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Poly[[μ -bis(4-nitrophenyl) phosphato- $\kappa^2 O, O'$]sodium]

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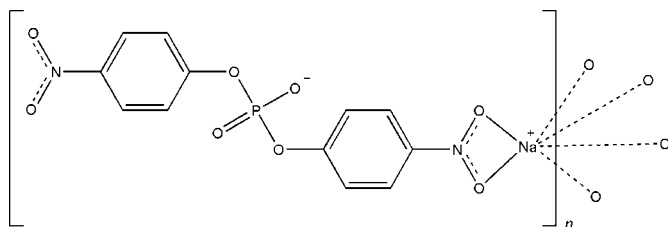
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(C-C) = 0.001$ Å; R factor = 0.030; wR factor = 0.090; data-to-parameter ratio = 31.1.

The title compound, $[Na(C_{12}H_8N_2O_8P)]$, consists of one Na^+ cation and one bis(*p*-nitrophenyl)phosphate anion with a considerable distortion of the phosphate tetrahedron due to the presence of two P—O ester bonds. The anion bridges five Na^+ cations whereby each cation is chelated by the nitro O atoms of one anion and bonded *via* a nitro O atom and phosphate O atoms to four other anions. This bridging arrangement leads to the formation of double layers parallel to (001). Adjacent layers are linked through weak C—H...O hydrogen bonds.

Related literature

For hydrolytic cleavage of the phosphodiester bond in bis(*p*-nitrophenyl)phosphate (BNPP) and related systems, see: Belousoff *et al.* (2009); Branum *et al.* (2001); Chang *et al.* (2009); Liu *et al.* (2004); Mancin *et al.* (2005); Oh *et al.* (1996); Sredhera & Cowan (2001). For crystal structures containing the BNPP entity, see: Bazzicalupi *et al.* (2004); Bond *et al.* (1985); Fry *et al.* (2003); Jurek & Martell (1999); Král *et al.* (2006); Pletcher *et al.* (1972); Sax *et al.* (1970, 1971); Warden *et al.* (2005); Yoo *et al.* (1975).



Experimental

Crystal data

$[Na(C_{12}H_8N_2O_8P)]$
 $M_r = 362.16$
 Triclinic, $P\bar{1}$
 $a = 6.963$ (2) Å
 $b = 9.844$ (3) Å

$c = 11.213$ (3) Å
 $\alpha = 103.93$ (3)°
 $\beta = 105.83$ (3)°
 $\gamma = 106.38$ (3)°
 $V = 666.1$ (3) Å³

$Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.29$ mm⁻¹

$T = 100$ K
 $0.30 \times 0.27 \times 0.25$ mm

Data collection

Agilent Xcalibur (Onyx with CCD camera) diffractometer
 Absorption correction: analytical (*CrysAlis PRO*; Agilent, 2011)
 $T_{min} = 0.918$, $T_{max} = 0.931$

13418 measured reflections
 6748 independent reflections
 5542 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.014$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.090$
 $S = 1.07$
 6748 reflections

217 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 0.66$ e Å⁻³
 $\Delta\rho_{min} = -0.33$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

P1—O31	1.4733 (8)	O2—Na	2.4618 (11)
P1—O41	1.4834 (7)	O4—Na ⁱ	2.3853 (11)
P1—O11	1.6266 (8)	O31—Na ⁱⁱ	2.2386 (10)
P1—O21	1.6287 (12)	O41—Na ⁱⁱⁱ	2.3135 (9)
O1—Na	2.9377 (18)	O41—Na ^{iv}	2.4065 (14)
O31—P1—O41	119.67 (5)	O31—P1—O21	110.48 (5)
O31—P1—O11	110.86 (4)	O41—P1—O21	110.21 (4)
O41—P1—O11	110.02 (4)	O11—P1—O21	92.20 (4)

Symmetry codes: (i) $x-1, y-2, z$; (ii) $x, y-1, z$; (iii) $x-1, y-1, z$; (iv) $-x+1, -y+2, -z+1$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2...O3 ^v	0.95	2.50	3.1865 (15)	129
C21—H21...O1 ^{vi}	0.95	2.53	3.3337 (18)	142

Symmetry codes: (v) $-x, -y, -z$; (vi) $-x, -y+1, -z$.

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Professor Dr Jerzy Lisowski for helpful discussions during preparation of this article.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2751).

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supporting information

Acta Cryst. (2013). E69, m464–m465 [doi:10.1107/S1600536813019260]

Poly[[μ -bis(4-nitrophenyl) phosphato- κ^2 O,O']sodium]**Aleksandra Gerus and Tadeusz Lis****S1. Comment**

Phosphate diester hydrolysis is a reaction of continuing interest since such process is of fundamental biological importance. Currently, there is much interest in developing artificial nucleases that hydrolyze the phosphate diester bonds in RNA and DNA (Sredhera & Cowan, 2001; Belousoff *et al.*, 2009; Branum *et al.*, 2001). Thus, there have been numerous model studies devoted to understanding how metalloenzymes hydrolyze phosphate diesters (Mancin *et al.*, 2005; Liu *et al.*, 2004). In most cases the substrate of choice is the "activated" phosphate diester bis(*p*-nitrophenyl)-phosphate (BNPP). It is considered as an activated phosphate diester because the *p*-nitro groups draw electron density away from the phosphorus atom as well as help to stabilize the negatively charged leaving group (Jurek & Martell, 1999). For this reason the bis(*p*-nitrophenyl)phosphate anion is a popular model substrate for kinetic studies of the hydrolytic cleavage of the phosphodiester bond similar to DNA (Chang *et al.*, 2009; Oh *et al.*, 1996).

BNPP is commercially available as a sodium salt. There are many references concerning solid state studies of BNPP acting as a ligand in complexes or as an anion in salts. The first publications referring to BNPP describe salts of local anesthetics (Sax *et al.*, 1970, 1971; Pletcher *et al.*, 1972; Yoo *et al.*, 1975). The structure of BNPP has been observed also in many macrocyclic complexes (Král *et al.*, 2006; Bazzicalupi *et al.*, 2004; Fry *et al.*, 2003; Warden *et al.*, 2005). Here we report the structure of BNPP as a sodium salt, [Na(C₁₂H₈N₂O₈P)], (I).

Compound (I) crystallizes with one bis(*p*-nitrophenyl)phosphate anion (Fig. 1) and one sodium cation in the asymmetric unit. The phenyl rings are almost coplanar. The interplanar angle between two phenyl rings amounts to 2.36 (3)°. The nitro group O1—N1—O2 is rotated 2.00 (4)° from the phenyl ring C1—C6 and the second nitro group O3—N2—O4 is rotated 9.01 (4)° from the phenyl ring C11—C16. The phosphate group is highly distorted from the ideal tetrahedral geometry (Table 1). In the anion there are two shorter P—O bonds of 1.4733 (8) Å and 1.4834 (7) Å, and two longer P—O ester bonds lengths of 1.6266 (8) Å and 1.6287 (12) Å. The shortest bond is P—O31. A little longer than the P—O31 bond is the P—O41 bond, bridging Na⁺ ions. Both O11 and O21 atoms involved in longer ester bonds are attached to aryl rings. The average P—O distance is 1.55 Å, but individual P—O bonds in the structure of compound (I) show how much the phosphate group is deformed. In previous reports containing BNPP anions the most similar deviations for P—O ester bond length in the phosphate group has been observed for these four examples (Sax *et al.*, 1970, 1971; Pletcher *et al.*, 1972; Yoo *et al.*, 1975).

The bond angles in the phosphate group distinctly deviate from the ideal value of 109.5°. The average value for the O—P—O angle is 108.9°, however, individual angles show considerable deviations. The smallest angle is 92.20 (4)° for O11—P1—O21, that is ArO—P—OAr. This deviation can be correlated with the corresponding bond lengths. Such a small angle has not been observed in any previous report of a BNPP structure. The most comparable value of an O—P—O angle is 95.3 (2)° (Bond *et al.*, 1985). The largest angle is 119.67 (5)° for O31—P—O41, and the four remaining angles are about 110°.

In (I), the coordination geometry of Na^+ ion is irregular, with an overall coordination number of six [5 + 1]. The Na^+ ion is coordinated by five symmetry-related BNPP anions *via* oxygen atoms. It is chelated by one anion in a bidentate mode (*via* O1 and O2), and coordinated by four anions in a monodentate manner (*via* O31^{iv}, O4ⁱⁱⁱ, O41^v and O41^{vi}) (Fig. 2). The Na—O distances are in the range 2.2386 (10) to 2.9377 (18) Å (Table 2). In the structure there is also a short Na...Na distance of 3.253 (2) Å, and two sodium cations are bridged by two O atoms (denoted as O41 in Fig. 2), forming a dimeric sub-structure with a four-membered ring (Figs. 2 and 4). The cations and anions are arranged in double layers parallel to (001) (Figs. 3 and 4). Adjacent layers are linked through weak C—H...O hydrogen bonds existing between H atoms of the aromatic rings and nitro O atoms (Fig. 3, Table 2).

S2. Experimental

The bis(*p*-nitrophenyl)phosphate sodium salt was purchased from Sigma-Aldrich. Yellow crystals were obtained after several days by slow evaporation of an aqueous solution.

S3. Refinement

All H atoms were introduced in geometrically calculated positions, with C—H = 0.95 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

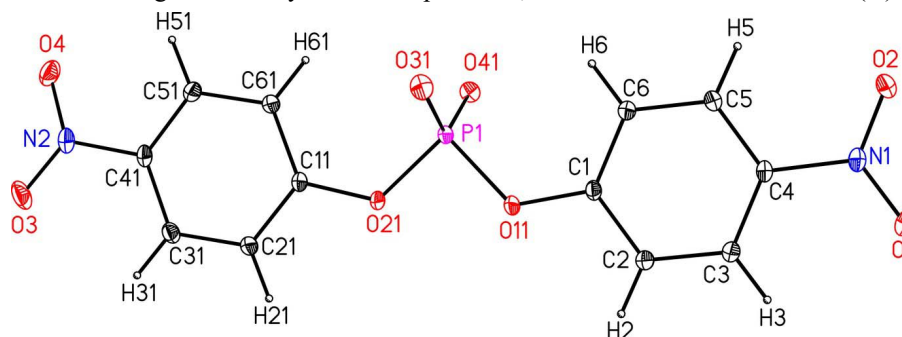
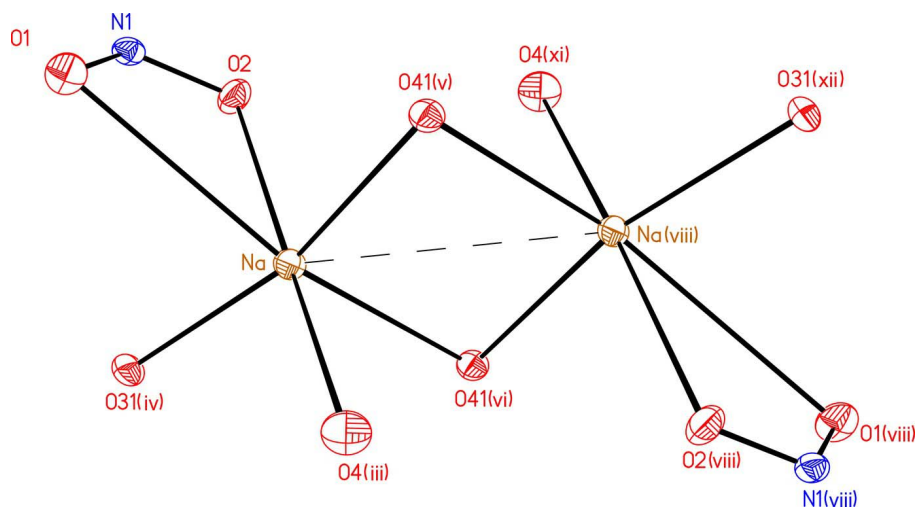
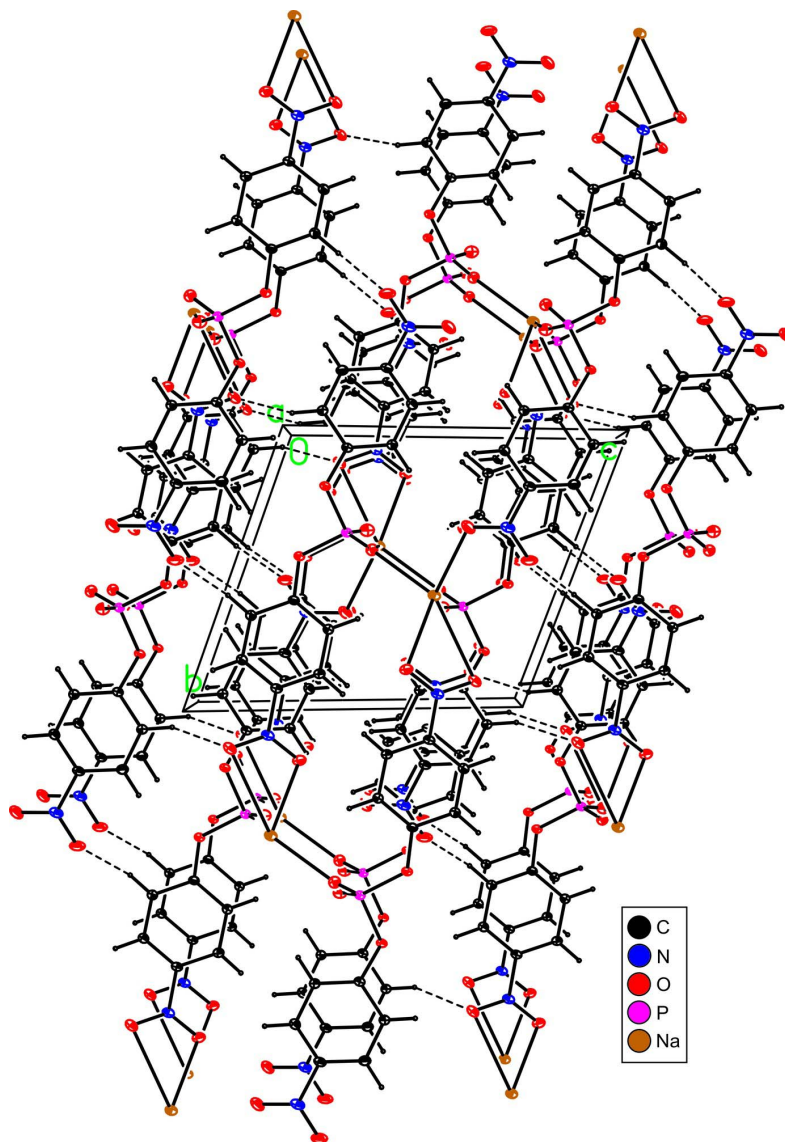


Figure 1

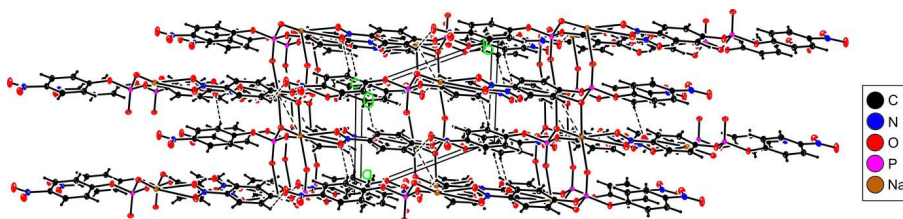
The molecular structure and numbering scheme for the BNPP anion. Displacement ellipsoids are shown at the 50% probability level.

**Figure 2**

Coordination sphere of the Na⁺ cation in (I). Displacement ellipsoids are shown at the 50% probability level. [Symmetry codes: (iii) $x + 1, y + 2, z$; (iv) $x, y + 1, z$; (v) $x + 1, y + 1, z$; (vi) $-x + 1, -y + 2, -z + 1$; (viii) $-x + 2, -y + 3, -z + 1$; (xi) $-x + 1, -y + 1, -z + 1$; (xii) $-x + 2, -y + 2, -z + 1$].

**Figure 3**

Projection of (I) along [100] showing the double layers. Dashed lines indicate C—H...O hydrogen bonds. Displacement ellipsoids are shown at the 50% probability level.

**Figure 4**

The packing diagram for crystal of the title salt (I). Displacement ellipsoids are shown at 50% probability level.

Poly[[μ -bis(4-nitrophenyl) phosphato- κ^2O,O']sodium]

Crystal data

[Na(C₁₂H₈N₂O₈P)] $M_r = 362.16$ Triclinic, $P\bar{1}$

Hall symbol: -P 1

 $a = 6.963$ (2) Å $b = 9.844$ (3) Å $c = 11.213$ (3) Å $\alpha = 103.93$ (3)° $\beta = 105.83$ (3)° $\gamma = 106.38$ (3)° $V = 666.1$ (3) Å³ $Z = 2$ $F(000) = 368$ $D_x = 1.806$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 8925 reflections

 $\theta = 3.2$ – 37.5 ° $\mu = 0.29$ mm⁻¹ $T = 100$ K

Block, yellow

 $0.30 \times 0.27 \times 0.25$ mm

Data collection

Agilent Xcalibur (Onyx with CCD camera)
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 ω and π scans

Absorption correction: analytical

(CrysAlis PRO; Agilent, 2011)

 $T_{\min} = 0.918$, $T_{\max} = 0.931$

13418 measured reflections

6748 independent reflections

5542 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.014$ $\theta_{\text{max}} = 37.6$ °, $\theta_{\text{min}} = 3.2$ ° $h = -11 \rightarrow 10$ $k = -16 \rightarrow 15$ $l = -19 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.030$ $wR(F^2) = 0.090$ $S = 1.07$

6748 reflections

217 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 0.1337P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} = 0.001$ $\Delta\rho_{\text{max}} = 0.66$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.33$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
P1	0.19163 (3)	0.36887 (2)	0.291283 (19)	0.00783 (4)
O1	0.52988 (11)	1.11256 (7)	0.18582 (7)	0.01642 (12)
O2	0.66594 (11)	1.15233 (7)	0.39510 (6)	0.01488 (11)

O3	-0.28509 (13)	-0.46498 (7)	0.15506 (8)	0.02195 (14)
O4	-0.14079 (12)	-0.34783 (8)	0.36644 (7)	0.01817 (13)
O11	0.18884 (10)	0.45097 (6)	0.18143 (6)	0.01210 (10)
O21	0.02554 (10)	0.20680 (6)	0.18007 (6)	0.01107 (10)
O31	0.40483 (10)	0.36277 (7)	0.34892 (6)	0.01340 (11)
O41	0.08681 (9)	0.42769 (7)	0.37940 (6)	0.01131 (10)
N1	0.55665 (11)	1.06716 (8)	0.27967 (7)	0.01084 (11)
N2	-0.18533 (12)	-0.34891 (8)	0.25185 (8)	0.01290 (12)
C1	0.28334 (12)	0.60309 (8)	0.21207 (7)	0.00932 (12)
C2	0.24915 (13)	0.65553 (9)	0.10570 (8)	0.01132 (12)
H2	0.1654	0.5862	0.0187	0.014*
C3	0.33698 (13)	0.80825 (9)	0.12681 (8)	0.01110 (12)
H3	0.3144	0.8448	0.0551	0.013*
C4	0.45900 (12)	0.90670 (8)	0.25538 (8)	0.00970 (12)
C5	0.49639 (13)	0.85587 (9)	0.36171 (8)	0.01053 (12)
H5	0.5815	0.9255	0.4484	0.013*
C6	0.40903 (13)	0.70311 (9)	0.34079 (8)	0.01043 (12)
H6	0.4341	0.6669	0.4126	0.013*
C11	-0.01420 (12)	0.07325 (8)	0.20306 (8)	0.00914 (11)
C21	-0.14071 (13)	-0.05705 (9)	0.09256 (8)	0.01090 (12)
H21	-0.1902	-0.0492	0.0077	0.013*
C31	-0.19405 (13)	-0.19754 (9)	0.10643 (8)	0.01187 (13)
H31	-0.2790	-0.2867	0.0320	0.014*
C41	-0.11984 (13)	-0.20435 (9)	0.23230 (8)	0.01057 (12)
C51	0.00777 (13)	-0.07667 (9)	0.34263 (8)	0.01163 (13)
H51	0.0579	-0.0854	0.4271	0.014*
C61	0.06168 (13)	0.06395 (9)	0.32862 (8)	0.01120 (12)
H61	0.1489	0.1526	0.4033	0.013*
Na	0.75570 (5)	1.41177 (4)	0.39243 (3)	0.01082 (7)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.00772 (8)	0.00661 (8)	0.00894 (8)	0.00226 (6)	0.00311 (6)	0.00274 (6)
O1	0.0212 (3)	0.0124 (3)	0.0172 (3)	0.0056 (2)	0.0065 (2)	0.0091 (2)
O2	0.0167 (3)	0.0091 (2)	0.0144 (3)	0.0027 (2)	0.0032 (2)	0.0020 (2)
O3	0.0321 (4)	0.0079 (3)	0.0231 (3)	0.0030 (3)	0.0129 (3)	0.0025 (2)
O4	0.0225 (3)	0.0154 (3)	0.0206 (3)	0.0075 (2)	0.0087 (3)	0.0116 (2)
O11	0.0172 (3)	0.0066 (2)	0.0100 (2)	0.00113 (19)	0.0046 (2)	0.00292 (18)
O21	0.0137 (2)	0.0062 (2)	0.0103 (2)	0.00136 (19)	0.00201 (19)	0.00335 (18)
O31	0.0084 (2)	0.0132 (3)	0.0176 (3)	0.0045 (2)	0.0038 (2)	0.0042 (2)
O41	0.0108 (2)	0.0121 (2)	0.0121 (2)	0.00466 (19)	0.00572 (19)	0.00352 (19)
N1	0.0107 (3)	0.0084 (3)	0.0147 (3)	0.0041 (2)	0.0052 (2)	0.0049 (2)
N2	0.0142 (3)	0.0093 (3)	0.0190 (3)	0.0054 (2)	0.0094 (2)	0.0063 (2)
C1	0.0102 (3)	0.0068 (3)	0.0107 (3)	0.0024 (2)	0.0041 (2)	0.0031 (2)
C2	0.0127 (3)	0.0092 (3)	0.0100 (3)	0.0020 (2)	0.0031 (2)	0.0035 (2)
C3	0.0123 (3)	0.0092 (3)	0.0111 (3)	0.0031 (2)	0.0036 (2)	0.0044 (2)
C4	0.0101 (3)	0.0072 (3)	0.0122 (3)	0.0031 (2)	0.0044 (2)	0.0038 (2)

C5	0.0119 (3)	0.0078 (3)	0.0106 (3)	0.0031 (2)	0.0035 (2)	0.0025 (2)
C6	0.0123 (3)	0.0086 (3)	0.0097 (3)	0.0031 (2)	0.0037 (2)	0.0035 (2)
C11	0.0094 (3)	0.0073 (3)	0.0110 (3)	0.0029 (2)	0.0039 (2)	0.0036 (2)
C21	0.0126 (3)	0.0084 (3)	0.0101 (3)	0.0025 (2)	0.0036 (2)	0.0028 (2)
C31	0.0136 (3)	0.0082 (3)	0.0124 (3)	0.0025 (2)	0.0054 (3)	0.0024 (2)
C41	0.0121 (3)	0.0074 (3)	0.0142 (3)	0.0040 (2)	0.0068 (2)	0.0046 (2)
C51	0.0130 (3)	0.0104 (3)	0.0118 (3)	0.0040 (2)	0.0040 (2)	0.0053 (2)
C61	0.0130 (3)	0.0086 (3)	0.0099 (3)	0.0024 (2)	0.0027 (2)	0.0031 (2)
Na	0.00911 (14)	0.00915 (14)	0.01433 (15)	0.00301 (11)	0.00447 (12)	0.00451 (12)

Geometric parameters (Å, °)

P1—O31	1.4733 (8)	C2—C3	1.3861 (12)
P1—O41	1.4834 (7)	C2—H2	0.9500
P1—O11	1.6266 (8)	C3—C4	1.3908 (14)
P1—O21	1.6287 (12)	C3—H3	0.9500
O1—N1	1.2282 (10)	C4—C5	1.3895 (12)
O1—Na	2.9377 (18)	C5—C6	1.3867 (12)
O2—N1	1.2399 (12)	C5—H5	0.9500
O2—Na	2.4618 (11)	C6—H6	0.9500
O3—N2	1.2288 (12)	C11—C61	1.3976 (12)
O4—N2	1.2335 (11)	C11—C21	1.3995 (14)
O4—Na ⁱ	2.3853 (11)	C21—C31	1.3857 (12)
O11—C1	1.3663 (11)	C21—H21	0.9500
O21—C11	1.3668 (10)	C31—C41	1.3894 (12)
O31—Na ⁱⁱ	2.2386 (10)	C31—H31	0.9500
O41—Na ⁱⁱⁱ	2.3135 (9)	C41—C51	1.3862 (14)
O41—Na ^{iv}	2.4065 (14)	C51—C61	1.3877 (12)
N1—C4	1.4552 (12)	C51—H51	0.9500
N2—C41	1.4560 (12)	C61—H61	0.9500
C1—C2	1.3987 (12)	Na—Na ^v	3.253 (2)
C1—C6	1.3998 (14)		
O31—P1—O41	119.67 (5)	C1—C6—H6	120.6
O31—P1—O11	110.86 (4)	O21—C11—C61	123.21 (8)
O41—P1—O11	110.02 (4)	O21—C11—C21	116.04 (7)
O31—P1—O21	110.48 (5)	C61—C11—C21	120.74 (8)
O41—P1—O21	110.21 (4)	C31—C21—C11	120.28 (8)
O11—P1—O21	92.20 (4)	C31—C21—H21	119.9
N1—O1—Na	83.76 (6)	C11—C21—H21	119.9
N1—O2—Na	106.72 (6)	C21—C31—C41	118.15 (8)
N2—O4—Na ⁱ	116.10 (7)	C21—C31—H31	120.9
C1—O11—P1	123.69 (6)	C41—C31—H31	120.9
C11—O21—P1	123.67 (6)	C51—C41—C31	122.37 (8)
P1—O31—Na ⁱⁱ	157.93 (4)	C51—C41—N2	117.95 (8)
P1—O41—Na ⁱⁱⁱ	143.20 (5)	C31—C41—N2	119.61 (8)
P1—O41—Na ^{iv}	129.49 (4)	C41—C51—C61	119.45 (8)
Na ⁱⁱⁱ —O41—Na ^{iv}	87.11 (4)	C41—C51—H51	120.3

O1—N1—O2	122.74 (7)	C61—C51—H51	120.3
O1—N1—C4	119.12 (8)	C51—C61—C11	119.01 (8)
O2—N1—C4	118.13 (8)	C51—C61—H61	120.5
O1—N1—Na	72.71 (6)	C11—C61—H61	120.5
O2—N1—Na	50.43 (5)	O31 ^{vi} —Na—O41 ^{vii}	165.08 (3)
C4—N1—Na	167.00 (5)	O31 ^{vi} —Na—O4 ^{viii}	99.55 (4)
O3—N2—O4	123.14 (8)	O41 ^{vii} —Na—O4 ^{viii}	81.55 (4)
O3—N2—C41	119.25 (8)	O31 ^{vi} —Na—O41 ^{iv}	101.98 (5)
O4—N2—C41	117.59 (8)	O41 ^{vii} —Na—O41 ^{iv}	92.89 (4)
O11—C1—C2	115.91 (8)	O4 ^{viii} —Na—O41 ^{iv}	80.28 (4)
O11—C1—C6	123.34 (8)	O31 ^{vi} —Na—O2	84.38 (4)
C2—C1—C6	120.75 (7)	O41 ^{vii} —Na—O2	92.94 (4)
C3—C2—C1	120.25 (8)	O4 ^{viii} —Na—O2	172.26 (3)
C3—C2—H2	119.9	O41 ^{iv} —Na—O2	105.55 (4)
C1—C2—H2	119.9	O31 ^{vi} —Na—O1	74.29 (5)
C2—C3—C4	118.44 (8)	O41 ^{vii} —Na—O1	93.25 (4)
C2—C3—H3	120.8	O4 ^{viii} —Na—O1	128.23 (3)
C4—C3—H3	120.8	O41 ^{iv} —Na—O1	151.44 (3)
C5—C4—C3	121.88 (8)	O2—Na—O1	46.28 (3)
C5—C4—N1	118.65 (8)	O31 ^{vi} —Na—N1	76.99 (4)
C3—C4—N1	119.43 (8)	O41 ^{vii} —Na—N1	94.92 (4)
C6—C5—C4	119.77 (8)	O4 ^{viii} —Na—N1	151.70 (3)
C6—C5—H5	120.1	O41 ^{iv} —Na—N1	128.02 (4)
C4—C5—H5	120.1	O2—Na—N1	22.85 (2)
C5—C6—C1	118.90 (8)	O1—Na—N1	23.53 (2)
C5—C6—H6	120.6		
O31—P1—O11—C1	-74.91 (8)	C4—C5—C6—C1	-0.33 (12)
O41—P1—O11—C1	59.73 (8)	O11—C1—C6—C5	-179.42 (7)
O21—P1—O11—C1	172.18 (6)	C2—C1—C6—C5	1.12 (12)
O31—P1—O21—C11	53.96 (7)	P1—O21—C11—C61	8.66 (11)
O41—P1—O21—C11	-80.51 (7)	P1—O21—C11—C21	-172.40 (6)
O11—P1—O21—C11	167.21 (6)	O21—C11—C21—C31	-178.45 (7)
P1—O11—C1—C2	-174.63 (6)	C61—C11—C21—C31	0.52 (12)
P1—O11—C1—C6	5.90 (11)	C11—C21—C31—C41	0.45 (12)
O11—C1—C2—C3	179.50 (7)	C21—C31—C41—C51	-1.26 (12)
C6—C1—C2—C3	-1.01 (12)	C21—C31—C41—N2	175.67 (7)
C1—C2—C3—C4	0.09 (12)	O3—N2—C41—C51	-174.72 (8)
C2—C3—C4—C5	0.72 (12)	O4—N2—C41—C51	6.77 (11)
C2—C3—C4—N1	178.70 (7)	O3—N2—C41—C31	8.22 (12)
O1—N1—C4—C5	177.82 (7)	O4—N2—C41—C31	-170.30 (8)
O2—N1—C4—C5	-1.43 (11)	C31—C41—C51—C61	1.08 (12)
O1—N1—C4—C3	-0.23 (11)	N2—C41—C51—C61	-175.90 (7)
O2—N1—C4—C3	-179.48 (7)	C41—C51—C61—C11	-0.07 (12)

C3—C4—C5—C6	-0.60 (12)	O21—C11—C61—C51	178.18 (7)
N1—C4—C5—C6	-178.60 (7)	C21—C11—C61—C51	-0.71 (12)

Symmetry codes: (i) $x-1, y-2, z$; (ii) $x, y-1, z$; (iii) $x-1, y-1, z$; (iv) $-x+1, -y+2, -z+1$; (v) $-x+2, -y+3, -z+1$; (vi) $x, y+1, z$; (vii) $x+1, y+1, z$; (viii) $x+1, y+2, z$.

Hydrogen-bond geometry (Å, °)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 \cdots O3 ^{ix}	0.95	2.50	3.1865 (15)	129
C21—H21 \cdots O1 ^x	0.95	2.53	3.3337 (18)	142

Symmetry codes: (ix) $-x, -y, -z$; (x) $-x, -y+1, -z$.