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1-Phenyl-4-(triphenylphosphanylidene)-pyrrolidine-2,3,5-trione

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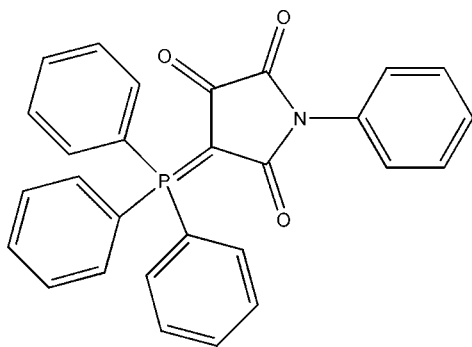
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.052; wR factor = 0.181; data-to-parameter ratio = 13.2.

In the title compound, $\text{C}_{28}\text{H}_{20}\text{NO}_3\text{P}$, the five-membered maleimide ring is almost planar. The interplanar angles between the maleimide ring and the three P-bound phenyl rings are 70.6 (2), 60.4 (2) and 54.68 (18)°, while the dihedral angle between the maleimide ring and the N-bound phenyl group is 55.43 (19)°.

Related literature

For related literature, see: Augustin *et al.* (1979); Trost & Schmidt (1988); Mao *et al.* (2005).



Experimental

Crystal data

 $\text{C}_{28}\text{H}_{20}\text{NO}_3\text{P}$ $M_r = 449.42$ Orthorhombic, $Pbca$ $a = 18.171$ (4) Å $b = 12.553$ (3) Å $c = 19.982$ (4) Å $V = 4557.9$ (16) Å³ $Z = 8$ Mo $K\alpha$ radiation $\mu = 0.15$ mm⁻¹ $T = 293$ (2) K $0.30 \times 0.20 \times 0.20$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer

Absorption correction: ψ scan (*XCAD4*; Harms & Wocadlo, 1995) $T_{\min} = 0.956$, $T_{\max} = 0.970$

3961 measured reflections

3961 independent reflections

2590 reflections with $I > 2\sigma(I)$

3 standard reflections

every 150 reflections

intensity decay: none

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.051$ $wR(F^2) = 0.180$ $S = 1.07$

3961 reflections

299 parameters

H-atom parameters constrained

 $\Delta\rho_{\max} = 0.40$ e Å⁻³ $\Delta\rho_{\min} = -0.34$ e Å⁻³

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

This work was supported by the Shaoxing Key Discipline of Organic Chemistry.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2239).

References

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supplementary materials

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1-Phenyl-4-(triphenylphosphanylidene)pyrrolidine-2,3,5-trione

D.-H. Fan

Comment

Organophosphorus compounds play an important role in organic synthesis. In some reactions, a nucleophilic tertiary phosphine initially adds to the triple bond of an electron-deficient alkyne and is finally eliminated from the reaction product after a series of transformations. As such, the tertiary phosphine plays the role of a catalyst (Trost *et al.*, 1988). In recent experiments, the title compound, (I), was synthesized unexpectedly when triphenylphosphine, Ph₃P, was used as a catalyst in a reaction with *N*-phenylmaleimide (Augustin *et al.*, 1979). In this reaction, the Ph₃P was not eliminated but instead reacted (Mao *et al.*, 2005). The structure of (I), Fig. 1, shows the interplanar angles between the maleimide ring and the three P-bound phenyl rings to be 70.6 (2), 60.4 (2) and 54.68 (18)°, respectively, and the dihedral angle between the maleimide ring and the N-bound phenyl group to be 55.4 (3)°.

Experimental

To a CH₂Cl₂ (5 ml) solution comprising Ph₃P (0.06 g, 0.00014 mmol), *N*-phenylmaleimide (0.173 g, 1.0 mmol) and 1-aminobenzotriazole (0.201 g, 1.5 mmol), lead tetraacetate (0.666 g, 1.5 mmol) in CH₂Cl₂ (5 ml) was added dropwise. After stirring at room temperature for 30 min, the solution was concentrated and separated by flash chromatography on a silica gel column with petroleum ether/ethyl acetate as eluent. Compound (I) was isolated as one of the products (yield 2.4%); m. pt. 526 K.

Refinement

The H atoms were fixed geometrically and were treated as riding on their parent C atoms, with C—H = 0.93 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

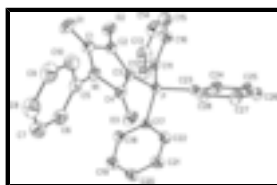


Fig. 1. The molecular structure of (I) showing 30% probability displacement ellipsoids and the atom labelling scheme.

1-Phenyl-4-(triphenylphosphanylidene)pyrrolidine-2,3,5-trione

Crystal data

C₂₈H₂₀NO₃P

$D_x = 1.310 \text{ Mg m}^{-3}$

supplementary materials

$M_r = 449.42$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 18.171$ (4) Å

$b = 12.553$ (3) Å

$c = 19.982$ (4) Å

$V = 4557.9$ (16) Å³

$Z = 8$

$F_{000} = 1872$

Melting point: 527 K

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 187 reflections

$\theta = 3.6$ – 45.0°

$\mu = 0.15$ mm⁻¹

$T = 293$ (2) K

Block, colorless

$0.30 \times 0.20 \times 0.20$ mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ (2) K

$\omega/2\theta$ scans

Absorption correction: ψ scan
(XCAD4; Harms & Wocadlo, 1995)

$T_{\min} = 0.956$, $T_{\max} = 0.970$

3961 measured reflections

3961 independent reflections

2590 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.000$

$\theta_{\text{max}} = 25.0^\circ$

$\theta_{\text{min}} = 2.0^\circ$

$h = 0 \rightarrow 21$

$k = 0 \rightarrow 14$

$l = -23 \rightarrow 0$

3 standard reflections

every 150 reflections

intensity decay: none

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.051$

$wR(F^2) = 0.180$

$S = 1.07$

3961 reflections

299 parameters

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

$$w = 1/[\sigma^2(F_o^2) + (0.0776P)^2 + 4.6891P]$$

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

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.40$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.34$ e Å⁻³

Extinction correction: SHELXTL (Sheldrick, 2008),

$$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$$

Extinction coefficient: 0.0079 (7)

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 $F^2 > 2\sigma(F^2)$ 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 | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|---------------|------------|--------------|----------------------------------|
| C1 | 0.14772 (19) | 0.5354 (3) | 0.47338 (17) | 0.0463 (9) |
| C2 | 0.14220 (18) | 0.6388 (3) | 0.43154 (16) | 0.0420 (8) |
| C3 | 0.10163 (18) | 0.6110 (3) | 0.37341 (15) | 0.0377 (8) |
| C4 | 0.07940 (18) | 0.5005 (3) | 0.37848 (16) | 0.0408 (8) |
| C5 | 0.0969 (2) | 0.3513 (3) | 0.46274 (16) | 0.0436 (8) |
| C6 | 0.0270 (2) | 0.3128 (3) | 0.46980 (19) | 0.0532 (10) |
| H6A | -0.0131 | 0.3545 | 0.4577 | 0.064* |
| C7 | 0.0162 (3) | 0.2110 (3) | 0.4952 (2) | 0.0619 (11) |
| H7A | -0.0313 | 0.1845 | 0.5003 | 0.074* |
| C8 | 0.0757 (3) | 0.1496 (3) | 0.5128 (2) | 0.0647 (11) |
| H8A | 0.0686 | 0.0816 | 0.5301 | 0.078* |
| C9 | 0.1461 (3) | 0.1888 (3) | 0.5048 (2) | 0.0645 (11) |
| H9A | 0.1863 | 0.1470 | 0.5166 | 0.077* |
| C10 | 0.1572 (2) | 0.2895 (3) | 0.47953 (19) | 0.0516 (9) |
| H10A | 0.2046 | 0.3157 | 0.4738 | 0.062* |
| C11 | 0.1025 (2) | 0.8272 (3) | 0.32675 (17) | 0.0448 (8) |
| C12 | 0.0544 (3) | 0.9069 (3) | 0.3436 (2) | 0.0627 (11) |
| H12A | 0.0041 | 0.8933 | 0.3448 | 0.075* |
| C13 | 0.0807 (4) | 1.0078 (4) | 0.3588 (3) | 0.0909 (17) |
| H13A | 0.0483 | 1.0624 | 0.3696 | 0.109* |
| C14 | 0.1563 (4) | 1.0261 (4) | 0.3575 (3) | 0.0956 (18) |
| H14A | 0.1744 | 1.0932 | 0.3685 | 0.115* |
| C15 | 0.2036 (3) | 0.9482 (4) | 0.3407 (2) | 0.0782 (14) |
| H15A | 0.2538 | 0.9621 | 0.3394 | 0.094* |
| C16 | 0.1779 (2) | 0.8478 (4) | 0.3253 (2) | 0.0607 (11) |
| H16A | 0.2108 | 0.7939 | 0.3140 | 0.073* |
| C17 | -0.02614 (17) | 0.6940 (3) | 0.30122 (16) | 0.0388 (8) |
| C18 | -0.07044 (19) | 0.6465 (3) | 0.34892 (18) | 0.0513 (9) |
| H18A | -0.0492 | 0.6132 | 0.3858 | 0.062* |
| C19 | -0.1459 (2) | 0.6482 (4) | 0.3422 (2) | 0.0695 (13) |
| H19A | -0.1755 | 0.6137 | 0.3733 | 0.083* |
| C20 | -0.1774 (2) | 0.7013 (4) | 0.2891 (2) | 0.0678 (12) |
| H20A | -0.2284 | 0.7045 | 0.2854 | 0.081* |
| C21 | -0.1342 (2) | 0.7497 (4) | 0.2415 (2) | 0.0635 (11) |
| H21A | -0.1560 | 0.7850 | 0.2057 | 0.076* |
| C22 | -0.05895 (19) | 0.7460 (3) | 0.24670 (19) | 0.0520 (9) |
| H22A | -0.0297 | 0.7779 | 0.2142 | 0.062* |
| C23 | 0.11017 (17) | 0.6596 (3) | 0.22757 (16) | 0.0404 (8) |
| C24 | 0.1195 (2) | 0.7381 (4) | 0.17908 (19) | 0.0568 (10) |
| H24A | 0.1071 | 0.8084 | 0.1885 | 0.068* |

supplementary materials

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|------|--------------|-------------|--------------|-------------|
| C25 | 0.1475 (2) | 0.7109 (4) | 0.11636 (19) | 0.0642 (12) |
| H25A | 0.1540 | 0.7631 | 0.0839 | 0.077* |
| C26 | 0.1653 (2) | 0.6068 (5) | 0.1026 (2) | 0.0694 (13) |
| H26A | 0.1839 | 0.5886 | 0.0607 | 0.083* |
| C27 | 0.1559 (2) | 0.5302 (4) | 0.1501 (2) | 0.0667 (12) |
| H27A | 0.1681 | 0.4600 | 0.1403 | 0.080* |
| C28 | 0.1284 (2) | 0.5556 (3) | 0.21299 (19) | 0.0536 (10) |
| H28A | 0.1224 | 0.5027 | 0.2451 | 0.064* |
| N1 | 0.10879 (16) | 0.4592 (2) | 0.43984 (14) | 0.0445 (7) |
| O1 | 0.17921 (16) | 0.5257 (2) | 0.52663 (13) | 0.0717 (9) |
| O2 | 0.16942 (15) | 0.7217 (2) | 0.45206 (13) | 0.0610 (8) |
| O3 | 0.04234 (15) | 0.4470 (2) | 0.34108 (12) | 0.0568 (7) |
| P | 0.07209 (4) | 0.69405 (7) | 0.30865 (4) | 0.0358 (3) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C1 | 0.0449 (19) | 0.056 (2) | 0.0382 (19) | 0.0003 (17) | -0.0043 (16) | -0.0005 (17) |
| C2 | 0.0376 (17) | 0.052 (2) | 0.0361 (18) | 0.0013 (16) | -0.0016 (15) | -0.0003 (16) |
| C3 | 0.0375 (17) | 0.0408 (19) | 0.0348 (17) | 0.0025 (15) | -0.0036 (14) | -0.0018 (14) |
| C4 | 0.0430 (19) | 0.045 (2) | 0.0341 (17) | 0.0074 (16) | -0.0041 (15) | -0.0012 (15) |
| C5 | 0.051 (2) | 0.045 (2) | 0.0353 (18) | 0.0036 (17) | 0.0005 (15) | 0.0006 (15) |
| C6 | 0.053 (2) | 0.055 (2) | 0.052 (2) | 0.0084 (19) | -0.0034 (18) | 0.0045 (18) |
| C7 | 0.071 (3) | 0.056 (3) | 0.059 (2) | -0.010 (2) | 0.000 (2) | 0.007 (2) |
| C8 | 0.086 (3) | 0.044 (2) | 0.064 (3) | 0.005 (2) | 0.001 (2) | 0.009 (2) |
| C9 | 0.077 (3) | 0.056 (3) | 0.061 (3) | 0.021 (2) | 0.001 (2) | 0.010 (2) |
| C10 | 0.048 (2) | 0.053 (2) | 0.054 (2) | 0.0111 (17) | 0.0017 (17) | 0.0042 (18) |
| C11 | 0.049 (2) | 0.048 (2) | 0.0376 (18) | -0.0043 (17) | 0.0016 (15) | 0.0031 (15) |
| C12 | 0.073 (3) | 0.050 (2) | 0.064 (3) | 0.005 (2) | 0.004 (2) | -0.007 (2) |
| C13 | 0.120 (5) | 0.050 (3) | 0.102 (4) | 0.004 (3) | 0.016 (3) | -0.016 (3) |
| C14 | 0.141 (6) | 0.056 (3) | 0.090 (4) | -0.035 (4) | -0.009 (4) | -0.009 (3) |
| C15 | 0.089 (4) | 0.077 (3) | 0.069 (3) | -0.040 (3) | 0.004 (3) | -0.004 (3) |
| C16 | 0.053 (2) | 0.065 (3) | 0.064 (3) | -0.015 (2) | 0.0049 (19) | -0.003 (2) |
| C17 | 0.0333 (17) | 0.0425 (18) | 0.0404 (18) | 0.0039 (15) | -0.0031 (14) | -0.0014 (15) |
| C18 | 0.0388 (19) | 0.075 (3) | 0.0404 (19) | -0.0013 (18) | 0.0010 (16) | 0.0088 (18) |
| C19 | 0.043 (2) | 0.108 (4) | 0.057 (2) | -0.007 (2) | 0.0007 (19) | 0.017 (2) |
| C20 | 0.033 (2) | 0.100 (4) | 0.070 (3) | 0.004 (2) | 0.0008 (19) | 0.012 (3) |
| C21 | 0.042 (2) | 0.077 (3) | 0.072 (3) | 0.003 (2) | -0.010 (2) | 0.021 (2) |
| C22 | 0.0396 (19) | 0.062 (2) | 0.055 (2) | 0.0029 (18) | -0.0015 (17) | 0.0202 (19) |
| C23 | 0.0318 (16) | 0.056 (2) | 0.0334 (17) | -0.0008 (16) | -0.0025 (14) | -0.0026 (15) |
| C24 | 0.049 (2) | 0.074 (3) | 0.047 (2) | 0.006 (2) | -0.0005 (17) | 0.009 (2) |
| C25 | 0.053 (2) | 0.106 (4) | 0.034 (2) | 0.004 (2) | -0.0038 (17) | 0.012 (2) |
| C26 | 0.052 (2) | 0.118 (4) | 0.038 (2) | -0.009 (3) | 0.0076 (18) | -0.018 (3) |
| C27 | 0.069 (3) | 0.081 (3) | 0.050 (2) | -0.002 (2) | 0.008 (2) | -0.025 (2) |
| C28 | 0.053 (2) | 0.065 (3) | 0.043 (2) | -0.0003 (19) | 0.0045 (17) | -0.0066 (18) |
| N1 | 0.0512 (17) | 0.0441 (17) | 0.0382 (15) | 0.0040 (14) | -0.0062 (13) | 0.0036 (13) |
| O1 | 0.087 (2) | 0.075 (2) | 0.0529 (17) | -0.0132 (17) | -0.0312 (16) | 0.0138 (14) |
| O2 | 0.0692 (18) | 0.0578 (17) | 0.0560 (16) | -0.0164 (14) | -0.0168 (14) | -0.0007 (13) |

| | | | | | | |
|----|-------------|-------------|-------------|--------------|--------------|--------------|
| O3 | 0.0769 (18) | 0.0463 (15) | 0.0472 (15) | -0.0062 (13) | -0.0173 (14) | -0.0067 (12) |
| P | 0.0330 (4) | 0.0412 (5) | 0.0331 (5) | 0.0014 (4) | 0.0001 (3) | 0.0001 (4) |

Geometric parameters (Å, °)

| | | | |
|-----------|-----------|--------------|-----------|
| C1—O1 | 1.214 (4) | C14—H14A | 0.9300 |
| C1—N1 | 1.365 (4) | C15—C16 | 1.379 (6) |
| C1—C2 | 1.547 (5) | C15—H15A | 0.9300 |
| C2—O2 | 1.223 (4) | C16—H16A | 0.9300 |
| C2—C3 | 1.419 (4) | C17—C18 | 1.383 (5) |
| C3—C4 | 1.448 (5) | C17—C22 | 1.403 (5) |
| C3—P | 1.746 (3) | C17—P | 1.791 (3) |
| C4—O3 | 1.210 (4) | C18—C19 | 1.379 (5) |
| C4—N1 | 1.434 (4) | C18—H18A | 0.9300 |
| C5—C6 | 1.367 (5) | C19—C20 | 1.377 (6) |
| C5—C10 | 1.383 (5) | C19—H19A | 0.9300 |
| C5—N1 | 1.447 (4) | C20—C21 | 1.376 (6) |
| C6—C7 | 1.388 (5) | C20—H20A | 0.9300 |
| C6—H6A | 0.9300 | C21—C22 | 1.372 (5) |
| C7—C8 | 1.375 (6) | C21—H21A | 0.9300 |
| C7—H7A | 0.9300 | C22—H22A | 0.9300 |
| C8—C9 | 1.380 (6) | C23—C28 | 1.377 (5) |
| C8—H8A | 0.9300 | C23—C24 | 1.393 (5) |
| C9—C10 | 1.376 (6) | C23—P | 1.814 (3) |
| C9—H9A | 0.9300 | C24—C25 | 1.395 (5) |
| C10—H10A | 0.9300 | C24—H24A | 0.9300 |
| C11—C12 | 1.371 (5) | C25—C26 | 1.374 (6) |
| C11—C16 | 1.394 (5) | C25—H25A | 0.9300 |
| C11—P | 1.798 (4) | C26—C27 | 1.362 (6) |
| C12—C13 | 1.387 (6) | C26—H26A | 0.9300 |
| C12—H12A | 0.9300 | C27—C28 | 1.389 (5) |
| C13—C14 | 1.395 (8) | C27—H27A | 0.9300 |
| C13—H13A | 0.9300 | C28—H28A | 0.9300 |
| C14—C15 | 1.344 (8) | | |
| O1—C1—N1 | 127.1 (4) | C11—C16—H16A | 120.1 |
| O1—C1—C2 | 126.1 (3) | C18—C17—C22 | 119.2 (3) |
| N1—C1—C2 | 106.8 (3) | C18—C17—P | 121.6 (3) |
| O2—C2—C3 | 133.9 (3) | C22—C17—P | 119.2 (3) |
| O2—C2—C1 | 120.4 (3) | C19—C18—C17 | 120.3 (4) |
| C3—C2—C1 | 105.7 (3) | C19—C18—H18A | 119.8 |
| C2—C3—C4 | 108.8 (3) | C17—C18—H18A | 119.8 |
| C2—C3—P | 128.3 (3) | C20—C19—C18 | 119.8 (4) |
| C4—C3—P | 122.5 (2) | C20—C19—H19A | 120.1 |
| O3—C4—N1 | 122.3 (3) | C18—C19—H19A | 120.1 |
| O3—C4—C3 | 130.1 (3) | C21—C20—C19 | 120.6 (4) |
| N1—C4—C3 | 107.6 (3) | C21—C20—H20A | 119.7 |
| C6—C5—C10 | 120.9 (3) | C19—C20—H20A | 119.7 |
| C6—C5—N1 | 120.2 (3) | C22—C21—C20 | 120.1 (4) |
| C10—C5—N1 | 118.9 (3) | C22—C21—H21A | 120.0 |

supplementary materials

| | | | |
|--------------|------------|-----------------|-------------|
| C5—C6—C7 | 119.6 (4) | C20—C21—H21A | 120.0 |
| C5—C6—H6A | 120.2 | C21—C22—C17 | 119.9 (3) |
| C7—C6—H6A | 120.2 | C21—C22—H22A | 120.0 |
| C8—C7—C6 | 120.0 (4) | C17—C22—H22A | 120.0 |
| C8—C7—H7A | 120.0 | C28—C23—C24 | 119.6 (3) |
| C6—C7—H7A | 120.0 | C28—C23—P | 120.5 (3) |
| C7—C8—C9 | 119.9 (4) | C24—C23—P | 119.9 (3) |
| C7—C8—H8A | 120.0 | C23—C24—C25 | 119.7 (4) |
| C9—C8—H8A | 120.0 | C23—C24—H24A | 120.1 |
| C10—C9—C8 | 120.4 (4) | C25—C24—H24A | 120.1 |
| C10—C9—H9A | 119.8 | C26—C25—C24 | 120.0 (4) |
| C8—C9—H9A | 119.8 | C26—C25—H25A | 120.0 |
| C9—C10—C5 | 119.2 (4) | C24—C25—H25A | 120.0 |
| C9—C10—H10A | 120.4 | C27—C26—C25 | 120.1 (4) |
| C5—C10—H10A | 120.4 | C27—C26—H26A | 120.0 |
| C12—C11—C16 | 119.8 (4) | C25—C26—H26A | 120.0 |
| C12—C11—P | 122.1 (3) | C26—C27—C28 | 121.0 (4) |
| C16—C11—P | 118.0 (3) | C26—C27—H27A | 119.5 |
| C11—C12—C13 | 120.0 (5) | C28—C27—H27A | 119.5 |
| C11—C12—H12A | 120.0 | C23—C28—C27 | 119.7 (4) |
| C13—C12—H12A | 120.0 | C23—C28—H28A | 120.2 |
| C12—C13—C14 | 119.1 (5) | C27—C28—H28A | 120.2 |
| C12—C13—H13A | 120.4 | C1—N1—C4 | 111.1 (3) |
| C14—C13—H13A | 120.4 | C1—N1—C5 | 125.3 (3) |
| C15—C14—C13 | 120.9 (5) | C4—N1—C5 | 123.6 (3) |
| C15—C14—H14A | 119.5 | C3—P—C17 | 111.55 (16) |
| C13—C14—H14A | 119.5 | C3—P—C11 | 108.15 (16) |
| C14—C15—C16 | 120.3 (5) | C17—P—C11 | 108.89 (17) |
| C14—C15—H15A | 119.8 | C3—P—C23 | 113.70 (16) |
| C16—C15—H15A | 119.8 | C17—P—C23 | 107.82 (15) |
| C15—C16—C11 | 119.8 (4) | C11—P—C23 | 106.52 (16) |
| C15—C16—H16A | 120.1 | | |
| O1—C1—C2—O2 | -1.9 (6) | C25—C26—C27—C28 | -0.1 (6) |
| N1—C1—C2—O2 | 176.3 (3) | C24—C23—C28—C27 | 0.0 (5) |
| O1—C1—C2—C3 | 179.0 (4) | P—C23—C28—C27 | 178.5 (3) |
| N1—C1—C2—C3 | -2.7 (4) | C26—C27—C28—C23 | 0.2 (6) |
| O2—C2—C3—C4 | -176.2 (4) | O1—C1—N1—C4 | 179.9 (4) |
| C1—C2—C3—C4 | 2.7 (4) | C2—C1—N1—C4 | 1.7 (4) |
| O2—C2—C3—P | -2.9 (6) | O1—C1—N1—C5 | 1.0 (6) |
| C1—C2—C3—P | 176.0 (3) | C2—C1—N1—C5 | -177.3 (3) |
| C2—C3—C4—O3 | 177.3 (4) | O3—C4—N1—C1 | -179.2 (3) |
| P—C3—C4—O3 | 3.5 (5) | C3—C4—N1—C1 | -0.1 (4) |
| C2—C3—C4—N1 | -1.7 (4) | O3—C4—N1—C5 | -0.2 (5) |
| P—C3—C4—N1 | -175.5 (2) | C3—C4—N1—C5 | 178.9 (3) |
| C10—C5—C6—C7 | 1.1 (6) | C6—C5—N1—C1 | 123.4 (4) |
| N1—C5—C6—C7 | -176.6 (3) | C10—C5—N1—C1 | -54.3 (5) |
| C5—C6—C7—C8 | -0.3 (6) | C6—C5—N1—C4 | -55.5 (5) |
| C6—C7—C8—C9 | -0.4 (7) | C10—C5—N1—C4 | 126.8 (4) |
| C7—C8—C9—C10 | 0.3 (7) | C2—C3—P—C17 | -119.4 (3) |

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| C8—C9—C10—C5 | 0.5 (6) | C4—C3—P—C17 | 53.1 (3) |
| C6—C5—C10—C9 | -1.2 (6) | C2—C3—P—C11 | 0.4 (4) |
| N1—C5—C10—C9 | 176.5 (3) | C4—C3—P—C11 | 172.9 (3) |
| C16—C11—C12—C13 | 0.4 (6) | C2—C3—P—C23 | 118.4 (3) |
| P—C11—C12—C13 | 178.4 (4) | C4—C3—P—C23 | -69.1 (3) |
| C11—C12—C13—C14 | -0.9 (8) | C18—C17—P—C3 | 9.6 (4) |
| C12—C13—C14—C15 | 1.3 (9) | C22—C17—P—C3 | -172.3 (3) |
| C13—C14—C15—C16 | -1.1 (8) | C18—C17—P—C11 | -109.7 (3) |
| C14—C15—C16—C11 | 0.5 (7) | C22—C17—P—C11 | 68.4 (3) |
| C12—C11—C16—C15 | -0.1 (6) | C18—C17—P—C23 | 135.1 (3) |
| P—C11—C16—C15 | -178.3 (3) | C22—C17—P—C23 | -46.8 (3) |
| C22—C17—C18—C19 | 1.5 (6) | C12—C11—P—C3 | -110.7 (3) |
| P—C17—C18—C19 | 179.6 (3) | C16—C11—P—C3 | 67.4 (3) |
| C17—C18—C19—C20 | -2.7 (7) | C12—C11—P—C17 | 10.7 (4) |
| C18—C19—C20—C21 | 2.2 (8) | C16—C11—P—C17 | -171.2 (3) |
| C19—C20—C21—C22 | -0.4 (7) | C12—C11—P—C23 | 126.7 (3) |
| C20—C21—C22—C17 | -0.9 (7) | C16—C11—P—C23 | -55.2 (3) |
| C18—C17—C22—C21 | 0.3 (6) | C28—C23—P—C3 | 29.6 (3) |
| P—C17—C22—C21 | -177.8 (3) | C24—C23—P—C3 | -151.9 (3) |
| C28—C23—C24—C25 | -0.3 (5) | C28—C23—P—C17 | -94.7 (3) |
| P—C23—C24—C25 | -178.8 (3) | C24—C23—P—C17 | 83.8 (3) |
| C23—C24—C25—C26 | 0.3 (6) | C28—C23—P—C11 | 148.6 (3) |
| C24—C25—C26—C27 | -0.1 (6) | C24—C23—P—C11 | -32.9 (3) |

