) | 0.72160 (10) | 0.12433 (4) | 0.02325 (19) |
| C22 | 1.20846 (14) | 0.63055 (12) | 0.10377 (5) | 0.0318 (2) |
| H22 | 1.180 (2) | 0.5479 (18) | 0.1056 (6) | 0.045 (5)* |
| C23 | 1.32338 (15) | 0.66224 (14) | 0.08106 (5) | 0.0371 (3) |
| H23 | 1.372 (2) | 0.597 (2) | 0.0673 (7) | 0.057 (6)* |
| C24 | 1.36496 (15) | 0.78400 (14) | 0.07826 (5) | 0.0358 (3) |
| H24 | 1.448 (2) | 0.8079 (19) | 0.0628 (6) | 0.049 (5)* |
| C25 | 1.29177 (17) | 0.87515 (14) | 0.09808 (6) | 0.0420 (3) |
| H25 | 1.318 (2) | 0.957 (2) | 0.0961 (7) | 0.061 (6)* |
| C26 | 1.17755 (16) | 0.84426 (12) | 0.12116 (6) | 0.0371 (3) |
| H26 | 1.132 (2) | 0.909 (2) | 0.1355 (7) | 0.055 (6)* |
| C31 | 1.06971 (12) | 0.63888 (11) | 0.21231 (4) | 0.0256 (2) |
| C32 | 1.16599 (14) | 0.72246 (13) | 0.23711 (5) | 0.0326 (2) |
| H32 | 1.197 (2) | 0.7950 (18) | 0.2228 (6) | 0.042 (5)* |
| C33 | 1.21154 (17) | 0.70324 (17) | 0.28318 (5) | 0.0419 (3) |
| H33 | 1.277 (2) | 0.7602 (18) | 0.2992 (6) | 0.045 (5)* |
| C34 | 1.16275 (19) | 0.60144 (19) | 0.30440 (5) | 0.0488 (4) |
| H34 | 1.191 (2) | 0.587 (2) | 0.3358 (7) | 0.056 (6)* |
| C35 | 1.0706 (2) | 0.51676 (18) | 0.27995 (6) | 0.0491 (4) |
| H35 | 1.041 (2) | 0.449 (2) | 0.2946 (7) | 0.061 (6)* |
| C36 | 1.02326 (16) | 0.53572 (13) | 0.23390 (5) | 0.0362 (3) |
| H36 | 0.953 (2) | 0.4794 (18) | 0.2163 (6) | 0.047 (5)* |
| C41 | 0.77800 (13) | 0.90632 (11) | 0.11987 (4) | 0.0268 (2) |
| C42 | 0.78720 (15) | 0.86532 (13) | 0.07605 (5) | 0.0334 (3) |
| H42 | 0.842 (2) | 0.7942 (18) | 0.0716 (6) | 0.041 (5)* |
| C43 | 0.71842 (18) | 0.93088 (16) | 0.03862 (5) | 0.0420 (3) |
| H43 | 0.727 (2) | 0.9039 (19) | 0.0095 (7) | 0.052 (5)* |
| C44 | 0.64070 (18) | 1.03665 (16) | 0.04451 (6) | 0.0470 (4) |
| H44 | 0.597 (2) | 1.082 (2) | 0.0194 (7) | 0.058 (6)* |
| C45 | 0.6267 (2) | 1.07566 (16) | 0.08773 (7) | 0.0506 (4) |
| H45 | 0.578 (3) | 1.150 (2) | 0.0926 (8) | 0.070 (7)* |
| C46 | 0.69448 (17) | 1.01113 (14) | 0.12517 (6) | 0.0406 (3) |
| H46 | 0.684 (3) | 1.038 (2) | 0.1553 (8) | 0.069 (7)* |
| C51 | 0.75546 (14) | 0.78245 (12) | 0.20420 (4) | 0.0296 (2) |
| C52 | 0.78649 (17) | 0.79087 (16) | 0.25158 (5) | 0.0407 (3) |
| H52 | 0.878 (3) | 0.839 (2) | 0.2671 (8) | 0.067 (7)* |
| C53 | 0.6955 (2) | 0.73483 (19) | 0.27841 (6) | 0.0523 (4) |
| H53 | 0.719 (3) | 0.744 (2) | 0.3110 (8) | 0.073 (7)* |
| C54 | 0.5732 (2) | 0.67193 (19) | 0.25838 (7) | 0.0581 (5) |
| H54 | 0.512 (3) | 0.633 (2) | 0.2772 (8) | 0.071 (7)* |
| C55 | 0.5397 (2) | 0.66580 (18) | 0.21142 (7) | 0.0523 (4) |
| H55 | 0.460 (2) | 0.623 (2) | 0.1988 (7) | 0.058 (6)* |
| C56 | 0.63044 (15) | 0.72019 (14) | 0.18414 (5) | 0.0375 (3) |
| H56 | 0.608 (2) | 0.7168 (18) | 0.1505 (6) | 0.044 (5)* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|---------------|--------------|---------------|
| N1 | 0.0314 (5) | 0.0258 (4) | 0.0285 (5) | -0.0062 (4) | 0.0052 (4) | -0.0046 (4) |
| P1 | 0.02921 (14) | 0.02131 (13) | 0.02575 (14) | -0.00134 (10) | 0.00446 (11) | 0.00031 (10) |
| P2 | 0.02190 (12) | 0.01984 (12) | 0.02357 (13) | 0.00031 (9) | 0.00413 (9) | -0.00128 (9) |
| P3 | 0.02697 (13) | 0.02346 (13) | 0.02645 (14) | 0.00363 (10) | 0.00405 (11) | -0.00289 (10) |
| C1 | 0.0255 (5) | 0.0250 (5) | 0.0293 (5) | -0.0026 (4) | 0.0054 (4) | -0.0024 (4) |
| C2 | 0.0473 (8) | 0.0408 (7) | 0.0325 (7) | 0.0040 (6) | 0.0102 (6) | -0.0065 (6) |
| C3 | 0.0592 (10) | 0.0503 (10) | 0.0526 (10) | 0.0056 (8) | 0.0156 (8) | -0.0225 (8) |
| C4 | 0.0397 (7) | 0.0323 (7) | 0.0766 (12) | 0.0038 (6) | 0.0104 (8) | -0.0161 (7) |
| C5 | 0.0372 (7) | 0.0297 (6) | 0.0628 (10) | 0.0048 (5) | 0.0063 (7) | 0.0041 (6) |
| C6 | 0.0359 (6) | 0.0307 (6) | 0.0374 (7) | 0.0035 (5) | 0.0083 (5) | 0.0025 (5) |
| C11 | 0.0249 (5) | 0.0220 (5) | 0.0331 (6) | 0.0018 (4) | 0.0009 (4) | -0.0004 (4) |
| C12 | 0.0308 (6) | 0.0335 (6) | 0.0378 (7) | -0.0013 (5) | 0.0066 (5) | 0.0010 (5) |
| C13 | 0.0349 (7) | 0.0404 (8) | 0.0605 (10) | -0.0025 (6) | 0.0159 (7) | 0.0065 (7) |
| C14 | 0.0275 (6) | 0.0296 (6) | 0.0824 (13) | -0.0023 (5) | 0.0047 (7) | 0.0017 (7) |
| C15 | 0.0327 (6) | 0.0313 (7) | 0.0621 (10) | 0.0017 (5) | -0.0115 (6) | -0.0075 (6) |
| C16 | 0.0333 (6) | 0.0302 (6) | 0.0383 (7) | 0.0035 (5) | -0.0038 (5) | -0.0041 (5) |
| C21 | 0.0229 (4) | 0.0222 (5) | 0.0249 (5) | 0.0011 (4) | 0.0042 (4) | -0.0002 (4) |
| C22 | 0.0330 (6) | 0.0257 (5) | 0.0389 (7) | 0.0029 (4) | 0.0133 (5) | -0.0014 (5) |
| C23 | 0.0362 (6) | 0.0369 (7) | 0.0418 (7) | 0.0059 (5) | 0.0179 (6) | -0.0011 (5) |
| C24 | 0.0294 (6) | 0.0439 (7) | 0.0362 (7) | 0.0003 (5) | 0.0112 (5) | 0.0068 (5) |
| C25 | 0.0428 (7) | 0.0304 (6) | 0.0570 (9) | -0.0060 (6) | 0.0216 (7) | 0.0032 (6) |
| C26 | 0.0395 (6) | 0.0231 (5) | 0.0533 (8) | -0.0019 (5) | 0.0214 (6) | -0.0032 (5) |
| C31 | 0.0246 (5) | 0.0256 (5) | 0.0265 (5) | 0.0029 (4) | 0.0035 (4) | 0.0013 (4) |
| C32 | 0.0288 (5) | 0.0358 (6) | 0.0319 (6) | -0.0015 (5) | 0.0006 (5) | -0.0008 (5) |
| C33 | 0.0358 (7) | 0.0542 (9) | 0.0329 (7) | 0.0022 (6) | -0.0042 (5) | -0.0036 (6) |
| C34 | 0.0501 (9) | 0.0644 (11) | 0.0297 (7) | 0.0090 (8) | -0.0009 (6) | 0.0087 (7) |
| C35 | 0.0574 (9) | 0.0501 (9) | 0.0395 (8) | 0.0004 (8) | 0.0065 (7) | 0.0178 (7) |
| C36 | 0.0414 (7) | 0.0321 (6) | 0.0347 (7) | -0.0024 (5) | 0.0043 (5) | 0.0063 (5) |
| C41 | 0.0270 (5) | 0.0227 (5) | 0.0306 (5) | 0.0023 (4) | 0.0044 (4) | 0.0014 (4) |
| C42 | 0.0363 (6) | 0.0321 (6) | 0.0314 (6) | 0.0050 (5) | 0.0039 (5) | 0.0009 (5) |
| C43 | 0.0453 (8) | 0.0467 (8) | 0.0322 (7) | -0.0005 (6) | -0.0002 (6) | 0.0070 (6) |
| C44 | 0.0443 (8) | 0.0412 (8) | 0.0506 (9) | 0.0016 (6) | -0.0088 (7) | 0.0160 (7) |
| C45 | 0.0508 (9) | 0.0344 (7) | 0.0634 (11) | 0.0167 (7) | -0.0021 (8) | 0.0064 (7) |
| C46 | 0.0440 (7) | 0.0319 (7) | 0.0451 (8) | 0.0143 (6) | 0.0045 (6) | -0.0007 (6) |
| C51 | 0.0309 (5) | 0.0318 (6) | 0.0275 (5) | 0.0088 (4) | 0.0089 (4) | 0.0001 (4) |
| C52 | 0.0431 (7) | 0.0515 (9) | 0.0290 (6) | 0.0117 (6) | 0.0105 (6) | 0.0003 (6) |
| C53 | 0.0608 (10) | 0.0637 (11) | 0.0370 (8) | 0.0184 (9) | 0.0226 (7) | 0.0118 (7) |
| C54 | 0.0637 (11) | 0.0529 (10) | 0.0678 (12) | 0.0132 (8) | 0.0425 (10) | 0.0185 (9) |
| C55 | 0.0424 (8) | 0.0508 (9) | 0.0690 (12) | -0.0034 (7) | 0.0252 (8) | 0.0009 (8) |
| C56 | 0.0329 (6) | 0.0409 (7) | 0.0408 (7) | 0.0017 (5) | 0.0118 (5) | -0.0006 (6) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|-------|-------------|---------|-------------|
| N1—P2 | 1.5690 (10) | C24—H24 | 0.99 (2) |
| N1—P1 | 1.6755 (11) | C25—C26 | 1.3892 (19) |

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|------------|-------------|-------------|-------------|
| P1—C1 | 1.8421 (12) | C25—H25 | 0.92 (2) |
| P1—C11 | 1.8476 (12) | C26—H26 | 0.95 (2) |
| P2—C31 | 1.8071 (12) | C31—C36 | 1.3882 (18) |
| P2—C21 | 1.8156 (11) | C31—C32 | 1.4023 (18) |
| P2—P3 | 2.2273 (5) | C32—C33 | 1.388 (2) |
| P3—C51 | 1.8196 (13) | C32—H32 | 0.958 (19) |
| P3—C41 | 1.8200 (13) | C33—C34 | 1.379 (3) |
| C1—C2 | 1.3873 (18) | C33—H33 | 0.94 (2) |
| C1—C6 | 1.3935 (19) | C34—C35 | 1.385 (3) |
| C2—C3 | 1.395 (2) | C34—H34 | 0.95 (2) |
| C2—H2 | 0.94 (2) | C35—C36 | 1.390 (2) |
| C3—C4 | 1.371 (3) | C35—H35 | 0.92 (2) |
| C3—H3 | 0.96 (2) | C36—H36 | 0.99 (2) |
| C4—C5 | 1.379 (3) | C41—C42 | 1.3917 (18) |
| C4—H4 | 0.95 (2) | C41—C46 | 1.3965 (18) |
| C5—C6 | 1.385 (2) | C42—C43 | 1.393 (2) |
| C5—H5 | 0.96 (2) | C42—H42 | 0.943 (19) |
| C6—H6 | 0.97 (2) | C43—C44 | 1.378 (2) |
| C11—C12 | 1.3895 (18) | C43—H43 | 0.93 (2) |
| C11—C16 | 1.3972 (18) | C44—C45 | 1.378 (3) |
| C12—C13 | 1.394 (2) | C44—H44 | 0.93 (2) |
| C12—H12 | 0.933 (18) | C45—C46 | 1.384 (2) |
| C13—C14 | 1.382 (3) | C45—H45 | 0.95 (2) |
| C13—H13 | 0.97 (2) | C46—H46 | 0.96 (2) |
| C14—C15 | 1.380 (3) | C51—C56 | 1.398 (2) |
| C14—H14 | 0.93 (2) | C51—C52 | 1.3991 (19) |
| C15—C16 | 1.391 (2) | C52—C53 | 1.386 (2) |
| C15—H15 | 0.97 (2) | C52—H52 | 1.04 (2) |
| C16—H16 | 0.957 (17) | C53—C54 | 1.382 (3) |
| C21—C22 | 1.3909 (16) | C53—H53 | 0.97 (2) |
| C21—C26 | 1.3915 (17) | C54—C55 | 1.387 (3) |
| C22—C23 | 1.3901 (18) | C54—H54 | 0.96 (2) |
| C22—H22 | 0.94 (2) | C55—C56 | 1.386 (2) |
| C23—C24 | 1.379 (2) | C55—H55 | 0.91 (2) |
| C23—H23 | 0.97 (2) | C56—H56 | 0.990 (19) |
| C24—C25 | 1.379 (2) | | |
| P2—N1—P1 | 129.01 (7) | C24—C25—C26 | 120.13 (13) |
| N1—P1—C1 | 102.74 (6) | C24—C25—H25 | 120.2 (14) |
| N1—P1—C11 | 101.80 (6) | C26—C25—H25 | 119.7 (14) |
| C1—P1—C11 | 94.35 (5) | C25—C26—C21 | 120.58 (12) |
| N1—P2—C31 | 108.08 (6) | C25—C26—H26 | 118.3 (13) |
| N1—P2—C21 | 116.14 (5) | C21—C26—H26 | 121.1 (13) |
| C31—P2—C21 | 107.15 (5) | C36—C31—C32 | 119.56 (12) |
| N1—P2—P3 | 122.96 (4) | C36—C31—P2 | 119.62 (10) |
| C31—P2—P3 | 95.39 (4) | C32—C31—P2 | 120.40 (9) |
| C21—P2—P3 | 104.38 (4) | C33—C32—C31 | 119.97 (13) |
| C51—P3—C41 | 104.57 (6) | C33—C32—H32 | 119.6 (11) |

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|-------------|-------------|-------------|-------------|
| C51—P3—P2 | 96.68 (4) | C31—C32—H32 | 120.4 (11) |
| C41—P3—P2 | 106.86 (4) | C34—C33—C32 | 119.90 (15) |
| C2—C1—C6 | 118.77 (13) | C34—C33—H33 | 121.4 (12) |
| C2—C1—P1 | 118.55 (10) | C32—C33—H33 | 118.7 (12) |
| C6—C1—P1 | 122.45 (10) | C33—C34—C35 | 120.53 (15) |
| C1—C2—C3 | 120.23 (16) | C33—C34—H34 | 121.2 (13) |
| C1—C2—H2 | 119.5 (13) | C35—C34—H34 | 118.3 (13) |
| C3—C2—H2 | 120.2 (13) | C34—C35—C36 | 120.01 (15) |
| C4—C3—C2 | 120.34 (16) | C34—C35—H35 | 119.2 (14) |
| C4—C3—H3 | 121.6 (14) | C36—C35—H35 | 120.8 (14) |
| C2—C3—H3 | 118.0 (15) | C31—C36—C35 | 120.00 (14) |
| C3—C4—C5 | 119.92 (15) | C31—C36—H36 | 118.7 (11) |
| C3—C4—H4 | 119.2 (13) | C35—C36—H36 | 121.3 (11) |
| C5—C4—H4 | 120.9 (13) | C42—C41—C46 | 118.52 (12) |
| C4—C5—C6 | 120.29 (16) | C42—C41—P3 | 125.94 (9) |
| C4—C5—H5 | 119.1 (13) | C46—C41—P3 | 114.86 (10) |
| C6—C5—H5 | 120.5 (13) | C41—C42—C43 | 120.11 (13) |
| C5—C6—C1 | 120.40 (14) | C41—C42—H42 | 120.0 (11) |
| C5—C6—H6 | 119.7 (12) | C43—C42—H42 | 119.8 (11) |
| C1—C6—H6 | 119.8 (12) | C44—C43—C42 | 120.54 (15) |
| C12—C11—C16 | 118.50 (12) | C44—C43—H43 | 119.9 (13) |
| C12—C11—P1 | 123.05 (10) | C42—C43—H43 | 119.6 (13) |
| C16—C11—P1 | 118.45 (10) | C45—C44—C43 | 119.81 (14) |
| C11—C12—C13 | 120.16 (14) | C45—C44—H44 | 119.6 (13) |
| C11—C12—H12 | 120.7 (11) | C43—C44—H44 | 120.6 (13) |
| C13—C12—H12 | 119.1 (11) | C44—C45—C46 | 120.09 (15) |
| C14—C13—C12 | 120.79 (16) | C44—C45—H45 | 121.3 (14) |
| C14—C13—H13 | 121.1 (12) | C46—C45—H45 | 118.4 (14) |
| C12—C13—H13 | 117.9 (13) | C45—C46—C41 | 120.86 (15) |
| C15—C14—C13 | 119.60 (14) | C45—C46—H46 | 120.0 (14) |
| C15—C14—H14 | 121.1 (13) | C41—C46—H46 | 119.1 (14) |
| C13—C14—H14 | 119.3 (13) | C56—C51—C52 | 119.65 (13) |
| C14—C15—C16 | 119.93 (15) | C56—C51—P3 | 123.44 (10) |
| C14—C15—H15 | 121.8 (13) | C52—C51—P3 | 116.88 (11) |
| C16—C15—H15 | 118.3 (13) | C53—C52—C51 | 119.98 (17) |
| C15—C16—C11 | 121.02 (15) | C53—C52—H52 | 119.4 (12) |
| C15—C16—H16 | 120.3 (11) | C51—C52—H52 | 120.6 (12) |
| C11—C16—H16 | 118.6 (11) | C54—C53—C52 | 120.06 (16) |
| C22—C21—C26 | 118.84 (11) | C54—C53—H53 | 122.1 (15) |
| C22—C21—P2 | 118.12 (9) | C52—C53—H53 | 117.8 (15) |
| C26—C21—P2 | 123.03 (9) | C53—C54—C55 | 120.31 (16) |
| C23—C22—C21 | 120.17 (12) | C53—C54—H54 | 119.3 (14) |
| C23—C22—H22 | 120.4 (12) | C55—C54—H54 | 120.4 (14) |
| C21—C22—H22 | 119.4 (12) | C56—C55—C54 | 120.30 (18) |
| C24—C23—C22 | 120.53 (12) | C56—C55—H55 | 120.5 (14) |
| C24—C23—H23 | 121.4 (13) | C54—C55—H55 | 119.2 (14) |
| C22—C23—H23 | 118.1 (13) | C55—C56—C51 | 119.66 (16) |
| C23—C24—C25 | 119.74 (12) | C55—C56—H56 | 121.4 (11) |

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|-------------|------------|-------------|------------|
| C23—C24—H24 | 121.5 (12) | C51—C56—H56 | 118.9 (11) |
| C25—C24—H24 | 118.7 (12) | | |
