

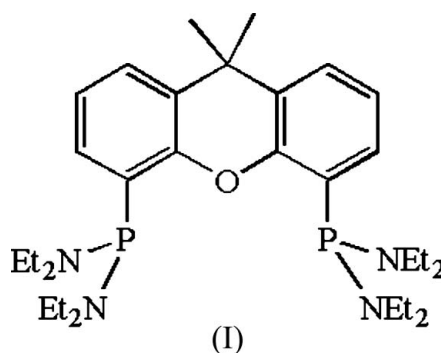
4,5-Bis[bis(diethylamino)phosphino]-
9,9-dimethylxantheneDavid J Adams, John Fawcett,
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Key indicators

Single-crystal X-ray study
 $T = 150$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.050
 wR factor = 0.139
Data-to-parameter ratio = 16.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.The structure of the title compound, $\text{C}_{31}\text{H}_{52}\text{N}_4\text{OP}_2$, reveals a
near-planar xanthene skeleton.Received 24 June 2005
Accepted 2 August 2005
Online 6 August 2005

Comment

Xantphos, and related bidentate ligands with the xanthene backbone, have been shown to be remarkable ligands for the rhodium-catalysed hydroformylation of long-chain alkenes, giving exceptionally high selectivity to the industrially useful linear aldehyde (linear/branched ratio = 50:1) (Kranenburg *et al.*, 1995). The title compound, (I), was prepared according to the literature procedure of Goertz *et al.* (2001) as an intermediate in work directed towards the synthesis of perfluoro-alkylated derivatives of Xantphos (Adams *et al.*, 2004). Crystals suitable for X-ray analysis were grown from hexane solution. The bond lengths and angles within the structure are unremarkable. The molecule has a pseudo- C_2 axis of symmetry through O1 and C6, such that the lone pairs on phosphorus point either in front or behind an approximately planar xanthene skeleton.

Experimental

The title compound was prepared according to the literature procedure of Goertz *et al.* (2001). Crystals suitable for X-ray analysis were grown from a hexane solution.

Crystal data

$\text{C}_{31}\text{H}_{52}\text{N}_4\text{OP}_2$
 $M_r = 558.71$
 Monoclinic, $P2_1/c$
 $a = 18.799$ (1) Å
 $b = 11.4968$ (6) Å
 $c = 15.2179$ (8) Å
 $\beta = 100.880$ (1)°
 $V = 3229.9$ (3) Å³
 $Z = 4$

$D_x = 1.149$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 6949
 reflections
 $\theta = 2.2$ – 26.9 °
 $\mu = 0.16$ mm⁻¹
 $T = 150$ (2) K
 Block, colourless
 $0.34 \times 0.21 \times 0.16$ mm

Data collection

Bruker APEX CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.93$, $T_{\max} = 0.96$
 22958 measured reflections

5685 independent reflections
 4653 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$
 $\theta_{\text{max}} = 25.0^\circ$
 $h = -22 \rightarrow 22$
 $k = -13 \rightarrow 13$
 $l = -18 \rightarrow 18$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.050$
 $wR(F^2) = 0.139$
 $S = 1.06$
 5685 reflections
 353 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0817P)^2 + 0.3182P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.002$
 $\Delta\rho_{\text{max}} = 0.53 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\text{min}} = -0.35 \text{ e } \text{Å}^{-3}$

All H atoms were included in calculated positions, riding on the bonded atom [C–H = 0.95 (CH), 0.98 (CH₃) and 0.99 Å (CH₂)], and with $U_{\text{iso}}(\text{H})$ values set at $1.5U_{\text{eq}}$ of the bonded C atom for methyl H atoms and at $1.2U_{\text{eq}}$ for all other H atoms.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Sheldrick, 2000); software used to prepare material for publication: SHELXTL.

The authors thank the EPSRC (DJA) and the Royal Society (AMS) for financial support.

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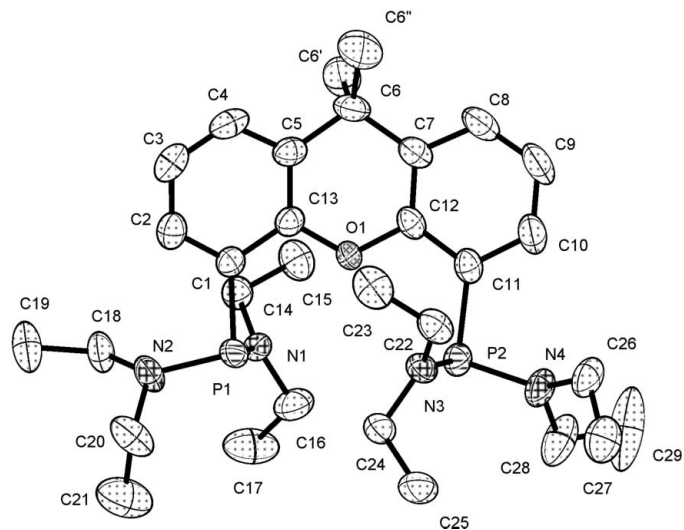


Figure 1
 The molecular structure of (I), showing the atom-labelling scheme and 50% probability displacement ellipsoids. H atoms have been omitted for clarity.

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supporting information

Acta Cryst. (2005). E61, o2831–o2832 [https://doi.org/10.1107/S1600536805024797]

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Crystal data

$C_{31}H_{52}N_4OP_2$

$M_r = 558.71$

Monoclinic, $P2_1/c$

$a = 18.799$ (1) Å

$b = 11.4968$ (6) Å

$c = 15.2179$ (8) Å

$\beta = 100.880$ (1)°

$V = 3229.9$ (3) Å³

$Z = 4$

$F(000) = 1216$

$D_x = 1.149$ Mg m⁻³

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

Cell parameters from 6949 reflections

$\theta = 2.2$ – 26.9 °

$\mu = 0.16$ mm⁻¹

$T = 150$ K

Block, colourless

$0.34 \times 0.21 \times 0.16$ mm

Data collection

Bruker APEX CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

$T_{\min} = 0.93$, $T_{\max} = 0.96$

22958 measured reflections

5685 independent reflections

4653 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.034$

$\theta_{\max} = 25.0$ °, $\theta_{\min} = 2.1$ °

$h = -22 \rightarrow 22$

$k = -13 \rightarrow 13$

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.139$

$S = 1.06$

5685 reflections

353 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0817P)^2 + 0.3182P]$

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

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

$\Delta\rho_{\max} = 0.53$ e Å⁻³

$\Delta\rho_{\min} = -0.35$ e Å⁻³

Special details

Experimental. absorption correction based on 11566 reflections (*SADABS*); R_{int} 0.042 before and 0.029 after correction.

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 | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|---------------|--------------|--------------|----------------------------------|
| P1 | 0.24064 (3) | 0.79839 (4) | 0.15134 (4) | 0.03314 (17) |
| P2 | 0.34099 (3) | 0.47707 (4) | 0.26900 (4) | 0.03378 (17) |
| O1 | 0.19529 (7) | 0.58133 (11) | 0.22875 (9) | 0.0323 (3) |
| N1 | 0.25398 (9) | 0.82334 (14) | 0.26194 (12) | 0.0335 (4) |
| N2 | 0.22386 (11) | 0.92669 (15) | 0.09521 (12) | 0.0421 (5) |
| N3 | 0.32498 (9) | 0.47476 (14) | 0.15649 (12) | 0.0341 (4) |
| N4 | 0.40281 (10) | 0.37232 (15) | 0.30858 (14) | 0.0460 (5) |
| C1 | 0.14864 (10) | 0.73710 (17) | 0.13477 (13) | 0.0299 (4) |
| C2 | 0.09075 (12) | 0.78508 (19) | 0.07518 (14) | 0.0378 (5) |
| H2 | 0.0981 | 0.8535 | 0.0431 | 0.045* |
| C3 | 0.02307 (12) | 0.7352 (2) | 0.06197 (15) | 0.0450 (6) |
| H3 | -0.0154 | 0.7682 | 0.0199 | 0.054* |
| C4 | 0.01100 (12) | 0.6380 (2) | 0.10931 (15) | 0.0431 (6) |
| H4 | -0.0364 | 0.6061 | 0.1010 | 0.052* |
| C5 | 0.06652 (11) | 0.58504 (18) | 0.16925 (14) | 0.0341 (5) |
| C6 | 0.05264 (12) | 0.48505 (19) | 0.22901 (17) | 0.0436 (6) |
| C6' | 0.02674 (16) | 0.5366 (3) | 0.3116 (2) | 0.0691 (9) |
| H61 | 0.0167 | 0.4733 | 0.3506 | 0.104* |
| H62 | -0.0175 | 0.5821 | 0.2918 | 0.104* |
| H63 | 0.0646 | 0.5872 | 0.3445 | 0.104* |
| C6'' | -0.00587 (16) | 0.4030 (3) | 0.1799 (3) | 0.0886 (11) |
| H64 | 0.0104 | 0.3692 | 0.1279 | 0.133* |
| H65 | -0.0508 | 0.4467 | 0.1599 | 0.133* |
| H66 | -0.0146 | 0.3406 | 0.2204 | 0.133* |
| C7 | 0.12274 (12) | 0.41934 (17) | 0.26105 (14) | 0.0356 (5) |
| C8 | 0.12244 (14) | 0.30780 (19) | 0.29698 (17) | 0.0491 (6) |
| H8 | 0.0776 | 0.2709 | 0.2989 | 0.059* |
| C9 | 0.18592 (16) | 0.2506 (2) | 0.32963 (18) | 0.0571 (7) |
| H9 | 0.1847 | 0.1759 | 0.3559 | 0.069* |
| C10 | 0.25162 (14) | 0.30120 (19) | 0.32450 (16) | 0.0464 (6) |
| H10 | 0.2952 | 0.2611 | 0.3483 | 0.056* |
| C11 | 0.25522 (11) | 0.40994 (17) | 0.28504 (13) | 0.0331 (5) |
| C12 | 0.18949 (11) | 0.46837 (16) | 0.25811 (13) | 0.0301 (5) |
| C13 | 0.13532 (10) | 0.63374 (17) | 0.17769 (13) | 0.0292 (4) |
| C14 | 0.19883 (12) | 0.85861 (18) | 0.31332 (14) | 0.0355 (5) |
| H14A | 0.1507 | 0.8556 | 0.2735 | 0.043* |
| H14B | 0.2080 | 0.9403 | 0.3327 | 0.043* |
| C15 | 0.19678 (14) | 0.7844 (2) | 0.39480 (15) | 0.0494 (6) |
| H15A | 0.1927 | 0.7023 | 0.3773 | 0.074* |
| H15B | 0.1549 | 0.8065 | 0.4210 | 0.074* |

| | | | | |
|------|--------------|--------------|--------------|-------------|
| H15C | 0.2414 | 0.7963 | 0.4390 | 0.074* |
| C16 | 0.32828 (12) | 0.8252 (2) | 0.31135 (18) | 0.0513 (6) |
| H16A | 0.3602 | 0.7907 | 0.2735 | 0.062* |
| H16B | 0.3315 | 0.7758 | 0.3653 | 0.062* |
| C17 | 0.35593 (16) | 0.9459 (3) | 0.3400 (2) | 0.0730 (9) |
| H17A | 0.3533 | 0.9954 | 0.2871 | 0.110* |
| H17B | 0.4063 | 0.9408 | 0.3718 | 0.110* |
| H17C | 0.3260 | 0.9796 | 0.3798 | 0.110* |
| C18 | 0.18840 (14) | 1.02350 (18) | 0.13247 (16) | 0.0449 (6) |
| H18A | 0.2254 | 1.0670 | 0.1749 | 0.054* |
| H18B | 0.1531 | 0.9914 | 0.1668 | 0.054* |
| C19 | 0.14921 (17) | 1.1079 (2) | 0.06274 (19) | 0.0656 (8) |
| H19A | 0.1838 | 1.1414 | 0.0291 | 0.098* |
| H19B | 0.1273 | 1.1702 | 0.0926 | 0.098* |
| H19C | 0.1112 | 1.0664 | 0.0216 | 0.098* |
| C20 | 0.27251 (16) | 0.9574 (2) | 0.03463 (18) | 0.0596 (7) |
| H20A | 0.2441 | 0.9963 | -0.0186 | 0.072* |
| H20B | 0.2928 | 0.8850 | 0.0141 | 0.072* |
| C21 | 0.33337 (19) | 1.0348 (3) | 0.0748 (2) | 0.0846 (10) |
| H21A | 0.3140 | 1.1095 | 0.0906 | 0.127* |
| H21B | 0.3652 | 1.0476 | 0.0316 | 0.127* |
| H21C | 0.3610 | 0.9983 | 0.1288 | 0.127* |
| C22 | 0.28363 (13) | 0.38731 (18) | 0.09829 (15) | 0.0408 (5) |
| H22A | 0.2685 | 0.3252 | 0.1359 | 0.049* |
| H22B | 0.3155 | 0.3516 | 0.0609 | 0.049* |
| C23 | 0.21694 (14) | 0.4359 (2) | 0.03769 (16) | 0.0546 (7) |
| H23A | 0.1860 | 0.4742 | 0.0740 | 0.082* |
| H23B | 0.1901 | 0.3725 | 0.0034 | 0.082* |
| H23C | 0.2317 | 0.4926 | -0.0036 | 0.082* |
| C24 | 0.36406 (12) | 0.55852 (19) | 0.11121 (16) | 0.0407 (5) |
| H24A | 0.3758 | 0.6276 | 0.1501 | 0.049* |
| H24B | 0.3319 | 0.5843 | 0.0554 | 0.049* |
| C25 | 0.43374 (14) | 0.5114 (2) | 0.0880 (2) | 0.0588 (7) |
| H25A | 0.4683 | 0.4941 | 0.1432 | 0.088* |
| H25B | 0.4546 | 0.5695 | 0.0532 | 0.088* |
| H25C | 0.4233 | 0.4401 | 0.0526 | 0.088* |
| C26 | 0.40659 (13) | 0.2562 (2) | 0.27059 (19) | 0.0525 (7) |
| H26A | 0.3605 | 0.2410 | 0.2286 | 0.063* |
| H26B | 0.4105 | 0.1986 | 0.3196 | 0.063* |
| C27 | 0.46806 (16) | 0.2363 (2) | 0.2219 (2) | 0.0665 (8) |
| H27A | 0.4620 | 0.2868 | 0.1691 | 0.100* |
| H27B | 0.4682 | 0.1548 | 0.2032 | 0.100* |
| H27C | 0.5140 | 0.2544 | 0.2618 | 0.100* |
| C28 | 0.46724 (15) | 0.4091 (2) | 0.37006 (19) | 0.0683 (9) |
| H28A | 0.4594 | 0.4893 | 0.3900 | 0.082* |
| H28B | 0.5080 | 0.4116 | 0.3373 | 0.082* |
| C29 | 0.4888 (3) | 0.3344 (3) | 0.4510 (2) | 0.1249 (18) |
| H29A | 0.4472 | 0.3240 | 0.4806 | 0.187* |

| | | | | |
|------|--------|--------|--------|--------|
| H29B | 0.5285 | 0.3717 | 0.4924 | 0.187* |
| H29C | 0.5048 | 0.2583 | 0.4331 | 0.187* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| P1 | 0.0327 (3) | 0.0226 (3) | 0.0477 (4) | 0.0019 (2) | 0.0167 (3) | 0.0019 (2) |
| P2 | 0.0341 (3) | 0.0233 (3) | 0.0428 (3) | 0.0034 (2) | 0.0045 (2) | -0.0032 (2) |
| O1 | 0.0293 (8) | 0.0204 (7) | 0.0463 (9) | -0.0018 (6) | 0.0047 (6) | 0.0051 (6) |
| N1 | 0.0250 (9) | 0.0262 (9) | 0.0489 (11) | 0.0013 (7) | 0.0062 (8) | 0.0015 (8) |
| N2 | 0.0568 (12) | 0.0292 (10) | 0.0465 (11) | 0.0027 (9) | 0.0252 (9) | 0.0080 (8) |
| N3 | 0.0348 (10) | 0.0258 (9) | 0.0436 (11) | -0.0028 (7) | 0.0125 (8) | -0.0012 (7) |
| N4 | 0.0386 (11) | 0.0278 (10) | 0.0656 (13) | 0.0065 (8) | -0.0051 (9) | -0.0067 (9) |
| C1 | 0.0307 (11) | 0.0280 (10) | 0.0331 (11) | 0.0050 (8) | 0.0114 (9) | -0.0011 (8) |
| C2 | 0.0434 (13) | 0.0347 (12) | 0.0358 (12) | 0.0090 (10) | 0.0087 (10) | 0.0006 (9) |
| C3 | 0.0364 (13) | 0.0523 (15) | 0.0432 (13) | 0.0134 (11) | -0.0007 (10) | -0.0033 (11) |
| C4 | 0.0260 (11) | 0.0506 (14) | 0.0525 (14) | 0.0007 (10) | 0.0070 (10) | -0.0117 (12) |
| C5 | 0.0289 (11) | 0.0331 (11) | 0.0418 (12) | -0.0006 (9) | 0.0103 (9) | -0.0084 (9) |
| C6 | 0.0341 (12) | 0.0368 (12) | 0.0630 (16) | -0.0093 (10) | 0.0174 (11) | -0.0005 (11) |
| C6' | 0.0724 (19) | 0.0618 (18) | 0.090 (2) | 0.0211 (15) | 0.0569 (17) | 0.0227 (15) |
| C6'' | 0.0591 (19) | 0.0610 (19) | 0.135 (3) | -0.0289 (16) | -0.0094 (19) | 0.0131 (19) |
| C7 | 0.0428 (13) | 0.0282 (11) | 0.0401 (12) | -0.0048 (9) | 0.0192 (10) | -0.0035 (9) |
| C8 | 0.0601 (16) | 0.0325 (12) | 0.0641 (16) | -0.0069 (11) | 0.0362 (13) | 0.0024 (11) |
| C9 | 0.080 (2) | 0.0314 (13) | 0.0695 (18) | 0.0031 (13) | 0.0380 (15) | 0.0164 (12) |
| C10 | 0.0589 (16) | 0.0330 (12) | 0.0504 (14) | 0.0099 (11) | 0.0181 (12) | 0.0119 (10) |
| C11 | 0.0433 (12) | 0.0247 (10) | 0.0328 (11) | 0.0042 (9) | 0.0113 (9) | -0.0006 (8) |
| C12 | 0.0416 (12) | 0.0212 (10) | 0.0297 (11) | -0.0012 (8) | 0.0122 (9) | -0.0019 (8) |
| C13 | 0.0277 (11) | 0.0273 (10) | 0.0332 (11) | 0.0032 (8) | 0.0069 (8) | -0.0030 (8) |
| C14 | 0.0368 (12) | 0.0313 (11) | 0.0381 (12) | 0.0019 (9) | 0.0067 (9) | 0.0003 (9) |
| C15 | 0.0621 (17) | 0.0458 (14) | 0.0399 (13) | -0.0022 (12) | 0.0085 (12) | 0.0050 (11) |
| C16 | 0.0311 (12) | 0.0524 (15) | 0.0677 (16) | -0.0042 (11) | 0.0023 (11) | -0.0056 (13) |
| C17 | 0.0571 (18) | 0.079 (2) | 0.083 (2) | -0.0322 (16) | 0.0133 (15) | -0.0303 (17) |
| C18 | 0.0589 (15) | 0.0285 (12) | 0.0488 (14) | 0.0102 (10) | 0.0141 (12) | 0.0087 (10) |
| C19 | 0.088 (2) | 0.0389 (14) | 0.0653 (18) | 0.0120 (14) | 0.0036 (15) | 0.0154 (13) |
| C20 | 0.082 (2) | 0.0461 (14) | 0.0577 (16) | -0.0171 (14) | 0.0310 (15) | 0.0000 (12) |
| C21 | 0.086 (2) | 0.073 (2) | 0.105 (3) | -0.0281 (18) | 0.042 (2) | -0.0244 (19) |
| C22 | 0.0522 (14) | 0.0318 (11) | 0.0419 (13) | -0.0053 (10) | 0.0183 (11) | -0.0057 (10) |
| C23 | 0.0701 (18) | 0.0523 (15) | 0.0380 (14) | -0.0116 (13) | 0.0013 (12) | -0.0032 (11) |
| C24 | 0.0380 (12) | 0.0297 (11) | 0.0583 (15) | 0.0004 (9) | 0.0189 (11) | 0.0027 (10) |
| C25 | 0.0481 (15) | 0.0462 (14) | 0.092 (2) | 0.0016 (12) | 0.0381 (15) | 0.0040 (14) |
| C26 | 0.0425 (14) | 0.0300 (12) | 0.0789 (18) | 0.0086 (10) | -0.0040 (12) | -0.0097 (12) |
| C27 | 0.072 (2) | 0.0449 (15) | 0.085 (2) | 0.0168 (14) | 0.0217 (16) | -0.0054 (14) |
| C28 | 0.0632 (18) | 0.0544 (16) | 0.0721 (19) | 0.0192 (14) | -0.0260 (15) | -0.0176 (14) |
| C29 | 0.199 (5) | 0.078 (2) | 0.072 (2) | 0.074 (3) | -0.039 (3) | -0.0197 (19) |

Geometric parameters (Å, °)

| | | | |
|----------|-------------|----------|-----------|
| P1—N1 | 1.6789 (19) | C14—H14B | 0.9900 |
| P1—N2 | 1.7038 (18) | C15—H15A | 0.9800 |
| P1—C1 | 1.840 (2) | C15—H15B | 0.9800 |
| P2—N3 | 1.6816 (18) | C15—H15C | 0.9800 |
| P2—N4 | 1.7027 (18) | C16—C17 | 1.517 (4) |
| P2—C11 | 1.845 (2) | C16—H16A | 0.9900 |
| O1—C13 | 1.381 (2) | C16—H16B | 0.9900 |
| O1—C12 | 1.384 (2) | C17—H17A | 0.9800 |
| N1—C16 | 1.456 (3) | C17—H17B | 0.9800 |
| N1—C14 | 1.469 (3) | C17—H17C | 0.9800 |
| N2—C20 | 1.459 (3) | C18—C19 | 1.521 (3) |
| N2—C18 | 1.465 (3) | C18—H18A | 0.9900 |
| N3—C24 | 1.460 (3) | C18—H18B | 0.9900 |
| N3—C22 | 1.463 (3) | C19—H19A | 0.9800 |
| N4—C28 | 1.447 (3) | C19—H19B | 0.9800 |
| N4—C26 | 1.462 (3) | C19—H19C | 0.9800 |
| C1—C2 | 1.392 (3) | C20—C21 | 1.487 (4) |
| C1—C13 | 1.401 (3) | C20—H20A | 0.9900 |
| C2—C3 | 1.375 (3) | C20—H20B | 0.9900 |
| C2—H2 | 0.9500 | C21—H21A | 0.9800 |
| C3—C4 | 1.371 (3) | C21—H21B | 0.9800 |
| C3—H3 | 0.9500 | C21—H21C | 0.9800 |
| C4—C5 | 1.390 (3) | C22—C23 | 1.516 (3) |
| C4—H4 | 0.9500 | C22—H22A | 0.9900 |
| C5—C13 | 1.393 (3) | C22—H22B | 0.9900 |
| C5—C6 | 1.519 (3) | C23—H23A | 0.9800 |
| C6—C7 | 1.517 (3) | C23—H23B | 0.9800 |
| C6—C6" | 1.532 (3) | C23—H23C | 0.9800 |
| C6—C6' | 1.549 (4) | C24—C25 | 1.520 (3) |
| C6'—H61 | 0.9800 | C24—H24A | 0.9900 |
| C6'—H62 | 0.9800 | C24—H24B | 0.9900 |
| C6'—H63 | 0.9800 | C25—H25A | 0.9800 |
| C6"—H64 | 0.9800 | C25—H25B | 0.9800 |
| C6"—H65 | 0.9800 | C25—H25C | 0.9800 |
| C6"—H66 | 0.9800 | C26—C27 | 1.503 (4) |
| C7—C12 | 1.384 (3) | C26—H26A | 0.9900 |
| C7—C8 | 1.394 (3) | C26—H26B | 0.9900 |
| C8—C9 | 1.371 (4) | C27—H27A | 0.9800 |
| C8—H8 | 0.9500 | C27—H27B | 0.9800 |
| C9—C10 | 1.381 (4) | C27—H27C | 0.9800 |
| C9—H9 | 0.9500 | C28—C29 | 1.494 (4) |
| C10—C11 | 1.394 (3) | C28—H28A | 0.9900 |
| C10—H10 | 0.9500 | C28—H28B | 0.9900 |
| C11—C12 | 1.398 (3) | C29—H29A | 0.9800 |
| C14—C15 | 1.512 (3) | C29—H29B | 0.9800 |
| C14—H14A | 0.9900 | C29—H29C | 0.9800 |

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| N1—P1—N2 | 109.46 (9) | N1—C16—C17 | 113.9 (2) |
| N1—P1—C1 | 99.29 (9) | N1—C16—H16A | 108.8 |
| N2—P1—C1 | 100.52 (9) | C17—C16—H16A | 108.8 |
| N3—P2—N4 | 109.15 (9) | N1—C16—H16B | 108.8 |
| N3—P2—C11 | 97.77 (9) | C17—C16—H16B | 108.8 |
| N4—P2—C11 | 102.27 (9) | H16A—C16—H16B | 107.7 |
| C13—O1—C12 | 119.03 (15) | C16—C17—H17A | 109.5 |
| C16—N1—C14 | 115.21 (18) | C16—C17—H17B | 109.5 |
| C16—N1—P1 | 117.86 (15) | H17A—C17—H17B | 109.5 |
| C14—N1—P1 | 126.45 (14) | C16—C17—H17C | 109.5 |
| C20—N2—C18 | 116.49 (18) | H17A—C17—H17C | 109.5 |
| C20—N2—P1 | 116.57 (16) | H17B—C17—H17C | 109.5 |
| C18—N2—P1 | 121.22 (14) | N2—C18—C19 | 114.2 (2) |
| C24—N3—C22 | 115.13 (17) | N2—C18—H18A | 108.7 |
| C24—N3—P2 | 117.43 (14) | C19—C18—H18A | 108.7 |
| C22—N3—P2 | 126.86 (14) | N2—C18—H18B | 108.7 |
| C28—N4—C26 | 115.18 (18) | C19—C18—H18B | 108.7 |
| C28—N4—P2 | 117.00 (15) | H18A—C18—H18B | 107.6 |
| C26—N4—P2 | 125.94 (16) | C18—C19—H19A | 109.5 |
| C2—C1—C13 | 116.95 (19) | C18—C19—H19B | 109.5 |
| C2—C1—P1 | 122.44 (16) | H19A—C19—H19B | 109.5 |
| C13—C1—P1 | 120.46 (15) | C18—C19—H19C | 109.5 |
| C3—C2—C1 | 121.2 (2) | H19A—C19—H19C | 109.5 |
| C3—C2—H2 | 119.4 | H19B—C19—H19C | 109.5 |
| C1—C2—H2 | 119.4 | N2—C20—C21 | 114.2 (2) |
| C4—C3—C2 | 120.2 (2) | N2—C20—H20A | 108.7 |
| C4—C3—H3 | 119.9 | C21—C20—H20A | 108.7 |
| C2—C3—H3 | 119.9 | N2—C20—H20B | 108.7 |
| C3—C4—C5 | 121.6 (2) | C21—C20—H20B | 108.7 |
| C3—C4—H4 | 119.2 | H20A—C20—H20B | 107.6 |
| C5—C4—H4 | 119.2 | C20—C21—H21A | 109.5 |
| C4—C5—C13 | 117.0 (2) | C20—C21—H21B | 109.5 |
| C4—C5—C6 | 122.15 (19) | H21A—C21—H21B | 109.5 |
| C13—C5—C6 | 120.70 (19) | C20—C21—H21C | 109.5 |
| C5—C6—C7 | 109.42 (17) | H21A—C21—H21C | 109.5 |
| C5—C6—C6" | 111.2 (2) | H21B—C21—H21C | 109.5 |
| C7—C6—C6" | 110.5 (2) | N3—C22—C23 | 113.50 (18) |
| C5—C6—C6' | 108.16 (19) | N3—C22—H22A | 108.9 |
| C7—C6—C6' | 108.5 (2) | C23—C22—H22A | 108.9 |
| C6"—C6—C6' | 109.0 (2) | N3—C22—H22B | 108.9 |
| C6—C6'—H61 | 109.5 | C23—C22—H22B | 108.9 |
| C6—C6'—H62 | 109.5 | H22A—C22—H22B | 107.7 |
| H61—C6'—H62 | 109.5 | C22—C23—H23A | 109.5 |
| C6—C6'—H63 | 109.5 | C22—C23—H23B | 109.5 |
| H61—C6'—H63 | 109.5 | H23A—C23—H23B | 109.5 |
| H62—C6'—H63 | 109.5 | C22—C23—H23C | 109.5 |
| C6—C6"—H64 | 109.5 | H23A—C23—H23C | 109.5 |

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| C6—C6"—H65 | 109.5 | H23B—C23—H23C | 109.5 |
| H64—C6"—H65 | 109.5 | N3—C24—C25 | 114.03 (18) |
| C6—C6"—H66 | 109.5 | N3—C24—H24A | 108.7 |
| H64—C6"—H66 | 109.5 | C25—C24—H24A | 108.7 |
| H65—C6"—H66 | 109.5 | N3—C24—H24B | 108.7 |
| C12—C7—C8 | 117.3 (2) | C25—C24—H24B | 108.7 |
| C12—C7—C6 | 121.64 (18) | H24A—C24—H24B | 107.6 |
| C8—C7—C6 | 121.09 (19) | C24—C25—H25A | 109.5 |
| C9—C8—C7 | 121.0 (2) | C24—C25—H25B | 109.5 |
| C9—C8—H8 | 119.5 | H25A—C25—H25B | 109.5 |
| C7—C8—H8 | 119.5 | C24—C25—H25C | 109.5 |
| C8—C9—C10 | 120.3 (2) | H25A—C25—H25C | 109.5 |
| C8—C9—H9 | 119.9 | H25B—C25—H25C | 109.5 |
| C10—C9—H9 | 119.9 | N4—C26—C27 | 115.7 (2) |
| C9—C10—C11 | 121.2 (2) | N4—C26—H26A | 108.4 |
| C9—C10—H10 | 119.4 | C27—C26—H26A | 108.4 |
| C11—C10—H10 | 119.4 | N4—C26—H26B | 108.4 |
| C10—C11—C12 | 116.43 (19) | C27—C26—H26B | 108.4 |
| C10—C11—P2 | 123.15 (17) | H26A—C26—H26B | 107.4 |
| C12—C11—P2 | 120.41 (15) | C26—C27—H27A | 109.5 |
| C7—C12—O1 | 121.31 (18) | C26—C27—H27B | 109.5 |
| C7—C12—C11 | 123.46 (18) | H27A—C27—H27B | 109.5 |
| O1—C12—C11 | 115.23 (17) | C26—C27—H27C | 109.5 |
| O1—C13—C5 | 121.45 (18) | H27A—C27—H27C | 109.5 |
| O1—C13—C1 | 115.70 (17) | H27B—C27—H27C | 109.5 |
| C5—C13—C1 | 122.85 (18) | N4—C28—C29 | 115.4 (3) |
| N1—C14—C15 | 114.25 (18) | N4—C28—H28A | 108.4 |
| N1—C14—H14A | 108.7 | C29—C28—H28A | 108.4 |
| C15—C14—H14A | 108.7 | N4—C28—H28B | 108.4 |
| N1—C14—H14B | 108.7 | C29—C28—H28B | 108.4 |
| C15—C14—H14B | 108.7 | H28A—C28—H28B | 107.5 |
| H14A—C14—H14B | 107.6 | C28—C29—H29A | 109.5 |
| C14—C15—H15A | 109.5 | C28—C29—H29B | 109.5 |
| C14—C15—H15B | 109.5 | H29A—C29—H29B | 109.5 |
| H15A—C15—H15B | 109.5 | C28—C29—H29C | 109.5 |
| C14—C15—H15C | 109.5 | H29A—C29—H29C | 109.5 |
| H15A—C15—H15C | 109.5 | H29B—C29—H29C | 109.5 |
| H15B—C15—H15C | 109.5 | | |
| N2—P1—N1—C16 | -101.02 (17) | C9—C10—C11—C12 | 5.2 (3) |
| C1—P1—N1—C16 | 154.27 (16) | C9—C10—C11—P2 | -175.46 (19) |
| N2—P1—N1—C14 | 70.55 (18) | N3—P2—C11—C10 | 113.93 (19) |
| C1—P1—N1—C14 | -34.16 (17) | N4—P2—C11—C10 | 2.3 (2) |
| N1—P1—N2—C20 | 122.28 (17) | N3—P2—C11—C12 | -66.72 (17) |
| C1—P1—N2—C20 | -133.86 (18) | N4—P2—C11—C12 | -178.34 (16) |
| N1—P1—N2—C18 | -30.1 (2) | C8—C7—C12—O1 | -175.96 (18) |
| C1—P1—N2—C18 | 73.8 (2) | C6—C7—C12—O1 | 2.4 (3) |
| N4—P2—N3—C24 | -97.65 (16) | C8—C7—C12—C11 | 3.2 (3) |

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| C11—P2—N3—C24 | 156.43 (15) | C6—C7—C12—C11 | -178.5 (2) |
| N4—P2—N3—C22 | 73.12 (19) | C13—O1—C12—C7 | -19.3 (3) |
| C11—P2—N3—C22 | -32.80 (18) | C13—O1—C12—C11 | 161.51 (17) |
| N3—P2—N4—C28 | 124.9 (2) | C10—C11—C12—C7 | -6.3 (3) |
| C11—P2—N4—C28 | -132.3 (2) | P2—C11—C12—C7 | 174.29 (16) |
| N3—P2—N4—C26 | -38.7 (2) | C10—C11—C12—O1 | 172.85 (18) |
| C11—P2—N4—C26 | 64.1 (2) | P2—C11—C12—O1 | -6.5 (2) |
| N1—P1—C1—C2 | 122.63 (17) | C12—O1—C13—C5 | 12.3 (3) |
| N2—P1—C1—C2 | 10.69 (19) | C12—O1—C13—C1 | -166.96 (16) |
| N1—P1—C1—C13 | -62.09 (17) | C4—C5—C13—O1 | -173.69 (18) |
| N2—P1—C1—C13 | -174.03 (16) | C6—C5—C13—O1 | 11.3 (3) |
| C13—C1—C2—C3 | 2.4 (3) | C4—C5—C13—C1 | 5.5 (3) |
| P1—C1—C2—C3 | 177.83 (16) | C6—C5—C13—C1 | -169.50 (19) |
| C1—C2—C3—C4 | 1.6 (3) | C2—C1—C13—O1 | 173.18 (17) |
| C2—C3—C4—C5 | -2.2 (3) | P1—C1—C13—O1 | -2.4 (2) |
| C3—C4—C5—C13 | -1.3 (3) | C2—C1—C13—C5 | -6.1 (3) |
| C3—C4—C5—C6 | 173.6 (2) | P1—C1—C13—C5 | 178.41 (15) |
| C4—C5—C6—C7 | 160.1 (2) | C16—N1—C14—C15 | -59.4 (2) |
| C13—C5—C6—C7 | -25.1 (3) | P1—N1—C14—C15 | 128.82 (18) |
| C4—C5—C6—C6" | 37.7 (3) | C14—N1—C16—C17 | -65.7 (3) |
| C13—C5—C6—C6" | -147.5 (2) | P1—N1—C16—C17 | 106.8 (2) |
| C4—C5—C6—C6' | -81.9 (3) | C20—N2—C18—C19 | 52.3 (3) |
| C13—C5—C6—C6' | 92.9 (2) | P1—N2—C18—C19 | -155.28 (19) |
| C5—C6—C7—C12 | 18.5 (3) | C18—N2—C20—C21 | 58.6 (3) |
| C6"—C6—C7—C12 | 141.4 (2) | P1—N2—C20—C21 | -95.2 (3) |
| C6'—C6—C7—C12 | -99.3 (2) | C24—N3—C22—C23 | -71.2 (2) |
| C5—C6—C7—C8 | -163.2 (2) | P2—N3—C22—C23 | 117.85 (19) |
| C6"—C6—C7—C8 | -40.4 (3) | C22—N3—C24—C25 | -77.7 (3) |
| C6'—C6—C7—C8 | 79.0 (3) | P2—N3—C24—C25 | 94.1 (2) |
| C12—C7—C8—C9 | 1.3 (3) | C28—N4—C26—C27 | -56.6 (3) |
| C6—C7—C8—C9 | -177.0 (2) | P2—N4—C26—C27 | 107.2 (2) |
| C7—C8—C9—C10 | -2.4 (4) | C26—N4—C28—C29 | -60.1 (4) |
| C8—C9—C10—C11 | -1.1 (4) | P2—N4—C28—C29 | 134.5 (2) |
