IUCrData

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4,4′,4″,4‴-({4′λ^5,6λ^5,6′λ^5-Spiro[dibenzo[*d*,*f*]-[1,3,2]dioxaphosphepine-6,2′-[1,3,5,2,4,6]triaza-triphosphinine]-4′,4′,6′,6′-tetrayl}tetrakis(oxy))-tetrabenzaldehyde

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Keywords: crystal structure; cyclotriphosphazene; van der Waals forces.

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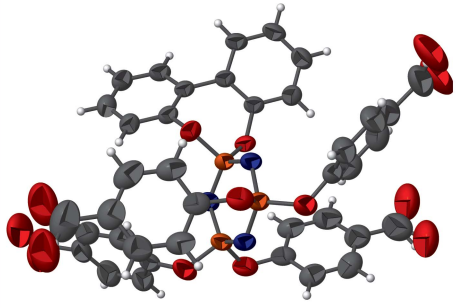
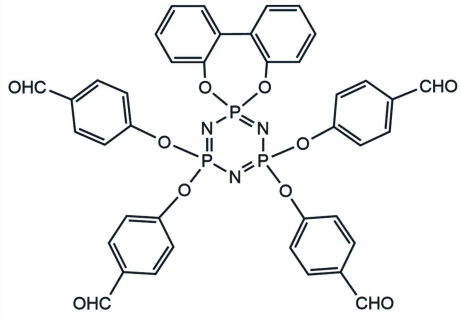
Structural data: full structural data are available from iucrdata.iucr.org

The complete molecule of the title compound, $C_{40}H_{28}N_3O_{10}P_3$, is generated by crystallographic twofold symmetry, with one P and one N atom lying on the rotation axis. The central P_3N_3 ring is close to planar, with an r.m.s. deviation of the six fitted atoms of 0.077 Å. The 2,2′-biphenoxy moiety generates a seven-membered spirocyclic structure with an endocyclic C—C—C—C torsion angle about the central biphenoxy C—C bond of 38.5 (4)°. The formyl-substituted phenyl rings subtend dihedral angles of 56.83 (10) and 61.02 (13)° with respect to the phosphazene core. The C═O and C—H groups of the formyl groups are disordered over two orientations in a 0.640 (4):0.360 (4) ratio. No directional interactions beyond normal van der Waals contacts could be identified in the crystal.

3D view



Chemical scheme



Structure description

Cyclic phosphazenes are an important family of inorganic ring systems with possible applications as flame retardants, anti-microbial agents, lithium-ion batteries, liquid crystals, organic light emitting diodes, membrane hydrogels, drug carriers, surfactants and phase-transfer catalysts (Uslu *et al.*, 2013). The title compound is a new cyclotriphosphazene. Herein, we report its synthesis and crystal structure.

The title compound (Fig. 1), crystallizing in *C*2/*c* space group with $Z = 4$, comprises a cyclotriphosphazene core, a 2,2′-biphenoxy group and four 4-formyl-phenoxy groups. The central phosphazene ring, which is generated by crystallographic twofold symmetry

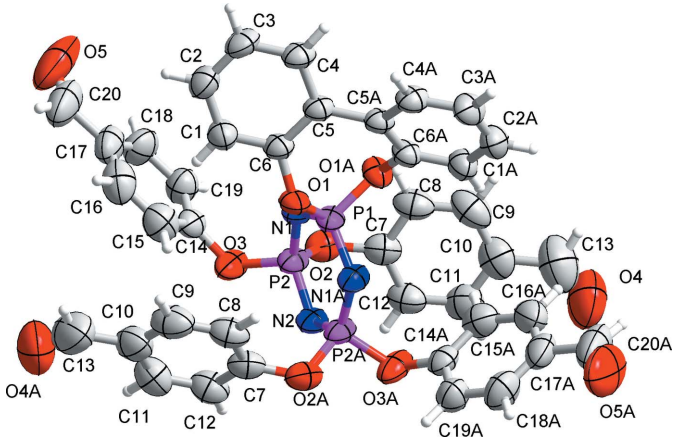


Figure 1
The molecular structure, showing 50% probability displacement ellipsoids (only the major disorder components of the formyl groups are shown).

(P1 and N2 lie on the axis) is close to planar, with an r.m.s. deviation of the six fitted atoms of 0.077 Å.

Incorporation of the 2,2'-biphenoxy moiety at P1 promotes a seven-membered spirocyclic structure with an endocyclic torsion angle about the central biphenoxy C—C bond of 38.5 (4)° for for C6—C5—C5^{i}—C6^{i} [symmetry code: (i) $1-x$, $y, \frac{1}{2}-z$]. The C7 and C14 benzene rings make dihedral angles of 56.83 (10) and 61.02 (13)°, respectively, with the cyclotriphosphazene ring. In the extended structure, there are no directional interactions, the crystal structure being enforced by van der Waals forces only.

Synthesis and crystallization

The title compound was synthesized by two steps: $[N_3P_3C_{l4}(O_2C_{12}H_8)]$ (T1) was synthesized as previously reported in the literature (Carriedo *et al.* 1996).

A mixture of 4-hydroxybenzaldehyde (2.6816 g, 0.0220 mol) and K_2CO_3 (5.8048 g, 0.0420 mol) in THF (50 ml) was stirred under reflux at room temperature for 0.5 h under nitrogen atmosphere. T1 (2.3047 g, 0.0050 mol) dissolved in 30 ml THF, was added dropwise into the mixture for 1 h at room temperature. The reaction mixture was heated slowly to reflux temperature and then allowed to stir strongly for 6 h. After that, the mixture was filtered twice to remove the white solid that formed. The filtrate was concentrated under vacuum to remove part of the solvent and was poured into a large amount of water to precipitate the crude product, which was recrystallized using a solvent of THF. Colourless prismatic crystals of the title compound were obtained by slow evaporation of the solvent.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The C═O and C—H moieties of both the C13 and C20 formyl groups are disordered over two overlapping orientations in 0.640 (4):0.360 (4) ratios.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{40}H_{28}N_3O_{10}P_3$
M_r	803.56
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	293
a, *b*, *c* (Å)	32.3691 (16), 10.7492 (2), 13.1332 (7)
β (°)	125.578 (7)
V (Å^3)	3716.6 (4)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.03
Crystal size (mm)	0.23 × 0.2 × 0.17
Data collection	
Diffractometer	Agilent Xcalibur Eos Gemini
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.812, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12837, 3323, 2939
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.597
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.143, 1.06
No. of reflections	3323
No. of parameters	262
No. of restraints	13
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.43, −0.31

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

Acknowledgements

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Funding information

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full crystallographic data

IUCrData (2017). **2**, x171712 [https://doi.org/10.1107/S2414314617017126]

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4,4′,4″,4‴-({4′λ^5,6λ^5,6′λ^5-Spiro[dibenzo[*d*,*f*][1,3,2]dioxaphosphepine-6,2′-[1,3,5,2,4,6]triazatriphosphinine]-4′,4′,6′,6′-tetrayl}tetrakis(oxy))tetrabenzaldehyde

Crystal data

$C_{40}H_{28}N_3O_{10}P_3$
M_r = 803.56
Monoclinic, *C*2/*c*
a = 32.3691 (16) Å
b = 10.7492 (2) Å
c = 13.1332 (7) Å
β = 125.578 (7)°
V = 3716.6 (4) Å^3
Z = 4
F(000) = 1656
D_x = 1.436 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 5579 reflections
θ = 4.2–70.6°
μ = 2.03 mm^{-1}
T = 293 K
Prism, colourless
0.23 × 0.2 × 0.17 mm

Data collection

Agilent Xcalibur Eos Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.2312 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.812, T_{max} = 1.000
12837 measured reflections
3323 independent reflections
2939 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 67.1°, θ_{min} = 4.4°
h = −38→35
k = −12→7
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.143
S = 1.06
3323 reflections
262 parameters
13 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0923P)^2 + 1.510P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00127 (14)

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.

Refinement. All C-bound hydrogen atoms were included in calculated positions with C—H = 0.93 Å and allowed to ride, with *U*iso(H) = 1.2*U*eq(C). DELU and ISOR restraints in *SHELXL2014* were applied to atoms C16 and C16. The aldehyde groups at C13 and C20 are disordered over two orientations in 0.640 (4): 0.360 (4) ratios. The disordered O atoms bonded to C13 and C20 were constrained with equal anisotropic displacement parameters.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.39125 (8)	0.3337 (2)	0.0572 (2)	0.0601 (5)	
H1	0.3735	0.4044	0.0117	0.072*	
C2	0.36550 (9)	0.2259 (2)	0.0461 (2)	0.0666 (6)	
H2	0.3302	0.2235	−0.0074	0.080*	
C3	0.39210 (9)	0.1229 (2)	0.1142 (3)	0.0656 (6)	
H3	0.3748	0.0503	0.1059	0.079*	
C4	0.44445 (9)	0.12598 (18)	0.1951 (2)	0.0572 (5)	
H4	0.4619	0.0557	0.2421	0.069*	
C5	0.47189 (8)	0.23294 (17)	0.20792 (19)	0.0477 (4)	
C6	0.44343 (8)	0.33485 (17)	0.13615 (19)	0.0493 (5)	
C7	0.54295 (10)	0.7863 (2)	0.5226 (2)	0.0635 (6)	
C8	0.56244 (12)	0.6753 (2)	0.5849 (3)	0.0752 (7)	
H8	0.5413	0.6076	0.5667	0.090*	
C9	0.61402 (15)	0.6669 (3)	0.6748 (3)	0.0913 (9)	
H9	0.6279	0.5925	0.7178	0.110*	
C10	0.64567 (13)	0.7686 (3)	0.7023 (3)	0.0876 (9)	
C11	0.62481 (12)	0.8787 (3)	0.6388 (3)	0.0849 (8)	
H11	0.6457	0.9470	0.6571	0.102*	
C12	0.57340 (11)	0.8885 (2)	0.5486 (2)	0.0744 (7)	
H12	0.5594	0.9629	0.5058	0.089*	
C13	0.7014 (2)	0.7618 (6)	0.7995 (5)	0.140 (2)	
H13	0.7126	0.6841	0.8371	0.168*	0.640 (4)
H13A	0.7175	0.8360	0.8394	0.168*	0.360 (4)
C14	0.37139 (9)	0.74268 (19)	0.1778 (2)	0.0572 (5)	
C15	0.34686 (12)	0.6838 (3)	0.0639 (3)	0.0816 (8)	
H15	0.3597	0.6863	0.0164	0.098*	
C16	0.30203 (12)	0.6200 (3)	0.0216 (3)	0.0908 (8)	
H16	0.2846	0.5794	−0.0552	0.109*	
C17	0.28356 (10)	0.6166 (3)	0.0920 (3)	0.0837 (7)	
C18	0.30870 (11)	0.6759 (3)	0.2045 (3)	0.0869 (9)	
H18	0.2957	0.6737	0.2518	0.104*	
C19	0.35297 (10)	0.7389 (3)	0.2488 (3)	0.0726 (7)	
H19	0.3703	0.7786	0.3261	0.087*	
C20	0.23542 (14)	0.5504 (4)	0.0424 (6)	0.1275 (17)	
H20	0.2165	0.5250	−0.0408	0.153*	0.640 (4)

H20A	0.2254	0.5426	0.0956	0.153*	0.360 (4)
N1	0.46628 (6)	0.60788 (16)	0.27931 (18)	0.0562 (5)	
N2	0.5000	0.82493 (19)	0.2500	0.0527 (6)	
O1	0.46806 (5)	0.44141 (12)	0.13432 (13)	0.0549 (4)	
O2	0.49050 (7)	0.79716 (15)	0.43020 (18)	0.0688 (5)	
O3	0.41462 (6)	0.81152 (14)	0.2194 (2)	0.0759 (6)	
O4	0.7329 (2)	0.8334 (7)	0.8366 (6)	0.165 (2)	0.640 (4)
O4A	0.7238 (4)	0.6851 (13)	0.8270 (10)	0.165 (2)	0.360 (4)
O5	0.21843 (19)	0.5264 (6)	0.1045 (8)	0.173 (2)	0.640 (4)
O5A	0.2100 (4)	0.5091 (10)	−0.0525 (15)	0.173 (2)	0.360 (4)
P1	0.5000	0.53226 (6)	0.2500	0.0489 (2)	
P2	0.46970 (2)	0.75408 (4)	0.29196 (6)	0.0529 (2)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0565 (12)	0.0501 (11)	0.0595 (12)	−0.0009 (9)	0.0257 (10)	−0.0006 (9)
C2	0.0550 (12)	0.0647 (14)	0.0738 (14)	−0.0110 (10)	0.0339 (11)	−0.0090 (11)
C3	0.0652 (13)	0.0478 (12)	0.0908 (16)	−0.0157 (10)	0.0492 (13)	−0.0081 (11)
C4	0.0653 (12)	0.0361 (10)	0.0784 (13)	−0.0028 (9)	0.0465 (11)	−0.0009 (9)
C5	0.0555 (11)	0.0335 (9)	0.0588 (11)	−0.0015 (8)	0.0358 (10)	−0.0027 (8)
C6	0.0555 (11)	0.0360 (9)	0.0550 (10)	−0.0052 (8)	0.0313 (9)	−0.0034 (8)
C7	0.0836 (16)	0.0536 (12)	0.0714 (14)	0.0020 (11)	0.0554 (13)	−0.0024 (10)
C8	0.105 (2)	0.0516 (13)	0.0810 (16)	−0.0016 (13)	0.0608 (17)	−0.0017 (11)
C9	0.119 (3)	0.0693 (17)	0.0797 (17)	0.0216 (17)	0.0549 (19)	0.0082 (14)
C10	0.094 (2)	0.091 (2)	0.0702 (16)	0.0075 (17)	0.0433 (16)	−0.0076 (14)
C11	0.093 (2)	0.0838 (19)	0.0741 (16)	−0.0188 (16)	0.0465 (15)	−0.0105 (14)
C12	0.0965 (19)	0.0578 (13)	0.0734 (15)	−0.0053 (13)	0.0520 (15)	0.0009 (11)
C13	0.121 (4)	0.139 (5)	0.118 (3)	0.037 (4)	0.046 (3)	−0.007 (3)
C14	0.0521 (11)	0.0437 (11)	0.0767 (14)	0.0099 (8)	0.0381 (11)	0.0088 (9)
C15	0.0864 (18)	0.0823 (19)	0.0831 (17)	0.0124 (14)	0.0533 (16)	0.0025 (14)
C16	0.0761 (17)	0.0814 (19)	0.0839 (18)	0.0100 (15)	0.0289 (13)	−0.0155 (15)
C17	0.0522 (12)	0.0652 (15)	0.110 (2)	0.0079 (11)	0.0341 (13)	0.0031 (15)
C18	0.0696 (16)	0.097 (2)	0.108 (2)	−0.0019 (15)	0.0602 (17)	0.0059 (18)
C19	0.0632 (14)	0.0820 (18)	0.0752 (15)	−0.0005 (12)	0.0418 (13)	−0.0019 (12)
C20	0.065 (2)	0.092 (3)	0.196 (5)	−0.0006 (18)	0.059 (3)	−0.005 (3)
N1	0.0547 (9)	0.0357 (9)	0.0829 (12)	0.0009 (7)	0.0427 (9)	0.0057 (8)
N2	0.0595 (14)	0.0292 (10)	0.0733 (15)	0.000	0.0409 (12)	0.000
O1	0.0606 (8)	0.0349 (7)	0.0574 (8)	−0.0061 (6)	0.0277 (7)	0.0038 (6)
O2	0.0819 (11)	0.0558 (9)	0.0927 (12)	0.0021 (8)	0.0644 (10)	−0.0036 (8)
O3	0.0621 (10)	0.0417 (8)	0.1282 (16)	0.0085 (7)	0.0579 (11)	0.0123 (8)
O4	0.097 (3)	0.187 (6)	0.139 (4)	−0.012 (3)	0.029 (3)	−0.024 (4)
O4A	0.097 (3)	0.187 (6)	0.139 (4)	−0.012 (3)	0.029 (3)	−0.024 (4)
O5	0.093 (3)	0.149 (4)	0.274 (7)	−0.045 (3)	0.104 (4)	−0.047 (4)
O5A	0.093 (3)	0.149 (4)	0.274 (7)	−0.045 (3)	0.104 (4)	−0.047 (4)
P1	0.0493 (4)	0.0284 (3)	0.0638 (4)	0.000	0.0300 (3)	0.000
P2	0.0546 (4)	0.0330 (3)	0.0794 (4)	0.00327 (18)	0.0436 (3)	0.0026 (2)

Geometric parameters (Å, º)

C1—H1	0.9300	C13—O4A	1.015 (12)
C1—C2	1.386 (3)	C14—C15	1.374 (4)
C1—C6	1.375 (3)	C14—C19	1.369 (4)
C2—H2	0.9300	C14—O3	1.384 (3)
C2—C3	1.367 (4)	C15—H15	0.9300
C3—H3	0.9300	C15—C16	1.395 (5)
C3—C4	1.381 (3)	C16—H16	0.9300
C4—H4	0.9300	C16—C17	1.363 (5)
C4—C5	1.402 (3)	C17—C18	1.361 (5)
C5—C5^{i}	1.481 (4)	C17—C20	1.475 (5)
C5—C6	1.388 (3)	C18—H18	0.9300
C6—O1	1.404 (2)	C18—C19	1.371 (4)
C7—C8	1.374 (4)	C19—H19	0.9300
C7—C12	1.380 (4)	C20—H20	0.9300
C7—O2	1.404 (3)	C20—H20A	0.9300
C8—H8	0.9300	C20—O5	1.248 (9)
C8—C9	1.377 (5)	C20—O5A	1.111 (14)
C9—H9	0.9300	N1—P1	1.5776 (18)
C9—C10	1.395 (5)	N1—P2	1.5773 (17)
C10—C11	1.377 (5)	N2—P2^{i}	1.5732 (11)
C10—C13	1.486 (6)	N2—P2	1.5731 (11)
C11—H11	0.9300	O1—P1	1.5821 (14)
C11—C12	1.375 (4)	O2—P2	1.5943 (19)
C12—H12	0.9300	O3—P2	1.5783 (17)
C13—H13	0.9300	P1—N1^{i}	1.5776 (18)
C13—H13A	0.9300	P1—O1^{i}	1.5821 (14)
C13—O4	1.136 (8)		

C2—C1—H1	120.4	C15—C14—O3	119.2 (2)
C6—C1—H1	120.4	C19—C14—C15	121.6 (2)
C6—C1—C2	119.1 (2)	C19—C14—O3	119.2 (2)
C1—C2—H2	120.1	C14—C15—H15	121.1
C3—C2—C1	119.8 (2)	C14—C15—C16	117.9 (3)
C3—C2—H2	120.1	C16—C15—H15	121.1
C2—C3—H3	119.7	C15—C16—H16	119.7
C2—C3—C4	120.5 (2)	C17—C16—C15	120.6 (3)
C4—C3—H3	119.7	C17—C16—H16	119.7
C3—C4—H4	119.3	C16—C17—C20	118.7 (4)
C3—C4—C5	121.3 (2)	C18—C17—C16	120.2 (3)
C5—C4—H4	119.3	C18—C17—C20	121.1 (4)
C4—C5—C5^{i}	120.48 (14)	C17—C18—H18	119.7
C6—C5—C4	116.23 (19)	C17—C18—C19	120.6 (3)
C6—C5—C5^{i}	123.28 (13)	C19—C18—H18	119.7
C1—C6—C5	122.96 (19)	C14—C19—C18	119.2 (3)
C1—C6—O1	117.06 (18)	C14—C19—H19	120.4
C5—C6—O1	119.77 (18)	C18—C19—H19	120.4

C8—C7—C12	122.0 (3)	C17—C20—H20	117.8
C8—C7—O2	119.5 (2)	C17—C20—H20A	116.9
C12—C7—O2	118.6 (2)	O5—C20—C17	124.4 (6)
C7—C8—H8	120.8	O5—C20—H20	117.8
C7—C8—C9	118.4 (3)	O5A—C20—C17	126.3 (8)
C9—C8—H8	120.8	O5A—C20—H20A	116.9
C8—C9—H9	119.6	P2—N1—P1	121.54 (11)
C8—C9—C10	120.8 (3)	P2—N2—P2^{i}	122.09 (14)
C10—C9—H9	119.6	C6—O1—P1	123.20 (13)
C9—C10—C13	121.7 (4)	C7—O2—P2	117.22 (14)
C11—C10—C9	119.3 (3)	C14—O3—P2	123.85 (13)
C11—C10—C13	119.0 (4)	N1—P1—N1^{i}	117.97 (13)
C10—C11—H11	119.7	N1—P1—O1^{i}	104.01 (9)
C12—C11—C10	120.6 (3)	N1^{i}—P1—O1^{i}	113.21 (9)
C12—C11—H11	119.7	N1^{i}—P1—O1	104.01 (9)
C7—C12—H12	120.5	N1—P1—O1	113.21 (9)
C11—C12—C7	119.0 (3)	O1^{i}—P1—O1	103.77 (10)
C11—C12—H12	120.5	N1—P2—O2	111.51 (10)
C10—C13—H13	113.8	N1—P2—O3	109.93 (9)
C10—C13—H13A	116.4	N2—P2—N1	117.73 (10)
O4—C13—C10	132.3 (7)	N2—P2—O2	108.79 (8)
O4—C13—H13	113.8	N2—P2—O3	108.35 (8)
O4A—C13—C10	127.1 (9)	O3—P2—O2	98.85 (11)
O4A—C13—H13A	116.4		

C1—C2—C3—C4	0.8 (4)	C13—C10—C11—C12	−179.8 (3)
C1—C6—O1—P1	114.63 (19)	C14—C15—C16—C17	−0.2 (4)
C2—C1—C6—C5	−1.2 (4)	C14—O3—P2—N1	14.2 (2)
C2—C1—C6—O1	173.4 (2)	C14—O3—P2—N2	144.1 (2)
C2—C3—C4—C5	−1.5 (4)	C14—O3—P2—O2	−102.7 (2)
C3—C4—C5—C5^{i}	−178.0 (2)	C15—C14—C19—C18	−0.7 (4)
C3—C4—C5—C6	0.8 (3)	C15—C14—O3—P2	−85.2 (3)
C4—C5—C6—C1	0.6 (3)	C15—C16—C17—C18	0.2 (5)
C4—C5—C6—O1	−173.89 (18)	C15—C16—C17—C20	178.6 (3)
C5^{i}—C5—C6—C1	179.3 (2)	C16—C17—C18—C19	−0.5 (5)
C5^{i}—C5—C6—O1	4.8 (3)	C16—C17—C20—O5	169.7 (5)
C5—C6—O1—P1	−70.6 (2)	C16—C17—C20—O5A	−6.1 (10)
C6—C1—C2—C3	0.5 (4)	C17—C18—C19—C14	0.7 (4)
C6—O1—P1—N1^{i}	162.08 (16)	C18—C17—C20—O5	−11.9 (6)
C6—O1—P1—N1	−68.66 (17)	C18—C17—C20—O5A	172.4 (9)
C6—O1—P1—O1^{i}	43.44 (13)	C19—C14—C15—C16	0.4 (4)
C7—C8—C9—C10	0.1 (4)	C19—C14—O3—P2	97.3 (3)
C7—O2—P2—N1	77.14 (18)	C20—C17—C18—C19	−178.9 (3)
C7—O2—P2—N2	−54.33 (18)	O2—C7—C8—C9	179.8 (2)
C7—O2—P2—O3	−167.25 (16)	O2—C7—C12—C11	−179.9 (2)
C8—C7—C12—C11	0.5 (4)	O3—C14—C15—C16	−177.0 (2)
C8—C7—O2—P2	−85.8 (2)	O3—C14—C19—C18	176.7 (2)
C8—C9—C10—C11	0.4 (5)	P1—N1—P2—N2	11.19 (17)

C8—C9—C10—C13	179.7 (4)	P1—N1—P2—O2	−115.56 (14)
C9—C10—C11—C12	−0.5 (5)	P1—N1—P2—O3	135.85 (14)
C9—C10—C13—O4	−178.3 (8)	P2—N1—P1—N1^{i}	−5.75 (9)
C9—C10—C13—O4A	28.3 (14)	P2—N1—P1—O1	−127.48 (12)
C10—C11—C12—C7	0.0 (4)	P2—N1—P1—O1^{i}	120.57 (13)
C11—C10—C13—O4	1.0 (10)	P2^{i}—N2—P2—N1	−5.44 (8)
C11—C10—C13—O4A	−152.4 (12)	P2^{i}—N2—P2—O2	122.61 (8)
C12—C7—C8—C9	−0.6 (4)	P2^{i}—N2—P2—O3	−130.89 (9)
C12—C7—O2—P2	94.5 (2)		

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