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ISSN 2414-3146

1,1-Bis(diphenylphosphoryl)hydrazine

Martha Höhne, Bhaskar R. Aluri, Anke Spannenberg, Bernd H. Müller, Normen Peulecke and Uwe Rosenthal*

Leibniz-Institut für Katalyse e. V. an der Universität Rostock, Albert-Einstein-Strasse 29a, 18059 Rostock, Germany. *Correspondence e-mail: uwe.rosenthal@catalysis.de

Received 27 April 2018
Accepted 3 May 2018

Edited by C. Rizzoli, Universita degli Studi di Parma, Italy

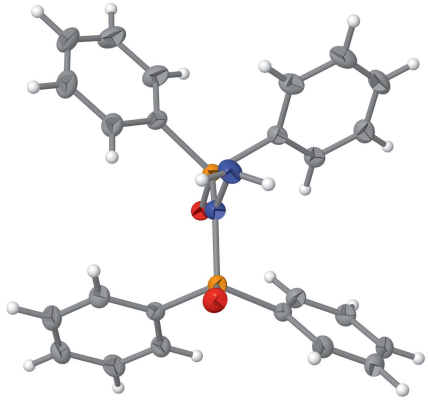
Keywords: crystal structure; diphosphazane; hydrazine.

CCDC reference: 1841174

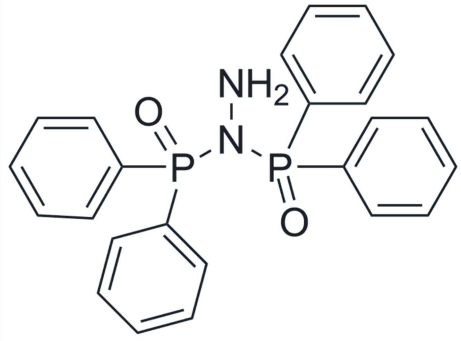
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{24}H_{22}N_2O_2P_2$, contains a diphosphazane backbone, as well as a hydrazine entity. The P—N—P diphosphazane unit and the N-amine N atom are almost coplanar, and the O atoms of the $Ph_2P(O)$ units are oriented *trans* to each other with respect to the P···P axis. In the crystal, centrosymmetrically related molecules are linked into dimers by pairs of N—H···O hydrogen bonds, forming rings of graph-set motif $R_2^2(10)$.

3D view



Chemical scheme



Structure description

The title compound (Fig. 1) contains a diphosphazane backbone, as well as a hydrazine entity. The P—N—P diphosphazane unit and the N-amine N atom are almost coplanar (r.m.s. deviation for P1/N1/P2/N2 = 0.045 Å). The N2 atom deviates from the P1/N1/P2 plane by 0.312 (4) Å. The geometry at atom N1 is nearly trigonal planar [$\Sigma(\angle N1)$ = 358.7°]. The O atoms of the $Ph_2P(O)$ units are oriented *trans* to each other with respect to the P···P axis, as was found in other $Ph_2P(O)—N(R)—(O)PPh_2$ compounds (Song *et al.*, 2009; Slawin *et al.*, 2001; Gümgüm *et al.*, 2006; Copolovici *et al.*, 2007). The P—N—P angle is 129.68 (6)°. The P—N bond lengths [P1—N1 = 1.6989 (10) Å and P2—N1 1.6769 (10) Å] are noticeably shortened compared to the calculated sum of the covalent radii by Pyykkö and show significant multiple-bond character [single: Σr_{cov}(P—N) = 1.82 Å; double: Σr_{cov}(P═N) = 1.62 Å] (Pyykkö, 2015). Nevertheless, these values are comparable to those observed in similar compounds with a $Ph_2P(O)—N(R)—(O)PPh_2$ skeleton (Song *et al.*, 2009; Slawin *et al.*, 2001; Gümgüm *et al.*, 2006). The N—N distance within the hydrazine entity is 1.4391 (13) Å. In the crystal, centrosymmetrically related molecules are linked into dimers by pairs of N—H···O hydrogen bonds (Table 1), forming rings of graph-set motif $R_2^2(10)$.

Synthesis and crystallization

A solution of *N*,*N*-bis(diphenylphosphine)hydrazine, [$Ph_2P—N(NH_2)—PPh_2$; 0.385 g, 0.965 mmol] and trimethylamine *N*-oxide (0.235 g, 2.115 mmol) in THF (10 ml) was

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{i}	0.909 (17)	2.089 (18)	2.9737 (15)	164.0 (14)

Symmetry code: (i) $-x+2, -y+1, -z$.

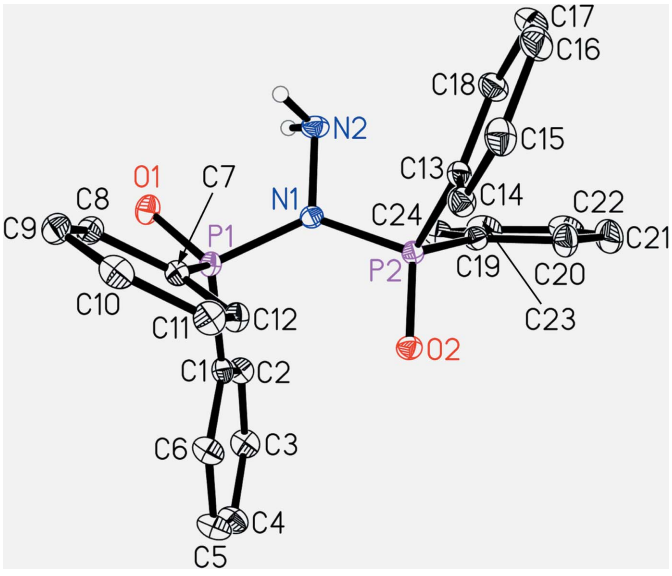


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level. Aromatic H atoms have been omitted for clarity.

stirred for 3 d at room temperature, followed by heating at 60°C for four weeks. Afterwards, the THF was removed in a vacuum and the product was recrystallized from mixed solvents of DCM/*n*-hexane (1:1 *v*/*v*). Yield 0.332 g (80%). ^{31}P NMR (162 MHz, THF-d_8, 298 K): δ 29.8. MS (ESI): m/z = 433 [M + H]$^+$. Elemental analysis calculated (%) for $C_{24}H_{22}N_2O_2P_2$: C 66.67, H 5.13, N 6.48, P 14.33; found: C 66.65, H 5.15, N 6.69, P 14.38. M.p. 211–212°C.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{22}N_2O_2P_2$
M_r	432.37
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	200
a, b, c (Å)	8.6901 (5), 10.1547 (5), 12.6282 (7)
α, β, γ (°)	71.352 (4), 84.442 (4), 81.817 (4)
V (Å^3)	1043.56 (10)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.23
Crystal size (mm)	0.50 × 0.30 × 0.25
Data collection	
Diffractometer	Stoe IPDS II
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15868, 5037, 4301
R_{int}	0.014
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.661
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.029, 0.081, 1.05
No. of reflections	5037
No. of parameters	279
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.28

Computer programs: *X-AREA* (Stoe & Cie, 2005), *XP* in *SHELXTL* and *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *publCIF* (Westrip, 2010).

Funding information

The publication of this article was funded by the Open Access Fund of the Leibniz Association.

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full crystallographic data

IUCrData (2018). **3**, x180679 [https://doi.org/10.1107/S241431461800679X]

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Crystal data

$C_{24}H_{22}N_2O_2P_2$
M_r = 432.37
Triclinic, $P\overline{1}$
a = 8.6901 (5) Å
b = 10.1547 (5) Å
c = 12.6282 (7) Å
α = 71.352 (4)°
β = 84.442 (4)°
γ = 81.817 (4)°
V = 1043.56 (10) Å^3
Z = 2
$F(000)$ = 452
D_x = 1.376 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5988 reflections
θ = 2.1–29.7°
μ = 0.23 mm^{-1}
T = 200 K
Prism, colourless
0.50 × 0.30 × 0.25 mm

Data collection

Stoe IPDS II diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
15868 measured reflections
5037 independent reflections
4301 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
θ_{max} = 28.0°, θ_{min} = 2.1°
h = −11→11
k = −13→13
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.081
S = 1.05
5037 reflections
279 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0504P)^2 + 0.1335P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.89750 (13)	0.48325 (12)	0.26480 (10)	0.0223 (2)
C2	0.77523 (15)	0.55487 (13)	0.19719 (11)	0.0274 (2)
H2C	0.7771	0.5531	0.1223	0.033*
C3	0.65113 (16)	0.62857 (15)	0.23907 (12)	0.0331 (3)
H3	0.5681	0.6775	0.1928	0.040*
C4	0.64754 (17)	0.63124 (15)	0.34843 (13)	0.0349 (3)
H4	0.5619	0.6814	0.3771	0.042*
C5	0.76835 (17)	0.56106 (16)	0.41553 (12)	0.0360 (3)
H5	0.7660	0.5630	0.4904	0.043*
C6	0.89352 (16)	0.48747 (14)	0.37381 (11)	0.0308 (3)
H6	0.9769	0.4398	0.4201	0.037*
C7	1.20749 (13)	0.32186 (12)	0.29927 (10)	0.0209 (2)
C8	1.35584 (14)	0.36535 (13)	0.27120 (10)	0.0258 (2)
H8	1.3740	0.4382	0.2037	0.031*
C9	1.47602 (14)	0.30254 (14)	0.34133 (12)	0.0296 (3)
H9	1.5761	0.3337	0.3228	0.036*
C10	1.45090 (15)	0.19430 (14)	0.43856 (11)	0.0296 (3)
H10	1.5346	0.1495	0.4854	0.036*
C11	1.30418 (16)	0.15118 (14)	0.46774 (11)	0.0287 (3)
H11	1.2871	0.0776	0.5350	0.034*
C12	1.18228 (14)	0.21521 (13)	0.39899 (10)	0.0245 (2)
H12	1.0814	0.1865	0.4197	0.029*
C13	1.01250 (14)	−0.02059 (12)	0.25987 (10)	0.0231 (2)
C14	1.08887 (15)	−0.08649 (13)	0.35836 (10)	0.0266 (2)
H14	1.0739	−0.0463	0.4175	0.032*
C15	1.18663 (16)	−0.21031 (14)	0.37088 (12)	0.0341 (3)
H15	1.2391	−0.2543	0.4381	0.041*
C16	1.20760 (17)	−0.26968 (15)	0.28517 (14)	0.0387 (3)
H16	1.2745	−0.3545	0.2936	0.046*
C17	1.13138 (19)	−0.20583 (16)	0.18727 (13)	0.0388 (3)
H17	1.1457	−0.2473	0.1289	0.047*
C18	1.03422 (17)	−0.08176 (14)	0.17395 (11)	0.0318 (3)
H18	0.9823	−0.0382	0.1064	0.038*
C19	0.72636 (14)	0.14265 (13)	0.17142 (10)	0.0247 (2)
C20	0.64662 (18)	0.02528 (17)	0.20351 (13)	0.0375 (3)
H20	0.6832	−0.0558	0.2616	0.045*
C21	0.51300 (19)	0.0271 (2)	0.15020 (16)	0.0476 (4)
H21	0.4577	−0.0525	0.1725	0.057*
C22	0.46105 (17)	0.1442 (2)	0.06523 (15)	0.0462 (4)
H22	0.3717	0.1442	0.0275	0.055*
C23	0.53780 (18)	0.26136 (19)	0.03472 (13)	0.0415 (3)
H23	0.4994	0.3428	−0.0225	0.050*
C24	0.67102 (15)	0.26122 (15)	0.08710 (11)	0.0305 (3)
H24	0.7243	0.3420	0.0653	0.037*
N1	0.98664 (11)	0.27181 (10)	0.16766 (8)	0.02110 (19)

N2	1.03825 (14)	0.24976 (12)	0.06221 (9)	0.0270 (2)
O1	1.12316 (11)	0.49585 (9)	0.09599 (7)	0.02781 (19)
O2	0.84523 (10)	0.16030 (9)	0.36001 (7)	0.02361 (17)
P1	1.05904 (3)	0.39960 (3)	0.20082 (2)	0.02008 (8)
P2	0.88965 (3)	0.14098 (3)	0.24925 (2)	0.01921 (8)
H2A	1.0080 (19)	0.3320 (18)	0.0093 (14)	0.031 (4)*
H2B	1.146 (2)	0.2365 (19)	0.0615 (15)	0.042 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0234 (5)	0.0172 (5)	0.0260 (6)	−0.0025 (4)	−0.0035 (4)	−0.0057 (4)
C2	0.0285 (6)	0.0265 (6)	0.0254 (6)	−0.0006 (5)	−0.0057 (5)	−0.0055 (5)
C3	0.0296 (6)	0.0318 (7)	0.0359 (7)	0.0049 (5)	−0.0089 (5)	−0.0093 (6)
C4	0.0321 (7)	0.0331 (7)	0.0418 (8)	0.0063 (5)	−0.0050 (6)	−0.0183 (6)
C5	0.0406 (7)	0.0387 (8)	0.0330 (7)	0.0060 (6)	−0.0076 (6)	−0.0199 (6)
C6	0.0320 (6)	0.0309 (7)	0.0312 (6)	0.0053 (5)	−0.0106 (5)	−0.0132 (5)
C7	0.0204 (5)	0.0200 (5)	0.0225 (5)	−0.0009 (4)	−0.0032 (4)	−0.0070 (4)
C8	0.0244 (6)	0.0244 (6)	0.0273 (6)	−0.0036 (5)	0.0010 (5)	−0.0065 (5)
C9	0.0200 (5)	0.0321 (7)	0.0385 (7)	−0.0019 (5)	−0.0009 (5)	−0.0142 (5)
C10	0.0268 (6)	0.0292 (6)	0.0340 (6)	0.0061 (5)	−0.0110 (5)	−0.0128 (5)
C11	0.0329 (6)	0.0250 (6)	0.0253 (6)	−0.0006 (5)	−0.0071 (5)	−0.0033 (5)
C12	0.0247 (6)	0.0239 (6)	0.0239 (5)	−0.0044 (4)	−0.0032 (4)	−0.0047 (5)
C13	0.0265 (6)	0.0189 (5)	0.0232 (5)	−0.0035 (4)	−0.0005 (4)	−0.0055 (4)
C14	0.0312 (6)	0.0221 (6)	0.0248 (6)	−0.0037 (5)	−0.0026 (5)	−0.0045 (5)
C15	0.0341 (7)	0.0242 (6)	0.0400 (7)	−0.0009 (5)	−0.0071 (6)	−0.0038 (5)
C16	0.0355 (7)	0.0236 (6)	0.0560 (9)	0.0010 (5)	0.0013 (6)	−0.0141 (6)
C17	0.0470 (8)	0.0319 (7)	0.0424 (8)	−0.0034 (6)	0.0043 (6)	−0.0208 (6)
C18	0.0417 (7)	0.0283 (6)	0.0274 (6)	−0.0043 (5)	−0.0019 (5)	−0.0116 (5)
C19	0.0234 (5)	0.0299 (6)	0.0231 (5)	−0.0042 (5)	−0.0027 (4)	−0.0108 (5)
C20	0.0374 (7)	0.0380 (8)	0.0402 (8)	−0.0138 (6)	−0.0055 (6)	−0.0113 (6)
C21	0.0359 (8)	0.0553 (10)	0.0637 (11)	−0.0171 (7)	−0.0041 (7)	−0.0300 (9)
C22	0.0263 (7)	0.0692 (11)	0.0568 (10)	0.0029 (7)	−0.0128 (6)	−0.0395 (9)
C23	0.0345 (7)	0.0535 (9)	0.0387 (8)	0.0101 (7)	−0.0147 (6)	−0.0203 (7)
C24	0.0294 (6)	0.0346 (7)	0.0279 (6)	0.0004 (5)	−0.0057 (5)	−0.0108 (5)
N1	0.0246 (5)	0.0213 (5)	0.0170 (4)	−0.0044 (4)	0.0001 (4)	−0.0050 (4)
N2	0.0331 (6)	0.0269 (6)	0.0195 (5)	−0.0014 (4)	0.0033 (4)	−0.0073 (4)
O1	0.0303 (4)	0.0240 (4)	0.0244 (4)	−0.0070 (3)	−0.0025 (3)	0.0009 (3)
O2	0.0250 (4)	0.0263 (4)	0.0199 (4)	−0.0039 (3)	−0.0005 (3)	−0.0076 (3)
P1	0.02100 (14)	0.01798 (14)	0.01910 (14)	−0.00280 (10)	−0.00280 (10)	−0.00205 (11)
P2	0.02125 (14)	0.01898 (14)	0.01705 (14)	−0.00319 (10)	−0.00204 (10)	−0.00449 (10)

Geometric parameters (Å, º)

C1—C6	1.3879 (17)	C14—H14	0.9500
C1—C2	1.3948 (17)	C15—C16	1.384 (2)
C1—P1	1.7957 (12)	C15—H15	0.9500
C2—C3	1.3841 (19)	C16—C17	1.383 (2)

C2—H2C	0.9500	C16—H16	0.9500
C3—C4	1.387 (2)	C17—C18	1.385 (2)
C3—H3	0.9500	C17—H17	0.9500
C4—C5	1.379 (2)	C18—H18	0.9500
C4—H4	0.9500	C19—C24	1.3890 (18)
C5—C6	1.3887 (19)	C19—C20	1.3916 (18)
C5—H5	0.9500	C19—P2	1.7980 (12)
C6—H6	0.9500	C20—C21	1.393 (2)
C7—C12	1.3959 (16)	C20—H20	0.9500
C7—C8	1.3987 (16)	C21—C22	1.377 (3)
C7—P1	1.7961 (12)	C21—H21	0.9500
C8—C9	1.3821 (18)	C22—C23	1.375 (3)
C8—H8	0.9500	C22—H22	0.9500
C9—C10	1.384 (2)	C23—C24	1.3875 (19)
C9—H9	0.9500	C23—H23	0.9500
C10—C11	1.3848 (19)	C24—H24	0.9500
C10—H10	0.9500	N1—N2	1.4391 (13)
C11—C12	1.3857 (17)	N1—P2	1.6769 (10)
C11—H11	0.9500	N1—P1	1.6989 (10)
C12—H12	0.9500	N2—H2A	0.909 (17)
C13—C14	1.3916 (17)	N2—H2B	0.927 (19)
C13—C18	1.3988 (17)	O1—P1	1.4843 (9)
C13—P2	1.7994 (12)	O2—P2	1.4810 (8)
C14—C15	1.3866 (19)		

C6—C1—C2	119.31 (11)	C17—C16—C15	120.17 (13)
C6—C1—P1	123.61 (9)	C17—C16—H16	119.9
C2—C1—P1	116.94 (9)	C15—C16—H16	119.9
C3—C2—C1	120.08 (12)	C16—C17—C18	120.31 (13)
C3—C2—H2C	120.0	C16—C17—H17	119.8
C1—C2—H2C	120.0	C18—C17—H17	119.8
C2—C3—C4	120.20 (12)	C17—C18—C13	120.02 (13)
C2—C3—H3	119.9	C17—C18—H18	120.0
C4—C3—H3	119.9	C13—C18—H18	120.0
C5—C4—C3	119.98 (13)	C24—C19—C20	119.65 (12)
C5—C4—H4	120.0	C24—C19—P2	121.71 (10)
C3—C4—H4	120.0	C20—C19—P2	118.42 (10)
C4—C5—C6	120.07 (13)	C19—C20—C21	119.81 (15)
C4—C5—H5	120.0	C19—C20—H20	120.1
C6—C5—H5	120.0	C21—C20—H20	120.1
C1—C6—C5	120.35 (12)	C22—C21—C20	120.01 (15)
C1—C6—H6	119.8	C22—C21—H21	120.0
C5—C6—H6	119.8	C20—C21—H21	120.0
C12—C7—C8	119.26 (11)	C23—C22—C21	120.35 (14)
C12—C7—P1	122.47 (9)	C23—C22—H22	119.8
C8—C7—P1	118.17 (9)	C21—C22—H22	119.8
C9—C8—C7	120.17 (12)	C22—C23—C24	120.31 (15)
C9—C8—H8	119.9	C22—C23—H23	119.8

C7—C8—H8	119.9	C24—C23—H23	119.8
C8—C9—C10	120.14 (12)	C23—C24—C19	119.85 (14)
C8—C9—H9	119.9	C23—C24—H24	120.1
C10—C9—H9	119.9	C19—C24—H24	120.1
C9—C10—C11	120.20 (12)	N2—N1—P2	111.01 (7)
C9—C10—H10	119.9	N2—N1—P1	118.03 (8)
C11—C10—H10	119.9	P2—N1—P1	129.68 (6)
C10—C11—C12	120.08 (12)	N1—N2—H2A	105.2 (10)
C10—C11—H11	120.0	N1—N2—H2B	105.7 (11)
C12—C11—H11	120.0	H2A—N2—H2B	108.7 (15)
C11—C12—C7	120.12 (11)	O1—P1—N1	107.98 (5)
C11—C12—H12	119.9	O1—P1—C1	112.80 (6)
C7—C12—H12	119.9	N1—P1—C1	105.50 (5)
C14—C13—C18	119.11 (12)	O1—P1—C7	111.04 (5)
C14—C13—P2	117.92 (9)	N1—P1—C7	109.40 (5)
C18—C13—P2	122.96 (10)	C1—P1—C7	109.90 (5)
C15—C14—C13	120.55 (12)	O2—P2—N1	110.58 (5)
C15—C14—H14	119.7	O2—P2—C19	113.78 (5)
C13—C14—H14	119.7	N1—P2—C19	105.17 (5)
C16—C15—C14	119.83 (13)	O2—P2—C13	112.32 (5)
C16—C15—H15	120.1	N1—P2—C13	107.58 (5)
C14—C15—H15	120.1	C19—P2—C13	106.97 (6)

C6—C1—C2—C3	−0.35 (19)	N2—N1—P1—C1	139.66 (9)
P1—C1—C2—C3	−176.26 (10)	P2—N1—P1—C1	−54.55 (9)
C1—C2—C3—C4	−0.2 (2)	N2—N1—P1—C7	−102.16 (9)
C2—C3—C4—C5	0.4 (2)	P2—N1—P1—C7	63.63 (9)
C3—C4—C5—C6	−0.1 (2)	C6—C1—P1—O1	−123.31 (11)
C2—C1—C6—C5	0.6 (2)	C2—C1—P1—O1	52.41 (11)
P1—C1—C6—C5	176.27 (11)	C6—C1—P1—N1	119.04 (11)
C4—C5—C6—C1	−0.4 (2)	C2—C1—P1—N1	−65.25 (10)
C12—C7—C8—C9	0.39 (18)	C6—C1—P1—C7	1.19 (12)
P1—C7—C8—C9	−176.16 (9)	C2—C1—P1—C7	176.91 (9)
C7—C8—C9—C10	1.34 (19)	C12—C7—P1—O1	−172.27 (9)
C8—C9—C10—C11	−1.92 (19)	C8—C7—P1—O1	4.17 (11)
C9—C10—C11—C12	0.75 (19)	C12—C7—P1—N1	−53.18 (11)
C10—C11—C12—C7	0.99 (19)	C8—C7—P1—N1	123.26 (9)
C8—C7—C12—C11	−1.55 (18)	C12—C7—P1—C1	62.22 (11)
P1—C7—C12—C11	174.85 (9)	C8—C7—P1—C1	−121.35 (10)
C18—C13—C14—C15	0.72 (19)	N2—N1—P2—O2	176.63 (8)
P2—C13—C14—C15	−179.18 (10)	P1—N1—P2—O2	10.06 (10)
C13—C14—C15—C16	−0.5 (2)	N2—N1—P2—C19	−60.13 (9)
C14—C15—C16—C17	0.0 (2)	P1—N1—P2—C19	133.29 (8)
C15—C16—C17—C18	0.3 (2)	N2—N1—P2—C13	53.64 (9)
C16—C17—C18—C13	−0.2 (2)	P1—N1—P2—C13	−112.94 (8)
C14—C13—C18—C17	−0.4 (2)	C24—C19—P2—O2	99.51 (11)
P2—C13—C18—C17	179.52 (11)	C20—C19—P2—O2	−75.13 (12)
C24—C19—C20—C21	0.6 (2)	C24—C19—P2—N1	−21.65 (12)

P2—C19—C20—C21	175.37 (12)	C20—C19—P2—N1	163.71 (11)
C19—C20—C21—C22	0.7 (2)	C24—C19—P2—C13	−135.85 (10)
C20—C21—C22—C23	−1.9 (2)	C20—C19—P2—C13	49.51 (12)
C21—C22—C23—C24	1.9 (2)	C14—C13—P2—O2	−18.63 (11)
C22—C23—C24—C19	−0.6 (2)	C18—C13—P2—O2	161.48 (10)
C20—C19—C24—C23	−0.7 (2)	C14—C13—P2—N1	103.29 (10)
P2—C19—C24—C23	−175.25 (10)	C18—C13—P2—N1	−76.60 (11)
N2—N1—P1—O1	18.81 (10)	C14—C13—P2—C19	−144.15 (10)
P2—N1—P1—O1	−175.40 (7)	C18—C13—P2—C19	35.95 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1^{i}	0.909 (17)	2.089 (18)	2.9737 (15)	164.0 (14)

Symmetry code: (i) −*x*+2, −*y*+1, −*z*.