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4-Diphenylphosphanyl-8-methyl-1,5-naphthyridine

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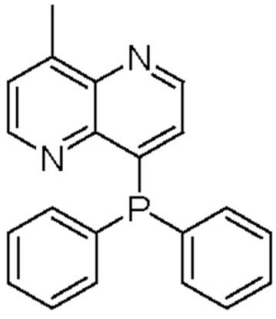
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.050; wR factor = 0.155; data-to-parameter ratio = 14.9.

In the title compound, $C_{21}H_{17}N_2P$, the dihedral angles between the 1,5-naphthyridine ring system (r.m.s. deviation = 0.005 Å) and the phenyl rings are 89.18 (8) and 77.39 (8)°. The phenyl rings are almost perpendicular, making a dihedral angle of 88.12 (8)°. The only possible intermolecular interaction is a very weak aromatic π–π stacking interaction [centroid–centroid separation = 3.898 (2) Å].

Related literature

For further synthetic details and background to the role of the title compound as an intermediate in the synthesis of OLED materials, see: Chen *et al.* (2012).



Experimental

Crystal data

$C_{21}H_{17}N_2P$
M_r = 328.34
Triclinic, $P\overline{1}$
a = 7.2320 (14) Å
b = 7.4470 (15) Å
c = 16.780 (3) Å
α = 99.78 (3)°
β = 93.35 (3)°
γ = 98.58 (3)°
V = 877.4 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.16 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.954, T_{max} = 0.984
3500 measured reflections
3224 independent reflections
2285 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.155
S = 1.00
3224 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7082).

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supporting information

Acta Cryst. (2013). E**69**, o928 [doi:10.1107/S1600536813013196]

4-Diphenylphosphanyl-8-methyl-1,5-naphthyridine

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S1. Comment

The tittle compound, (I), is an intermediate for manufacturing OLED materials (Chen *et al.*, 2012). We now report its crystal structure (Fig. 1).

The 1,5-naphthyridine ring system is nearly planar with an r.m.s. deviation of 0.005Å; its mean plane is oriented with respect to the two phenyl rings at 89.18 (8) and 77.39 (8)°. The two phenyl rings are twisted to each other with a dihedral angle of 88.12 (8)°. The crystal packing of the molecules in the crystal is influenced by van der Waals forces (Fig. 2).

S2. Experimental

The title compund was synthesized according to the published procedure (Chen *et al.*, 2012). Yellow blocks were obtained by dissolving it (0.5 g) in tetrahydrofuran (20 ml) and evaporating the solvent slowly at room temperature for about 5 d.

S3. Refinement

H atoms were positioned geometrically and refined as riding groups, with C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.2 for aromatic H, and x = 1.5 for other H.

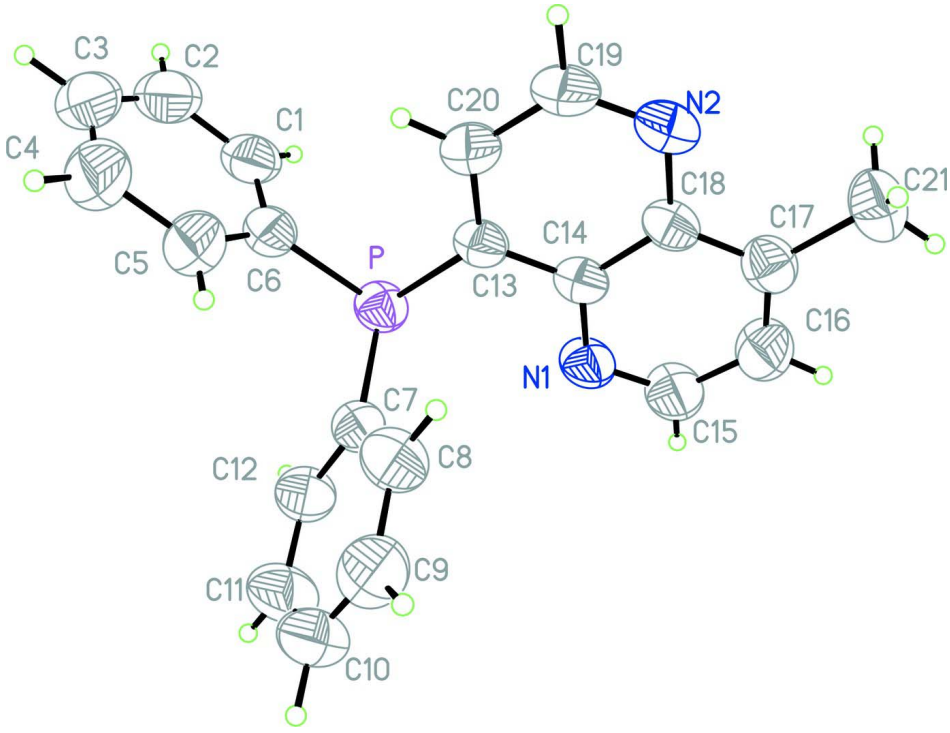

Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

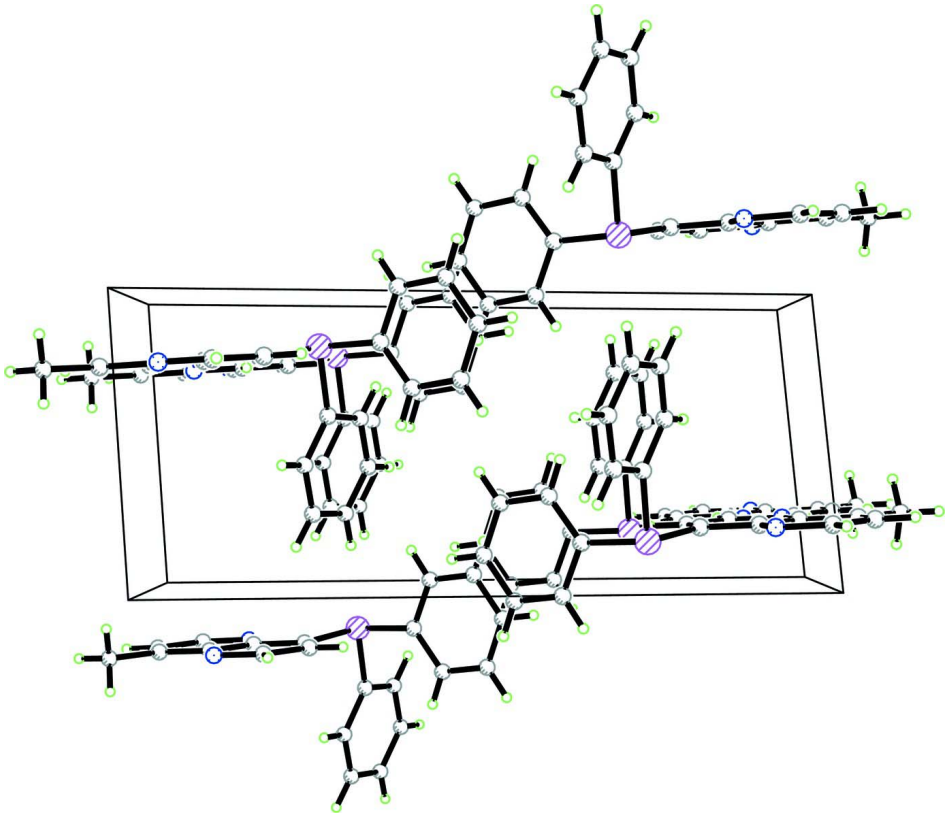

Figure 2

A packing diagram of (I).

4-Diphenylphosphanyl-8-methyl-1,5-naphthyridine

Crystal data

$C_{21}H_{17}N_2P$
$M_r = 328.34$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.2320\ (14)$ Å
$b = 7.4470\ (15)$ Å
$c = 16.780\ (3)$ Å
$\alpha = 99.78\ (3)°$
$\beta = 93.35\ (3)°$
$\gamma = 98.58\ (3)°$
$V = 877.4\ (3)$ Å^3
$Z = 2$
$F(000) = 344$
$D_x = 1.243$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10–14°$
$\mu = 0.16$ mm^{-1}
$T = 293$ K
Block, yellow
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.954$, $T_{max} = 0.984$
3500 measured reflections
3224 independent reflections
2285 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 25.4°$, $\theta_{min} = 1.2°$
$h = 0\rightarrow8$
$k = -8\rightarrow8$
$l = -20\rightarrow20$
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.155$
$S = 1.00$
3224 reflections
217 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
$w = 1/[\sigma^2(F_o^2) + (0.096P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
P	0.18105 (10)	0.17196 (9)	0.71974 (4)	0.0529 (2)
N1	0.2284 (3)	0.3164 (3)	0.89550 (13)	0.0603 (6)
C1	−0.0068 (5)	−0.0965 (4)	0.59708 (17)	0.0711 (8)
H1B	−0.1116	−0.0650	0.6223	0.085*
N2	0.2453 (3)	−0.1579 (3)	0.92992 (13)	0.0569 (6)
C2	−0.0308 (6)	−0.2312 (5)	0.5287 (2)	0.0906 (11)
H2B	−0.1507	−0.2917	0.5087	0.109*
C3	0.1213 (7)	−0.2762 (5)	0.4901 (2)	0.0976 (13)
H3A	0.1048	−0.3655	0.4432	0.117*
C4	0.2974 (6)	−0.1907 (5)	0.5202 (2)	0.0914 (11)
H4A	0.4009	−0.2230	0.4942	0.110*
C5	0.3227 (5)	−0.0553 (4)	0.58980 (18)	0.0734 (8)
H5A	0.4433	0.0028	0.6098	0.088*
C6	0.1710 (4)	−0.0060 (3)	0.62951 (15)	0.0579 (7)
C7	0.4103 (3)	0.3111 (3)	0.71826 (14)	0.0501 (6)
C8	0.5758 (4)	0.2855 (4)	0.75679 (17)	0.0644 (7)
H8A	0.5754	0.1889	0.7854	0.077*
C9	0.7416 (4)	0.4013 (4)	0.75339 (19)	0.0757 (8)
H9A	0.8516	0.3842	0.7806	0.091*
C10	0.7445 (5)	0.5412 (4)	0.7101 (2)	0.0822 (10)
H10A	0.8568	0.6181	0.7071	0.099*
C11	0.5835 (5)	0.5682 (4)	0.6713 (2)	0.0844 (10)
H11A	0.5859	0.6635	0.6419	0.101*
C12	0.4175 (4)	0.4557 (3)	0.67539 (17)	0.0652 (7)
H12A	0.3080	0.4764	0.6491	0.078*

C13	0.2210 (3)	0.0390 (3)	0.79998 (14)	0.0476 (6)
C14	0.2313 (3)	0.1306 (3)	0.88168 (14)	0.0468 (6)
C15	0.2393 (5)	0.3962 (4)	0.97172 (18)	0.0744 (9)
H15A	0.2379	0.5226	0.9827	0.089*
C16	0.2527 (4)	0.3065 (4)	1.03778 (18)	0.0736 (8)
H16A	0.2609	0.3736	1.0903	0.088*
C17	0.2539 (3)	0.1222 (4)	1.02590 (15)	0.0557 (6)
C18	0.2437 (3)	0.0284 (3)	0.94493 (15)	0.0478 (6)
C19	0.2366 (4)	−0.2382 (3)	0.85361 (17)	0.0638 (7)
H19A	0.2389	−0.3645	0.8426	0.077*
C20	0.2241 (4)	−0.1471 (3)	0.78760 (16)	0.0576 (6)
H20A	0.2179	−0.2133	0.7350	0.069*
C21	0.2657 (4)	0.0179 (4)	1.09549 (16)	0.0724 (8)
H21A	0.2718	0.1022	1.1460	0.109*
H21B	0.3761	−0.0394	1.0935	0.109*
H21C	0.1565	−0.0752	1.0911	0.109*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P	0.0594 (4)	0.0457 (4)	0.0574 (4)	0.0135 (3)	0.0070 (3)	0.0149 (3)
N1	0.0850 (16)	0.0364 (11)	0.0630 (14)	0.0140 (10)	0.0175 (12)	0.0113 (10)
C1	0.086 (2)	0.0568 (16)	0.0678 (18)	−0.0071 (15)	−0.0020 (16)	0.0218 (14)
N2	0.0624 (14)	0.0436 (11)	0.0676 (14)	0.0070 (10)	0.0070 (11)	0.0191 (10)
C2	0.124 (3)	0.066 (2)	0.070 (2)	−0.022 (2)	−0.013 (2)	0.0194 (17)
C3	0.166 (4)	0.0558 (19)	0.061 (2)	−0.009 (2)	0.003 (2)	0.0081 (15)
C4	0.136 (3)	0.065 (2)	0.077 (2)	0.024 (2)	0.029 (2)	0.0121 (17)
C5	0.091 (2)	0.0604 (17)	0.0681 (18)	0.0135 (15)	0.0148 (16)	0.0055 (14)
C6	0.0759 (18)	0.0475 (14)	0.0505 (14)	0.0035 (13)	0.0023 (13)	0.0162 (11)
C7	0.0615 (15)	0.0364 (12)	0.0539 (14)	0.0121 (11)	0.0124 (12)	0.0061 (10)
C8	0.0623 (17)	0.0624 (17)	0.0735 (18)	0.0144 (14)	0.0100 (14)	0.0214 (14)
C9	0.0608 (18)	0.087 (2)	0.076 (2)	0.0133 (16)	0.0077 (15)	0.0024 (17)
C10	0.082 (2)	0.069 (2)	0.088 (2)	−0.0125 (17)	0.0211 (19)	0.0113 (17)
C11	0.100 (3)	0.0589 (18)	0.096 (2)	−0.0019 (17)	0.017 (2)	0.0296 (17)
C12	0.0796 (19)	0.0476 (14)	0.0709 (18)	0.0105 (14)	0.0071 (14)	0.0175 (13)
C13	0.0499 (14)	0.0399 (12)	0.0547 (14)	0.0068 (10)	0.0084 (11)	0.0121 (10)
C14	0.0460 (13)	0.0402 (12)	0.0560 (14)	0.0065 (10)	0.0102 (11)	0.0121 (10)
C15	0.113 (3)	0.0438 (15)	0.0681 (18)	0.0187 (15)	0.0194 (17)	0.0057 (13)
C16	0.098 (2)	0.0628 (18)	0.0591 (17)	0.0169 (16)	0.0137 (16)	0.0018 (14)
C17	0.0519 (15)	0.0614 (16)	0.0563 (15)	0.0096 (12)	0.0090 (12)	0.0152 (12)
C18	0.0437 (13)	0.0456 (13)	0.0576 (14)	0.0082 (10)	0.0116 (11)	0.0158 (11)
C19	0.082 (2)	0.0361 (13)	0.0733 (18)	0.0077 (12)	0.0043 (15)	0.0130 (12)
C20	0.0713 (17)	0.0409 (13)	0.0591 (15)	0.0070 (12)	0.0045 (13)	0.0072 (11)
C21	0.0725 (19)	0.090 (2)	0.0609 (17)	0.0143 (16)	0.0112 (14)	0.0279 (15)

Geometric parameters (Å, º)

P—C7	1.823 (3)	C9—C10	1.367 (4)
P—C6	1.825 (3)	C9—H9A	0.9300
P—C13	1.836 (2)	C10—C11	1.358 (5)
N1—C15	1.308 (3)	C10—H10A	0.9300
N1—C14	1.367 (3)	C11—C12	1.369 (4)
C1—C2	1.374 (4)	C11—H11A	0.9300
C1—C6	1.392 (4)	C12—H12A	0.9300
C1—H1B	0.9300	C13—C20	1.370 (3)
N2—C19	1.312 (3)	C13—C14	1.416 (3)
N2—C18	1.369 (3)	C14—C18	1.413 (3)
C2—C3	1.364 (5)	C15—C16	1.394 (4)
C2—H2B	0.9300	C15—H15A	0.9300
C3—C4	1.362 (5)	C16—C17	1.355 (4)
C3—H3A	0.9300	C16—H16A	0.9300
C4—C5	1.391 (4)	C17—C18	1.411 (3)
C4—H4A	0.9300	C17—C21	1.513 (3)
C5—C6	1.380 (4)	C19—C20	1.399 (3)
C5—H5A	0.9300	C19—H19A	0.9300
C7—C8	1.381 (4)	C20—H20A	0.9300
C7—C12	1.390 (3)	C21—H21A	0.9600
C8—C9	1.379 (4)	C21—H21B	0.9600
C8—H8A	0.9300	C21—H21C	0.9600
C7—P—C6	102.31 (12)	C10—C11—H11A	119.8
C7—P—C13	102.97 (11)	C12—C11—H11A	119.8
C6—P—C13	100.69 (11)	C11—C12—C7	121.0 (3)
C15—N1—C14	115.8 (2)	C11—C12—H12A	119.5
C2—C1—C6	121.5 (3)	C7—C12—H12A	119.5
C2—C1—H1B	119.3	C20—C13—C14	116.6 (2)
C6—C1—H1B	119.3	C20—C13—P	125.1 (2)
C19—N2—C18	116.9 (2)	C14—C13—P	117.97 (16)
C3—C2—C1	119.9 (3)	N1—C14—C18	122.9 (2)
C3—C2—H2B	120.0	N1—C14—C13	117.7 (2)
C1—C2—H2B	120.0	C18—C14—C13	119.5 (2)
C4—C3—C2	120.2 (3)	N1—C15—C16	125.1 (2)
C4—C3—H3A	119.9	N1—C15—H15A	117.4
C2—C3—H3A	119.9	C16—C15—H15A	117.4
C3—C4—C5	120.1 (4)	C17—C16—C15	120.3 (3)
C3—C4—H4A	119.9	C17—C16—H16A	119.8
C5—C4—H4A	119.9	C15—C16—H16A	119.8
C6—C5—C4	120.8 (3)	C16—C17—C18	117.2 (2)
C6—C5—H5A	119.6	C16—C17—C21	122.4 (3)
C4—C5—H5A	119.6	C18—C17—C21	120.4 (2)
C5—C6—C1	117.5 (3)	N2—C18—C17	119.3 (2)
C5—C6—P	125.9 (2)	N2—C18—C14	122.1 (2)
C1—C6—P	116.6 (2)	C17—C18—C14	118.6 (2)

C8—C7—C12	117.7 (2)	N2—C19—C20	124.6 (2)
C8—C7—P	125.38 (19)	N2—C19—H19A	117.7
C12—C7—P	116.9 (2)	C20—C19—H19A	117.7
C9—C8—C7	120.8 (3)	C13—C20—C19	120.4 (2)
C9—C8—H8A	119.6	C13—C20—H20A	119.8
C7—C8—H8A	119.6	C19—C20—H20A	119.8
C10—C9—C8	120.1 (3)	C17—C21—H21A	109.5
C10—C9—H9A	120.0	C17—C21—H21B	109.5
C8—C9—H9A	120.0	H21A—C21—H21B	109.5
C11—C10—C9	120.0 (3)	C17—C21—H21C	109.5
C11—C10—H10A	120.0	H21A—C21—H21C	109.5
C9—C10—H10A	120.0	H21B—C21—H21C	109.5
C10—C11—C12	120.4 (3)		

C6—C1—C2—C3	−1.3 (5)	C7—P—C13—C14	76.6 (2)
C1—C2—C3—C4	1.4 (5)	C6—P—C13—C14	−178.00 (19)
C2—C3—C4—C5	−0.9 (5)	C15—N1—C14—C18	0.5 (4)
C3—C4—C5—C6	0.3 (5)	C15—N1—C14—C13	−179.6 (2)
C4—C5—C6—C1	−0.2 (4)	C20—C13—C14—N1	−180.0 (2)
C4—C5—C6—P	−178.5 (2)	P—C13—C14—N1	−6.0 (3)
C2—C1—C6—C5	0.7 (4)	C20—C13—C14—C18	−0.1 (3)
C2—C1—C6—P	179.2 (2)	P—C13—C14—C18	173.91 (17)
C7—P—C6—C5	19.7 (3)	C14—N1—C15—C16	−0.2 (5)
C13—P—C6—C5	−86.2 (2)	N1—C15—C16—C17	−0.5 (5)
C7—P—C6—C1	−158.59 (19)	C15—C16—C17—C18	0.9 (4)
C13—P—C6—C1	95.5 (2)	C15—C16—C17—C21	−179.2 (3)
C6—P—C7—C8	−91.8 (2)	C19—N2—C18—C17	−179.6 (2)
C13—P—C7—C8	12.4 (2)	C19—N2—C18—C14	0.7 (3)
C6—P—C7—C12	88.9 (2)	C16—C17—C18—N2	179.7 (2)
C13—P—C7—C12	−166.89 (19)	C21—C17—C18—N2	−0.2 (3)
C12—C7—C8—C9	0.7 (4)	C16—C17—C18—C14	−0.6 (4)
P—C7—C8—C9	−178.5 (2)	C21—C17—C18—C14	179.5 (2)
C7—C8—C9—C10	−1.4 (4)	N1—C14—C18—N2	179.6 (2)
C8—C9—C10—C11	1.0 (5)	C13—C14—C18—N2	−0.3 (3)
C9—C10—C11—C12	0.0 (5)	N1—C14—C18—C17	−0.1 (4)
C10—C11—C12—C7	−0.7 (5)	C13—C14—C18—C17	180.0 (2)
C8—C7—C12—C11	0.3 (4)	C18—N2—C19—C20	−0.7 (4)
P—C7—C12—C11	179.6 (2)	C14—C13—C20—C19	0.1 (4)
C7—P—C13—C20	−110.0 (2)	P—C13—C20—C19	−173.4 (2)
C6—P—C13—C20	−4.6 (3)	N2—C19—C20—C13	0.3 (4)