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Crystal structure of hexamethyl 4,4′,4″,4‴,4⁗,4⁗′-[(1,3,5,2λ^5,4λ^5,6λ^5-triazatriphosphinine-2,2,4,4,6,6-hexayl)hexakis(oxy)]hexabenzoate

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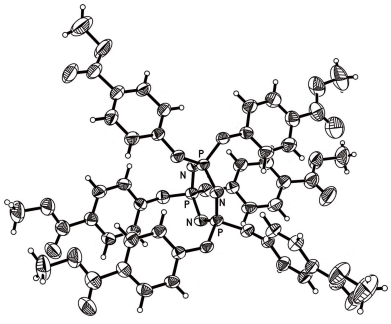
The title compound, $C_{48}H_{42}N_3O_{18}P_3$, achieved in a two-step synthesis, comprises a cyclotriphosphazene core and six 4-methoxycarbonylphenoxy groups. Each P atom is attached to two substituents located up and down with respect to the plane of the phosphazene ring, the central P_3N_3 ring having a twist-boat conformation. The three O/P/O planes and five of the six benzene rings are nearly perpendicular to the mean plane through the phosphazene ring [dihedral angles = 82.98 (8)–88.92 (8)°], while the remaining benzene ring forms a dihedral angle of 25.72 (7)°. The crystal packing is stabilized by van der Waals interactions only.

1. Chemical context

In the past few decades, a rich variety of cyclotriphosphazenes with interesting properties and applications have been synthesized by replacing the Cl atoms of hexachlorocyclotriphosphazene with various nucleophiles. The properties of cyclotriphosphazenes depend on the inorganic skeleton, as well as on the nature of the substituents attached to the P atoms (Patil *et al.*, 2011). Hexakis(allyl 4-hydroxybenzoate)cyclotriphosphazene (HABC) possessing six reactive peripheral allyl groups is used as a functional phosphazene-based oligomer for the synthesis of optical resin, through radical homopolymerization of itself and copolymerization with methyl methacrylate (Guo *et al.*, 2009). The title compound, HMPC, was obtained accidentally from the recrystallization of the crude product of HABC. Subsequently, as a retardant additive, HMPC was blended with a polymer of methyl methacrylate to obtain the flame-retardant polymer MC–PMMA. In this context, we report here the synthesis and crystal structure of HMPC.

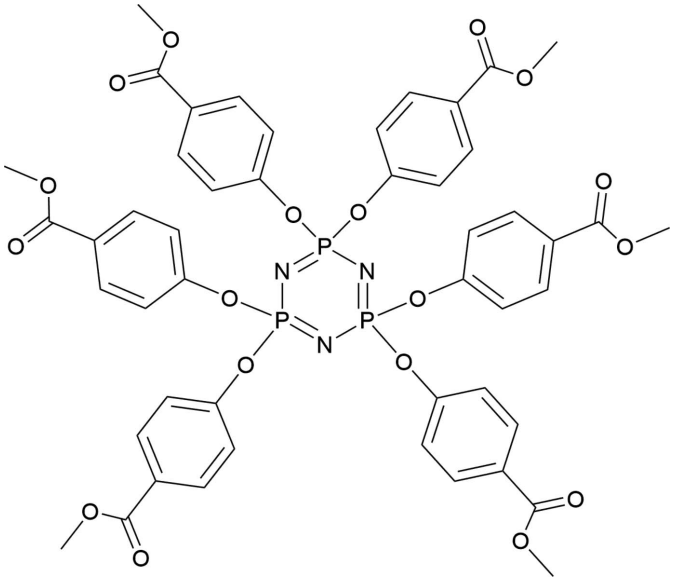


2. Structural commentary

The molecule of HMPC (Fig. 1) comprises a cyclotriphosphazene core and six 4-methoxycarbonyl phenoxy groups, and each P atom is attached to two substituents. Three of the six 4-methoxycarbonylphenoxy substituents are on one side of the phosphazene ring, while the other three groups are located on the opposite side. The central phosphazene ring is slightly nonplanar, having a boat distortion, with atoms P1 and N2 lying 0.1223 (7) and 0.138 (2) Å, respectively, on the same side of the plane defined by atoms N1/N3/P2/P3, in agreement

with the values reported in the literature for hexakis(4-formylphenoxy)cyclotriphosphazene (Patil *et al.*, 2011).

The P—O bond lengths are in the range 1.584 (2)–1.591 (19) Å, with a mean value of 1.584 (2) Å, which is 0.12 Å shorter than the normal single-bond distance (Cruickshank, 1961), suggesting considerable exocyclic π-bonding. The P—N bond lengths are within a narrow range [1.576 (3)–1.581 (2) Å], indicating electron delocalization within the ring. The N—P—N angles [116.53 (13)–117.92 (12)°] are significantly smaller than the P—N—P angles [121.25 (15)–122.53 (14)°]. The O13—P3—O16 angle [94.40 (12)°] is smaller than the corresponding angles at P1 [99.65 (11)°] and P2 [98.77 (11)°].



The 4-methoxycarbonylphenoxy groups of the HMPC molecule show significant deviations from a threefold symmetrical arrangement. The three PO_2 planes (O1/P1/O4, O7/P2/O10 and O13/P3/O16) are nearly perpendicular to the mean plane through the phosphazene ring [dihedral angles = 88.22 (6), 83.79 (9) and 84.84 (6)°, respectively]. Five of the six benzene rings lie approximately perpendicular to the phosphazene ring [dihedral angles = 82.92 (17)–88.16 (13)°; Table 1], whereas the remaining benzene ring (C17–C22) forms a dihedral angle of 28.21 (14)°. Each benzene ring and its terminal carbonyl group are approximately coplanar, the largest deviation from coplanarity being for the C33–C38 and C36/C39/O14/O15 planes [dihedral angle = 9.96 (14)°].

3. Supramolecular features

In the title compound, there are no usual hydrogen-bonding or stacking interactions, the crystal structure being enforced by van der Waals forces only.

4. Database survey

In a search in the Cambridge Structural Database (Groom *et al.*, 2016), 15 structures were found incorporating the same cyclophosphazene motif substituted by six phenoxy groups. Of these, only one structure contained alkoxycarbonylphenoxy groups bonded to each P atom of a phosphazene skeleton (Zhu *et al.*, 2015). In that structure, the atoms of two terminal propenyl groups are disordered over two sets of sites, with refined site-occupancy ratios of 0.249 (12):0.751 (12) and 0.476 (9):0.524 (9); no intermolecular interactions were observed.

Table 1
Dihedral angles between the phosphazene ring and attached benzene rings (°).

Atoms	Angle	Atoms	Angle
C1–C6	84.95 (19)	C25–C30	88.16 (13)
C9–C14	84.12 (16)	C33–C38	83.22 (13)
C17–C22	28.21 (14)	C41–C46	82.92 (17)

5. Synthesis and crystallization

All of the chemicals and solvents were of reagent grade. Hexachlorocyclotriphosphazine (HCCP) was purchased from Zhengzhou ALFA Chemical Co. Ltd, recrystallized from dry hexane and sublimated twice. Anhydrous K_2CO_3 was activated at 413 K for 2 h. Methyl 4-hydroxybenzoate was synthesized according to the literature method of Guo *et al.* (2009).

A three-necked round-bottomed flask was equipped with a nitrogen inlet, an addition funnel and a condenser. To a mixture of hexachlorocyclotriphosphazene (1.04 g, 3 mmol) and anhydrous K_2CO_3 (3.5 g, 253 mmol) in tetrahydrofuran (50 ml), a solution of methyl 4-hydroxybenzoate (3.20 g, 21 mmol in tetrahydrofuran) was added dropwise at room temperature. The reaction mixture was heated at *ca* 338 K for 48 h under nitrogen and thin-layer chromatography (TLC) was used to monitor the reaction. The resulting suspension

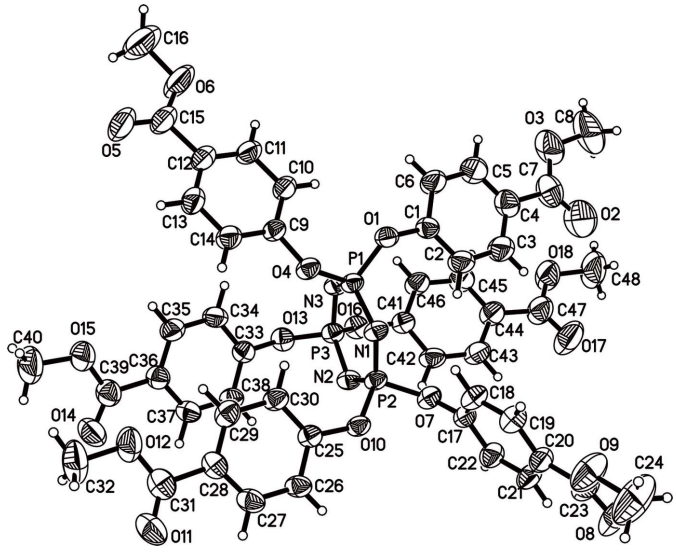


Figure 1
The molecular structure of the title compound showing 50% probability displacement ellipsoids.

was filtered and the filtrate concentrated, leading to the formation of a pale-yellow viscous liquid. This was dissolved in 20 ml ethyl acetate and the solution added dropwise to methanol. Colourless needle-shaped crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of the solvent.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were constrained, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for other H atoms. A rotating model was used for the methyl groups. An ISOR restraint in *SHELXL2014* (Sheldrick, 2015) was applied to the methyl C16 atom. Ten low-angle reflections with $F_o << F_c$, whose intensities may have been significantly reduced by the beam stop, were omitted from the final cycles of refinement.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{48}H_{42}N_3O_{18}P_3$
M_r	1041.75
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	291
a, b, c (Å)	11.4012 (4), 13.8443 (5), 17.0264 (8)
α, β, γ (°)	99.134 (3), 95.917 (3), 103.941 (3)
V (Å^3)	2547.07 (18)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.73
Crystal size (mm)	0.2 × 0.18 × 0.16
Data collection	
Diffractometer	Agilent Xcalibur Eos Gemini
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.889, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18292, 9102, 6523
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.597
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.058, 0.181, 1.03
No. of reflections	9102
No. of parameters	654
No. of restraints	6
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.52, −0.28

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2104* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

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supporting information

Acta Cryst. (2017). E**73**, 1252-1254 [https://doi.org/10.1107/S2056989017010325]

Crystal structure of hexamethyl 4,4′,4″,4‴,4⁗,4⁗′-[(1,3,5,2λ^5,4λ^5,6λ^5-triaza-triphosphinine-2,2,4,4,6,6-hexayl)hexakis(oxy)]hexabenzoate

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Computing details

Data collection: *CrysAlis PRO* (Agilent, 2014); cell refinement: *CrysAlis PRO* (Agilent, 2014); data reduction: *CrysAlis PRO* (Agilent, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2104* (Sheldrick, 2015); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

Hexamethyl 4,4′,4″,4‴,4⁗,4⁗′-[(1,3,5,2λ^5,4λ^5,6λ^5-triazatriphosphinine-2,2,4,4,6,6-hexayl)hexakis(oxy)]hexabenzoate

Crystal data

$C_{48}H_{42}N_3O_{18}P_3$
M_r = 1041.75
Triclinic, $P\overline{1}$
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b = 13.8443 (5) Å
c = 17.0264 (8) Å
α = 99.134 (3)°
β = 95.917 (3)°
γ = 103.941 (3)°
V = 2547.07 (18) Å^3
Z = 2
$F(000)$ = 1080
D_x = 1.358 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 5102 reflections
θ = 3.9–70.0°
μ = 1.73 mm^{-1}
T = 291 K
, colourless
0.2 × 0.18 × 0.16 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} = 0.889, T_{max} = 1.000
18292 measured reflections
9102 independent reflections
6523 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 67.1°, θ_{min} = 3.4°
h = −11→13
k = −16→16
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.181
S = 1.03
9102 reflections
654 parameters
6 restraints
Primary atom site location: structure-invariant direct methods

Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1121P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.52$ 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	0.8359 (3)	0.6168 (2)	0.10677 (19)	0.0668 (7)
C2	0.8017 (5)	0.6546 (3)	0.1773 (3)	0.1040 (14)
H2	0.7986	0.7218	0.1886	0.125*
C3	0.7718 (5)	0.5920 (4)	0.2314 (3)	0.1157 (17)
H3	0.7484	0.6174	0.2795	0.139*
C4	0.7758 (4)	0.4932 (3)	0.2158 (3)	0.0933 (11)
C5	0.8101 (6)	0.4568 (3)	0.1449 (3)	0.1198 (17)
H5	0.8140	0.3898	0.1337	0.144*
C6	0.8392 (5)	0.5189 (3)	0.0895 (3)	0.1104 (16)
H6	0.8607	0.4932	0.0408	0.132*
C7	0.7458 (6)	0.4277 (5)	0.2764 (4)	0.1261 (18)
C8	0.7271 (8)	0.2647 (5)	0.3072 (5)	0.194 (4)
H8A	0.7212	0.1970	0.2802	0.291*
H8B	0.6515	0.2672	0.3266	0.291*
H8C	0.7923	0.2843	0.3517	0.291*
C9	0.8940 (3)	0.7251 (2)	−0.12018 (17)	0.0631 (6)
C10	0.8708 (4)	0.6214 (3)	−0.1324 (2)	0.0832 (9)
H10	0.8485	0.5864	−0.0916	0.100*
C11	0.8814 (5)	0.5699 (3)	−0.2073 (2)	0.0973 (12)
H11	0.8652	0.4996	−0.2170	0.117*
C12	0.9155 (4)	0.6220 (3)	−0.2668 (2)	0.0944 (11)
C13	0.9382 (4)	0.7255 (3)	−0.2527 (2)	0.0983 (12)
H13	0.9607	0.7607	−0.2933	0.118*
C14	0.9282 (4)	0.7780 (3)	−0.1791 (2)	0.0837 (10)
H14	0.9445	0.8484	−0.1695	0.100*
C15	0.9305 (7)	0.5705 (4)	−0.3476 (3)	0.134 (2)
C16	0.9187 (9)	0.4122 (6)	−0.4322 (4)	0.214 (4)
H16A	0.9199	0.4590	−0.4646	0.321*
H16B	0.8492	0.3557	−0.4450	0.321*
H16C	0.9920	0.3836	−0.4381	0.321*
C17	0.8042 (3)	0.9714 (2)	0.26749 (17)	0.0637 (7)
C18	0.9268 (3)	0.9832 (3)	0.2737 (2)	0.0805 (9)
H18	0.9599	0.9525	0.2320	0.097*
C19	1.0025 (4)	1.0417 (3)	0.3428 (2)	0.0868 (10)
H19	1.0867	1.0514	0.3473	0.104*

C20	0.9508 (4)	1.0853 (3)	0.4051 (2)	0.0821 (9)
C21	0.8279 (4)	1.0716 (3)	0.3971 (2)	0.0915 (11)
H21	0.7940	1.1017	0.4387	0.110*
C22	0.7527 (4)	1.0146 (3)	0.3292 (2)	0.0828 (9)
H22	0.6685	1.0052	0.3248	0.099*
C23	1.0275 (5)	1.1485 (4)	0.4813 (3)	0.1073 (14)
C24	1.2295 (7)	1.2371 (7)	0.5482 (4)	0.222 (4)
H24A	1.3126	1.2378	0.5426	0.333*
H24B	1.2090	1.2113	0.5956	0.333*
H24C	1.2202	1.3048	0.5529	0.333*
C25	0.7969 (3)	1.0760 (2)	0.04436 (18)	0.0621 (6)
C26	0.7774 (3)	1.1707 (2)	0.0538 (2)	0.0733 (8)
H26	0.7537	1.1983	0.1011	0.088*
C27	0.7933 (3)	1.2244 (2)	−0.0070 (2)	0.0814 (9)
H27	0.7801	1.2888	−0.0006	0.098*
C28	0.8281 (3)	1.1854 (3)	−0.0771 (2)	0.0756 (8)
C29	0.8469 (3)	1.0887 (3)	−0.0863 (2)	0.0796 (9)
H29	0.8695	1.0609	−0.1340	0.096*
C30	0.8322 (3)	1.0334 (2)	−0.0248 (2)	0.0725 (8)
H30	0.8460	0.9693	−0.0305	0.087*
C31	0.8456 (4)	1.2499 (3)	−0.1411 (3)	0.0929 (11)
C32	0.8839 (7)	1.2588 (5)	−0.2720 (3)	0.161 (3)
H32A	0.9126	1.2234	−0.3161	0.242*
H32B	0.9409	1.3236	−0.2518	0.242*
H32C	0.8056	1.2683	−0.2902	0.242*
C33	0.5371 (3)	0.8246 (2)	−0.12920 (19)	0.0662 (7)
C34	0.6005 (4)	0.7933 (3)	−0.1888 (2)	0.0815 (9)
H34	0.6208	0.7318	−0.1920	0.098*
C35	0.6331 (4)	0.8545 (3)	−0.2430 (2)	0.0853 (10)
H35	0.6774	0.8350	−0.2827	0.102*
C36	0.6008 (3)	0.9452 (2)	−0.2394 (2)	0.0738 (8)
C37	0.5407 (3)	0.9764 (2)	−0.1778 (2)	0.0746 (8)
H37	0.5207	1.0380	−0.1742	0.089*
C38	0.5102 (3)	0.9169 (2)	−0.1216 (2)	0.0709 (7)
H38	0.4718	0.9389	−0.0792	0.085*
C39	0.6214 (4)	1.0076 (3)	−0.3021 (3)	0.0902 (10)
C40	0.6989 (7)	1.0189 (6)	−0.4250 (4)	0.170 (3)
H40A	0.6492	0.9724	−0.4710	0.254*
H40B	0.7827	1.0350	−0.4338	0.254*
H40C	0.6719	1.0798	−0.4168	0.254*
C41	0.4629 (3)	0.6495 (2)	0.1052 (2)	0.0692 (7)
C42	0.4727 (4)	0.7170 (2)	0.1749 (2)	0.0861 (10)
H42	0.4812	0.7854	0.1743	0.103*
C43	0.4698 (4)	0.6821 (3)	0.2460 (3)	0.0963 (12)
H43	0.4778	0.7277	0.2939	0.116*
C44	0.4553 (4)	0.5804 (3)	0.2475 (3)	0.0927 (11)
C45	0.4436 (5)	0.5145 (3)	0.1758 (3)	0.1006 (13)
H45	0.4327	0.4458	0.1759	0.121*

C46	0.4477 (4)	0.5485 (2)	0.1038 (2)	0.0882 (10)
H46	0.4402	0.5036	0.0556	0.106*
C47	0.4519 (6)	0.5466 (4)	0.3263 (3)	0.1229 (17)
C48	0.4132 (10)	0.4064 (5)	0.3942 (4)	0.212 (4)
H48A	0.3850	0.3338	0.3812	0.317*
H48B	0.3574	0.4330	0.4242	0.317*
H48C	0.4928	0.4259	0.4258	0.317*
N1	0.8413 (2)	0.85679 (17)	0.08693 (14)	0.0609 (5)
N2	0.6062 (2)	0.86386 (17)	0.05940 (15)	0.0623 (5)
N3	0.6736 (2)	0.70238 (16)	−0.01228 (15)	0.0640 (6)
O1	0.87654 (19)	0.67662 (15)	0.05182 (13)	0.0678 (5)
O2	0.7203 (6)	0.4592 (4)	0.3418 (3)	0.200 (3)
O3	0.7516 (4)	0.3338 (3)	0.2515 (3)	0.1446 (15)
O4	0.89006 (19)	0.78510 (14)	−0.04713 (12)	0.0672 (5)
O5	0.9558 (5)	0.6131 (3)	−0.4018 (2)	0.175 (2)
O6	0.9121 (7)	0.4724 (3)	−0.3521 (2)	0.212 (3)
O7	0.72241 (19)	0.91374 (15)	0.20060 (12)	0.0689 (5)
O8	0.9856 (4)	1.1792 (3)	0.53921 (19)	0.1426 (14)
O9	1.1461 (4)	1.1706 (3)	0.4758 (2)	0.1500 (16)
O10	0.78245 (19)	1.02854 (13)	0.11051 (12)	0.0656 (5)
O11	0.8401 (3)	1.3358 (2)	−0.1305 (2)	0.1172 (11)
O12	0.8724 (3)	1.1990 (3)	−0.20758 (19)	0.1173 (10)
O13	0.49148 (19)	0.75886 (16)	−0.07913 (14)	0.0731 (5)
O14	0.5805 (3)	1.0779 (3)	−0.3076 (2)	0.1237 (12)
O15	0.6883 (3)	0.9731 (3)	−0.35497 (19)	0.1156 (10)
O16	0.45734 (19)	0.68050 (16)	0.03086 (14)	0.0735 (5)
O17	0.4720 (6)	0.6033 (3)	0.3903 (2)	0.197 (3)
O18	0.4200 (4)	0.4473 (3)	0.3187 (2)	0.1383 (14)
P1	0.81205 (6)	0.75616 (5)	0.02155 (4)	0.05769 (19)
P2	0.73803 (6)	0.90996 (5)	0.10884 (4)	0.05735 (19)
P3	0.56765 (6)	0.75527 (5)	0.00331 (5)	0.0604 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0705 (17)	0.0575 (15)	0.0731 (18)	0.0171 (13)	0.0139 (13)	0.0119 (13)
C2	0.163 (4)	0.075 (2)	0.098 (3)	0.051 (2)	0.058 (3)	0.030 (2)
C3	0.176 (5)	0.101 (3)	0.096 (3)	0.058 (3)	0.062 (3)	0.034 (2)
C4	0.101 (3)	0.079 (2)	0.099 (3)	0.0106 (19)	0.016 (2)	0.033 (2)
C5	0.197 (5)	0.0553 (19)	0.106 (3)	0.025 (3)	0.028 (3)	0.020 (2)
C6	0.193 (5)	0.0594 (19)	0.084 (2)	0.037 (2)	0.040 (3)	0.0129 (17)
C7	0.136 (4)	0.126 (4)	0.127 (4)	0.024 (3)	0.030 (3)	0.066 (4)
C8	0.225 (8)	0.137 (5)	0.209 (7)	−0.011 (5)	−0.007 (6)	0.117 (5)
C9	0.0649 (16)	0.0627 (15)	0.0627 (15)	0.0167 (12)	0.0199 (12)	0.0080 (12)
C10	0.117 (3)	0.0666 (18)	0.0684 (19)	0.0225 (18)	0.0316 (18)	0.0120 (15)
C11	0.152 (4)	0.0656 (19)	0.081 (2)	0.032 (2)	0.045 (2)	0.0087 (17)
C12	0.131 (3)	0.089 (2)	0.072 (2)	0.038 (2)	0.038 (2)	0.0095 (18)
C13	0.139 (4)	0.092 (3)	0.074 (2)	0.034 (2)	0.045 (2)	0.0244 (19)

C14	0.107 (3)	0.0666 (18)	0.084 (2)	0.0230 (17)	0.040 (2)	0.0178 (16)
C15	0.227 (7)	0.106 (3)	0.088 (3)	0.061 (4)	0.074 (4)	0.016 (3)
C16	0.328 (8)	0.169 (5)	0.155 (5)	0.083 (5)	0.110 (5)	−0.014 (4)
C17	0.0808 (18)	0.0504 (13)	0.0599 (15)	0.0099 (12)	0.0247 (13)	0.0119 (11)
C18	0.088 (2)	0.081 (2)	0.0686 (18)	0.0204 (17)	0.0250 (16)	−0.0036 (16)
C19	0.091 (2)	0.088 (2)	0.075 (2)	0.0173 (18)	0.0147 (17)	0.0037 (18)
C20	0.113 (3)	0.0716 (19)	0.0609 (17)	0.0218 (18)	0.0194 (17)	0.0089 (14)
C21	0.120 (3)	0.097 (3)	0.0629 (19)	0.037 (2)	0.0337 (19)	0.0036 (17)
C22	0.093 (2)	0.090 (2)	0.0704 (19)	0.0284 (18)	0.0293 (17)	0.0135 (17)
C23	0.142 (4)	0.092 (3)	0.076 (2)	0.018 (3)	0.016 (3)	−0.001 (2)
C24	0.183 (7)	0.250 (10)	0.144 (6)	−0.014 (7)	−0.034 (5)	−0.079 (6)
C25	0.0599 (15)	0.0486 (13)	0.0720 (17)	0.0011 (11)	0.0186 (12)	0.0094 (12)
C26	0.0802 (19)	0.0521 (15)	0.090 (2)	0.0130 (13)	0.0311 (16)	0.0136 (14)
C27	0.083 (2)	0.0612 (17)	0.106 (3)	0.0174 (15)	0.0278 (19)	0.0248 (17)
C28	0.0622 (17)	0.0729 (19)	0.091 (2)	0.0077 (14)	0.0139 (15)	0.0277 (17)
C29	0.079 (2)	0.079 (2)	0.075 (2)	0.0061 (16)	0.0244 (16)	0.0116 (16)
C30	0.084 (2)	0.0537 (15)	0.0767 (19)	0.0086 (13)	0.0284 (16)	0.0075 (13)
C31	0.073 (2)	0.094 (3)	0.112 (3)	0.0093 (18)	0.022 (2)	0.038 (2)
C32	0.192 (7)	0.183 (6)	0.112 (4)	0.018 (5)	0.030 (4)	0.081 (4)
C33	0.0641 (16)	0.0580 (15)	0.0710 (17)	0.0091 (12)	0.0065 (13)	0.0092 (13)
C34	0.099 (2)	0.0618 (17)	0.093 (2)	0.0309 (16)	0.0268 (19)	0.0159 (16)
C35	0.100 (3)	0.081 (2)	0.086 (2)	0.0351 (19)	0.038 (2)	0.0176 (18)
C36	0.0721 (18)	0.0702 (18)	0.082 (2)	0.0176 (14)	0.0183 (15)	0.0195 (15)
C37	0.0750 (19)	0.0611 (16)	0.093 (2)	0.0214 (14)	0.0203 (16)	0.0191 (15)
C38	0.0690 (17)	0.0643 (17)	0.0809 (19)	0.0183 (13)	0.0215 (15)	0.0104 (14)
C39	0.090 (2)	0.094 (3)	0.096 (3)	0.025 (2)	0.026 (2)	0.031 (2)
C40	0.214 (7)	0.221 (7)	0.137 (5)	0.102 (6)	0.097 (5)	0.104 (5)
C41	0.0680 (17)	0.0570 (15)	0.0798 (19)	0.0053 (12)	0.0246 (14)	0.0132 (14)
C42	0.109 (3)	0.0528 (16)	0.100 (3)	0.0181 (16)	0.044 (2)	0.0126 (16)
C43	0.127 (3)	0.071 (2)	0.089 (2)	0.017 (2)	0.044 (2)	0.0059 (18)
C44	0.114 (3)	0.070 (2)	0.090 (2)	0.0083 (19)	0.033 (2)	0.0135 (18)
C45	0.144 (4)	0.0541 (17)	0.098 (3)	0.0048 (19)	0.033 (3)	0.0176 (18)
C46	0.119 (3)	0.0511 (16)	0.085 (2)	0.0026 (16)	0.030 (2)	0.0061 (15)
C47	0.175 (5)	0.096 (3)	0.095 (3)	0.017 (3)	0.041 (3)	0.023 (3)
C48	0.386 (14)	0.140 (6)	0.104 (4)	0.041 (7)	0.035 (6)	0.053 (4)
N1	0.0613 (13)	0.0505 (11)	0.0661 (13)	0.0092 (9)	0.0160 (10)	0.0008 (10)
N2	0.0612 (13)	0.0499 (11)	0.0745 (14)	0.0119 (9)	0.0187 (11)	0.0063 (10)
N3	0.0686 (14)	0.0436 (10)	0.0733 (14)	0.0076 (9)	0.0146 (11)	0.0002 (10)
O1	0.0766 (12)	0.0607 (11)	0.0730 (12)	0.0249 (9)	0.0250 (10)	0.0135 (9)
O2	0.296 (7)	0.189 (5)	0.171 (4)	0.082 (5)	0.116 (5)	0.114 (4)
O3	0.188 (4)	0.090 (2)	0.150 (3)	0.006 (2)	0.009 (3)	0.062 (2)
O4	0.0779 (12)	0.0522 (10)	0.0688 (12)	0.0100 (9)	0.0254 (10)	0.0053 (9)
O5	0.322 (7)	0.128 (3)	0.095 (2)	0.068 (4)	0.103 (3)	0.022 (2)
O6	0.443 (9)	0.108 (3)	0.113 (3)	0.089 (4)	0.143 (4)	0.014 (2)
O7	0.0771 (12)	0.0576 (10)	0.0671 (12)	0.0039 (9)	0.0276 (10)	0.0077 (9)
O8	0.185 (4)	0.153 (3)	0.0691 (18)	0.024 (3)	0.029 (2)	−0.0143 (19)
O9	0.129 (3)	0.162 (4)	0.111 (3)	0.004 (3)	−0.010 (2)	−0.044 (2)
O10	0.0823 (13)	0.0441 (9)	0.0663 (11)	0.0078 (8)	0.0231 (9)	0.0036 (8)

O11	0.123 (2)	0.101 (2)	0.149 (3)	0.0353 (18)	0.037 (2)	0.064 (2)
O12	0.136 (3)	0.126 (3)	0.093 (2)	0.018 (2)	0.0320 (19)	0.0453 (19)
O13	0.0694 (12)	0.0624 (11)	0.0809 (14)	0.0041 (9)	0.0096 (10)	0.0150 (10)
O14	0.145 (3)	0.117 (2)	0.149 (3)	0.063 (2)	0.061 (2)	0.073 (2)
O15	0.139 (3)	0.130 (2)	0.106 (2)	0.052 (2)	0.057 (2)	0.0526 (19)
O16	0.0669 (12)	0.0598 (11)	0.0865 (14)	−0.0005 (9)	0.0163 (10)	0.0150 (10)
O17	0.366 (8)	0.116 (3)	0.096 (3)	0.025 (4)	0.074 (4)	0.014 (2)
O18	0.222 (4)	0.090 (2)	0.093 (2)	0.011 (2)	0.031 (2)	0.0313 (17)
P1	0.0640 (4)	0.0458 (3)	0.0621 (4)	0.0113 (3)	0.0187 (3)	0.0054 (3)
P2	0.0641 (4)	0.0429 (3)	0.0623 (4)	0.0068 (3)	0.0215 (3)	0.0051 (3)
P3	0.0596 (4)	0.0465 (3)	0.0706 (4)	0.0050 (3)	0.0146 (3)	0.0083 (3)

Geometric parameters (Å, º)

C1—C2	1.366 (5)	C27—C28	1.367 (5)
C1—C6	1.351 (5)	C28—C29	1.392 (5)
C1—O1	1.388 (4)	C28—C31	1.514 (5)
C2—H2	0.9300	C29—H29	0.9300
C2—C3	1.375 (5)	C29—C30	1.393 (5)
C3—H3	0.9300	C30—H30	0.9300
C3—C4	1.364 (6)	C31—O11	1.193 (5)
C4—C5	1.364 (6)	C31—O12	1.339 (5)
C4—C7	1.492 (6)	C32—H32A	0.9600
C5—H5	0.9300	C32—H32B	0.9600
C5—C6	1.387 (6)	C32—H32C	0.9600
C6—H6	0.9300	C32—O12	1.474 (5)
C7—O2	1.220 (7)	C33—C34	1.379 (5)
C7—O3	1.322 (7)	C33—C38	1.374 (4)
C8—H8A	0.9600	C33—O13	1.391 (4)
C8—H8B	0.9600	C34—H34	0.9300
C8—H8C	0.9600	C34—C35	1.370 (5)
C8—O3	1.451 (6)	C35—H35	0.9300
C9—C10	1.373 (4)	C35—C36	1.384 (5)
C9—C14	1.368 (4)	C36—C37	1.379 (5)
C9—O4	1.393 (3)	C36—C39	1.479 (5)
C10—H10	0.9300	C37—H37	0.9300
C10—C11	1.390 (5)	C37—C38	1.376 (5)
C11—H11	0.9300	C38—H38	0.9300
C11—C12	1.370 (5)	C39—O14	1.189 (5)
C12—C13	1.371 (5)	C39—O15	1.342 (5)
C12—C15	1.493 (5)	C40—H40A	0.9600
C13—H13	0.9300	C40—H40B	0.9600
C13—C14	1.376 (5)	C40—H40C	0.9600
C14—H14	0.9300	C40—O15	1.439 (5)
C15—O5	1.194 (6)	C41—C42	1.366 (5)
C15—O6	1.312 (6)	C41—C46	1.363 (4)
C16—H16A	0.9140	C41—O16	1.400 (4)
C16—H16B	0.9484	C42—H42	0.9300

C16—H16C	1.0149	C42—C43	1.372 (5)
C16—O6	1.500 (6)	C43—H43	0.9300
C17—C18	1.359 (5)	C43—C44	1.383 (5)
C17—C22	1.379 (4)	C44—C45	1.375 (5)
C17—O7	1.392 (4)	C44—C47	1.491 (6)
C18—H18	0.9300	C45—H45	0.9300
C18—C19	1.392 (5)	C45—C46	1.383 (5)
C19—H19	0.9300	C46—H46	0.9300
C19—C20	1.391 (5)	C47—O17	1.203 (6)
C20—C21	1.357 (6)	C47—O18	1.316 (6)
C20—C23	1.499 (6)	C48—H48A	0.9600
C21—H21	0.9300	C48—H48B	0.9600
C21—C22	1.369 (5)	C48—H48C	0.9600
C22—H22	0.9300	C48—O18	1.485 (6)
C23—O8	1.202 (5)	N1—P1	1.581 (2)
C23—O9	1.330 (6)	N1—P2	1.578 (2)
C24—H24A	0.9600	N2—P2	1.576 (3)
C24—H24B	0.9600	N2—P3	1.583 (2)
C24—H24C	0.9600	N3—P1	1.578 (2)
C24—O9	1.500 (6)	N3—P3	1.580 (2)
C25—C26	1.369 (4)	O1—P1	1.585 (2)
C25—C30	1.375 (4)	O4—P1	1.584 (2)
C25—O10	1.396 (3)	O7—P2	1.585 (2)
C26—H26	0.9300	O10—P2	1.5919 (19)
C26—C27	1.371 (5)	O13—P3	1.587 (2)
C27—H27	0.9300	O16—P3	1.588 (2)

C2—C1—O1	122.8 (3)	C29—C30—H30	120.9
C6—C1—C2	120.8 (3)	O11—C31—C28	122.8 (4)
C6—C1—O1	116.3 (3)	O11—C31—O12	126.0 (4)
C1—C2—H2	120.4	O12—C31—C28	111.1 (4)
C1—C2—C3	119.1 (4)	H32A—C32—H32B	109.5
C3—C2—H2	120.4	H32A—C32—H32C	109.5
C2—C3—H3	119.4	H32B—C32—H32C	109.5
C4—C3—C2	121.2 (4)	O12—C32—H32A	109.5
C4—C3—H3	119.4	O12—C32—H32B	109.5
C3—C4—C5	118.7 (4)	O12—C32—H32C	109.5
C3—C4—C7	120.0 (5)	C34—C33—O13	119.6 (3)
C5—C4—C7	121.2 (4)	C38—C33—C34	121.4 (3)
C4—C5—H5	119.7	C38—C33—O13	118.8 (3)
C4—C5—C6	120.6 (4)	C33—C34—H34	120.6
C6—C5—H5	119.7	C35—C34—C33	118.7 (3)
C1—C6—C5	119.5 (4)	C35—C34—H34	120.6
C1—C6—H6	120.2	C34—C35—H35	119.6
C5—C6—H6	120.2	C34—C35—C36	120.8 (3)
O2—C7—C4	122.8 (6)	C36—C35—H35	119.6
O2—C7—O3	124.6 (5)	C35—C36—C39	122.5 (3)
O3—C7—C4	112.5 (5)	C37—C36—C35	119.3 (3)

H8A—C8—H8B	109.5	C37—C36—C39	118.1 (3)
H8A—C8—H8C	109.5	C36—C37—H37	119.8
H8B—C8—H8C	109.5	C38—C37—C36	120.5 (3)
O3—C8—H8A	109.5	C38—C37—H37	119.8
O3—C8—H8B	109.5	C33—C38—C37	119.1 (3)
O3—C8—H8C	109.5	C33—C38—H38	120.5
C10—C9—O4	123.6 (3)	C37—C38—H38	120.5
C14—C9—C10	121.7 (3)	O14—C39—C36	124.8 (4)
C14—C9—O4	114.5 (3)	O14—C39—O15	123.2 (4)
C9—C10—H10	120.8	O15—C39—C36	112.0 (3)
C9—C10—C11	118.4 (3)	H40A—C40—H40B	109.5
C11—C10—H10	120.8	H40A—C40—H40C	109.5
C10—C11—H11	119.8	H40B—C40—H40C	109.5
C12—C11—C10	120.5 (3)	O15—C40—H40A	109.5
C12—C11—H11	119.8	O15—C40—H40B	109.5
C11—C12—C13	119.8 (3)	O15—C40—H40C	109.5
C11—C12—C15	122.6 (4)	C42—C41—O16	120.7 (3)
C13—C12—C15	117.6 (4)	C46—C41—C42	122.1 (3)
C12—C13—H13	119.6	C46—C41—O16	116.9 (3)
C12—C13—C14	120.7 (3)	C41—C42—H42	120.6
C14—C13—H13	119.6	C41—C42—C43	118.8 (3)
C9—C14—C13	118.9 (3)	C43—C42—H42	120.6
C9—C14—H14	120.6	C42—C43—H43	119.5
C13—C14—H14	120.6	C42—C43—C44	121.1 (4)
O5—C15—C12	124.3 (5)	C44—C43—H43	119.5
O5—C15—O6	124.0 (4)	C43—C44—C47	118.8 (4)
O6—C15—C12	111.6 (4)	C45—C44—C43	118.4 (4)
H16A—C16—H16B	114.6	C45—C44—C47	122.8 (4)
H16A—C16—H16C	108.6	C44—C45—H45	119.3
H16B—C16—H16C	105.9	C44—C45—C46	121.3 (3)
O6—C16—H16A	101.8	C46—C45—H45	119.3
O6—C16—H16B	107.9	C41—C46—C45	118.3 (3)
O6—C16—H16C	118.4	C41—C46—H46	120.9
C18—C17—C22	121.2 (3)	C45—C46—H46	120.9
C18—C17—O7	123.0 (3)	O17—C47—C44	124.1 (5)
C22—C17—O7	115.7 (3)	O17—C47—O18	122.9 (5)
C17—C18—H18	120.2	O18—C47—C44	112.9 (4)
C17—C18—C19	119.6 (3)	H48A—C48—H48B	109.5
C19—C18—H18	120.2	H48A—C48—H48C	109.5
C18—C19—H19	120.4	H48B—C48—H48C	109.5
C20—C19—C18	119.2 (4)	O18—C48—H48A	109.5
C20—C19—H19	120.4	O18—C48—H48B	109.5
C19—C20—C23	121.7 (4)	O18—C48—H48C	109.5
C21—C20—C19	119.6 (4)	P2—N1—P1	121.25 (15)
C21—C20—C23	118.7 (4)	P2—N2—P3	122.18 (15)
C20—C21—H21	119.2	P1—N3—P3	122.53 (14)
C20—C21—C22	121.6 (3)	C1—O1—P1	125.06 (18)
C22—C21—H21	119.2	C7—O3—C8	116.7 (5)

C17—C22—H22	120.6	C9—O4—P1	128.66 (18)
C21—C22—C17	118.7 (4)	C15—O6—C16	116.2 (5)
C21—C22—H22	120.6	C17—O7—P2	127.46 (17)
O8—C23—C20	123.5 (5)	C23—O9—C24	116.0 (5)
O8—C23—O9	124.1 (5)	C25—O10—P2	126.87 (17)
O9—C23—C20	112.3 (4)	C31—O12—C32	111.9 (4)
H24A—C24—H24B	109.5	C33—O13—P3	122.39 (19)
H24A—C24—H24C	109.5	C39—O15—C40	116.6 (4)
H24B—C24—H24C	109.5	C41—O16—P3	124.1 (2)
O9—C24—H24A	109.5	C47—O18—C48	116.8 (4)
O9—C24—H24B	109.5	N1—P1—O1	110.93 (13)
O9—C24—H24C	109.5	N1—P1—O4	105.08 (11)
C26—C25—C30	121.5 (3)	N3—P1—N1	117.61 (12)
C26—C25—O10	115.3 (3)	N3—P1—O1	109.56 (12)
C30—C25—O10	123.2 (3)	N3—P1—O4	112.49 (13)
C25—C26—H26	120.3	O4—P1—O1	99.65 (11)
C25—C26—C27	119.4 (3)	N1—P2—O7	110.81 (13)
C27—C26—H26	120.3	N1—P2—O10	110.56 (12)
C26—C27—H27	119.3	N2—P2—N1	117.92 (12)
C28—C27—C26	121.3 (3)	N2—P2—O7	106.22 (12)
C28—C27—H27	119.3	N2—P2—O10	110.78 (12)
C27—C28—C29	118.8 (3)	O7—P2—O10	98.77 (11)
C27—C28—C31	118.3 (3)	N2—P3—O13	110.06 (13)
C29—C28—C31	122.9 (4)	N2—P3—O16	112.16 (12)
C28—C29—H29	119.7	N3—P3—N2	116.53 (13)
C28—C29—C30	120.7 (3)	N3—P3—O13	110.80 (13)
C30—C29—H29	119.7	N3—P3—O16	110.73 (12)
C25—C30—C29	118.3 (3)	O13—P3—O16	94.40 (12)
C25—C30—H30	120.9		

C1—C2—C3—C4	0.0 (8)	C33—C34—C35—C36	−1.4 (6)
C1—O1—P1—N1	77.4 (3)	C33—O13—P3—N2	56.8 (3)
C1—O1—P1—N3	−54.1 (3)	C33—O13—P3—N3	−73.5 (3)
C1—O1—P1—O4	−172.2 (2)	C33—O13—P3—O16	172.4 (2)
C2—C1—C6—C5	−1.5 (8)	C34—C33—C38—C37	4.0 (5)
C2—C1—O1—P1	−46.9 (5)	C34—C33—O13—P3	90.7 (3)
C2—C3—C4—C5	−0.1 (9)	C34—C35—C36—C37	3.4 (6)
C2—C3—C4—C7	178.5 (5)	C34—C35—C36—C39	−172.7 (4)
C3—C4—C5—C6	−0.6 (8)	C35—C36—C37—C38	−1.7 (6)
C3—C4—C7—O2	−2.1 (10)	C35—C36—C39—O14	169.1 (5)
C3—C4—C7—O3	178.8 (5)	C35—C36—C39—O15	−8.4 (6)
C4—C5—C6—C1	1.4 (9)	C36—C37—C38—C33	−2.0 (5)
C4—C7—O3—C8	178.4 (5)	C36—C39—O15—C40	171.3 (5)
C5—C4—C7—O2	176.5 (7)	C37—C36—C39—O14	−7.1 (7)
C5—C4—C7—O3	−2.6 (8)	C37—C36—C39—O15	175.5 (4)
C6—C1—C2—C3	0.8 (7)	C38—C33—C34—C35	−2.4 (6)
C6—C1—O1—P1	137.2 (3)	C38—C33—O13—P3	−93.9 (3)
C7—C4—C5—C6	−179.2 (5)	C39—C36—C37—C38	174.6 (3)

C9—C10—C11—C12	0.7 (7)	C41—C42—C43—C44	−1.0 (7)
C9—O4—P1—N1	−177.2 (2)	C41—O16—P3—N2	−62.6 (3)
C9—O4—P1—N3	−48.1 (3)	C41—O16—P3—N3	69.4 (3)
C9—O4—P1—O1	67.9 (3)	C41—O16—P3—O13	−176.4 (2)
C10—C9—C14—C13	0.7 (6)	C42—C41—C46—C45	−0.7 (6)
C10—C9—O4—P1	−27.7 (4)	C42—C41—O16—P3	67.6 (4)
C10—C11—C12—C13	−0.6 (8)	C42—C43—C44—C45	−0.1 (7)
C10—C11—C12—C15	178.8 (5)	C42—C43—C44—C47	−179.6 (5)
C11—C12—C13—C14	0.6 (8)	C43—C44—C45—C46	0.8 (7)
C11—C12—C15—O5	177.2 (7)	C43—C44—C47—O17	−7.0 (10)
C11—C12—C15—O6	−2.7 (9)	C43—C44—C47—O18	170.6 (5)
C12—C13—C14—C9	−0.6 (7)	C44—C45—C46—C41	−0.4 (7)
C12—C15—O6—C16	177.1 (6)	C44—C47—O18—C48	−179.6 (6)
C13—C12—C15—O5	−3.3 (10)	C45—C44—C47—O17	173.6 (7)
C13—C12—C15—O6	176.8 (6)	C45—C44—C47—O18	−8.8 (8)
C14—C9—C10—C11	−0.8 (6)	C46—C41—C42—C43	1.4 (6)
C14—C9—O4—P1	155.0 (3)	C46—C41—O16—P3	−117.7 (3)
C15—C12—C13—C14	−178.9 (5)	C47—C44—C45—C46	−179.7 (5)
C17—C18—C19—C20	1.3 (6)	O1—C1—C2—C3	−174.9 (4)
C17—O7—P2—N1	69.3 (3)	O1—C1—C6—C5	174.4 (4)
C17—O7—P2—N2	−161.5 (2)	O2—C7—O3—C8	−0.7 (10)
C17—O7—P2—O10	−46.7 (3)	O4—C9—C10—C11	−177.9 (4)
C18—C17—C22—C21	1.0 (5)	O4—C9—C14—C13	178.1 (4)
C18—C17—O7—P2	−42.0 (4)	O5—C15—O6—C16	−2.8 (13)
C18—C19—C20—C21	−1.0 (6)	O7—C17—C18—C19	−179.6 (3)
C18—C19—C20—C23	179.6 (4)	O7—C17—C22—C21	179.5 (3)
C19—C20—C21—C22	0.8 (6)	O8—C23—O9—C24	0.9 (9)
C19—C20—C23—O8	−172.6 (5)	O10—C25—C26—C27	178.0 (3)
C19—C20—C23—O9	10.5 (6)	O10—C25—C30—C29	−178.3 (3)
C20—C21—C22—C17	−0.8 (6)	O11—C31—O12—C32	−5.5 (7)
C20—C23—O9—C24	177.7 (5)	O13—C33—C34—C35	172.9 (3)
C21—C20—C23—O8	8.1 (7)	O13—C33—C38—C37	−171.3 (3)
C21—C20—C23—O9	−168.8 (4)	O14—C39—O15—C40	−6.3 (8)
C22—C17—C18—C19	−1.3 (5)	O16—C41—C42—C43	175.8 (3)
C22—C17—O7—P2	139.6 (3)	O16—C41—C46—C45	−175.3 (4)
C23—C20—C21—C22	−179.8 (4)	O17—C47—O18—C48	−1.9 (11)
C25—C26—C27—C28	0.0 (5)	P1—N1—P2—N2	−4.0 (2)
C25—O10—P2—N1	72.8 (3)	P1—N1—P2—O7	118.61 (17)
C25—O10—P2—N2	−59.8 (3)	P1—N1—P2—O10	−132.93 (16)
C25—O10—P2—O7	−171.0 (2)	P1—N3—P3—N2	−3.4 (2)
C26—C25—C30—C29	−0.6 (5)	P1—N3—P3—O13	123.41 (18)
C26—C25—O10—P2	149.5 (2)	P1—N3—P3—O16	−133.21 (18)
C26—C27—C28—C29	0.4 (5)	P2—N1—P1—N3	−8.3 (2)
C26—C27—C28—C31	−179.1 (3)	P2—N1—P1—O1	−135.53 (16)
C27—C28—C29—C30	−0.9 (5)	P2—N1—P1—O4	117.68 (17)
C27—C28—C31—O11	6.3 (6)	P2—N2—P3—N3	−9.8 (2)
C27—C28—C31—O12	−176.3 (3)	P2—N2—P3—O13	−137.04 (17)
C28—C29—C30—C25	1.0 (5)	P2—N2—P3—O16	119.26 (17)

C28—C31—O12—C32	177.2 (4)	P3—N2—P2—N1	13.5 (2)
C29—C28—C31—O11	−173.1 (4)	P3—N2—P2—O7	−111.43 (18)
C29—C28—C31—O12	4.2 (5)	P3—N2—P2—O10	142.30 (16)
C30—C25—C26—C27	0.1 (5)	P3—N3—P1—N1	12.3 (3)
C30—C25—O10—P2	−32.7 (4)	P3—N3—P1—O1	140.13 (17)
C31—C28—C29—C30	178.6 (3)	P3—N3—P1—O4	−110.02 (18)