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Bis(2-amino-3-nitropyridinium) dihydrogendiphosphate

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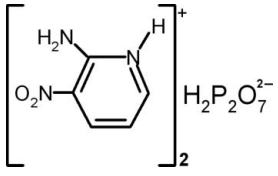
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.033; wR factor = 0.091; data-to-parameter ratio = 10.3.

The structure of the title compound, $2C_5H_6N_3O_2^+\cdot H_2P_2O_7^{2-}$, contains infinite $(H_2P_2O_7^{2-})_n$ layers stacked perpendicular to the a axis. The 2-amino-3-nitropyridinium cations are arranged in pairs and are anchored between these layers, linking them by N—H···O and C—H···O hydrogen-bonding and electrostatic interactions between anionic and cationic species to form a three-dimensional network.

Related literature

For related structures of 2-amino-3-nitropyridinium, see: Akriche & Rzaigui (2000, 2009*a*,*b*,*c*); Nicoud *et al.* (1997). For bond lengths in related structures, see: Aakeröy *et al.* (1998). For related structures of diphosphate anions, see: Akriche & Rzaigui (2005); Charfi & Jouini (2005); Brodski *et al.* (2004); Mrad *et al.* (2006); Soumhi *et al.* (1998).



Experimental

Crystal data

$2C_5H_6N_3O_2^+\cdot H_2O_7P_2^{2-}$
M_r = 456.21
Orthorhombic, $Pca2_1$
a = 34.250 (5) Å
b = 5.763 (2) Å
c = 8.991 (3) Å
V = 1774.8 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 298 K
0.29 × 0.25 × 0.19 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
2726 measured reflections
2724 independent reflections
2279 reflections with $I > 2\sigma(I)$
R_{int} = 0.008
2 standard reflections every 120 min
intensity decay: 3%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.091
S = 1.09
2724 reflections
265 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack (1983), 443 Friedel pairs
Flack parameter: −0.15 (11)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O5^{i}	0.82	1.73	2.549 (3)	178
O7—H7···O1^{ii}	0.82	1.73	2.537 (3)	166
N1—H1···O1	0.86	1.87	2.706 (3)	165
N2—H2A···O3	0.86	1.88	2.726 (4)	168
N2—H2B···O9	0.86	2.05	2.645 (4)	126
N4—H4···O6	0.86	1.72	2.582 (4)	174
N5—H5A···O5	0.86	1.95	2.786 (4)	165
N5—H5B···O10	0.86	2.07	2.669 (5)	126
N5—H5B···O3^{iii}	0.86	2.22	2.843 (4)	130
C2—H2C···O7^{iv}	0.93	2.46	3.280 (4)	147
C3—H3···O6^{iv}	0.93	2.34	3.208 (4)	155
C8—H8···O9^{v}	0.93	2.52	3.097 (4)	120

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

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: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2529).

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supporting information

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Bis(2-amino-3-nitropyridinium) dihydrogendiphosphate

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S1. Comment

In the framework of our systematic research using the 2-amino-3-nitropyridine (2 A3NP) molecule, we report here the new non-centrosymetric compound, $2(C_5H_6N_3O_2)^+$, $H_2P_2O_7^{2-}$ (I) obtained by the interaction of the 2 A3NP molecule and diphosphoric acid.

The asymmetric unit of the title compound is built up from one anion $H_2P_2O_7^{2-}$ and two $(C_5H_6N_3O_2)^+$ cations as shown in Fig. 1.

The dihydrogendiphosphate anions are connected through strong hydrogen bonds characterized by relatively short distances (with distances O2···O5 = 2.549 (3) Å and O7···O1 = 2.537 (3) Å (Table 1)), to form corrugated layers parallel to *bc* plane at *x* = 0 and *x*= 1/2 (Fig. 2). Two crystallographically independent cations coexist in this structure. They are arranged in pairs and anchored onto both adjacent anionic layers *via* N—H···O and C—H···O hydrogen bonds to keep up the three-dimensionel network cohesion.

As expected, the $H_2P_2O_7^{2-}$ group with bent configuration shows its standard geometry, the longest bonds length P2–O4 = 1.592 (2) Å and P1–O4 = 1.613 (2) Å, correspond to the bridging oxygen atom, the intermediate ones, P1–O2 = 1.552 (2) Å and P2–O7 = 1.545 (2) Å, correspond to the P–OH bonding and the shortest ones spreading between 1.481 (2) Å and 1.515 (2) Å, correspond to the external oxygen atoms. The average values of the P–O distances and O–P–O angles are 1.536 Å and 109.3°. The P–P distance is 2.898 (1) Å and the P–O–P angle is close to 129.4 (1) °. All these distances and angles are similar to those commonly observed in others diphosphate anions (Akriche & Rzaigui, 2005; Charfi & Jouini, 2005; Brodski, *et al.*, 2004; Mrad, *et al.*, 2006). Despite the limited number of organic cation diphosphates (about twenty seven related structures of diphosphate anions), we can distinguish only one non-centrosymmetric structure (Soumhi, *et al.*, 1998) such as the title compound (I).

In this atomic arrangement, one can distinguish the inter-cation contact C8—H8···O9 (H8···O9 = 2.52 Å) which induces the aggregation of the two independent organic cations in pairs $(2\ A3NP^+)_2$. This kind of arrangement is also observed in the related structure of 2-amino-3-nitropyridinium hydrogenselenate (Akriche & Rzaigui, 2009*b*). These pairs are located between the anionic layers to link them by manifesting different interactions (Fig. 2). The geometric features of organic cations are usual and comparable with values of other 2-amino-3-nitropyridinium compounds (Akriche & Rzaigui, 2000; Nicoud *et al.*,1997; Akriche & Rzaigui, 2009*a*, 2009*b*, 2009*c*). It is worth noticing, the C—NH_2 (1.316 (4) Å) and C—NO_2 (1.440 (4) and 1.454 (5) Å) distances in the 2 A3NP cations are respectively shortened and lengthened with respect to the C—NH_2 (1.337 (4) Å) and C—NO_2 (1.429 (4) Å) observed in the 2-amino-3-nitropyridine molecular crystal (Aakeröy, *et al.*, 1998). All the 2-amino-3-nitropyridinium cations encapsulated in various anionic subnetworks show the same changes in C—NH_2 and C—NO_2 distances, revealing a weak increase of pi bond character in C—NH_2 and a decrease in C—NO_2.

S2. Experimental

Single crystals of the title compound were prepared at room temperature by slow evaporation of a mixture of an aqueous solution (20 ml) of diphosphoric acid (5 mmol) and an ethanolic solution (10 ml) of 2-amino-3-nitropyridine (4 mmol, 354 mg). The diphosphoric acid was produced from $Na_4P_2O_7$ by using a cation-exchange resin (Amberlite IR 120). The resulting solution was evaporated slowly at room temperature for several days until the formation of good quality of prismatic single crystals.

S3. Refinement

All H atoms attached to C, N and O atoms were fixed geometrically and treated as riding, with C—H = 0.93 Å, N—H = 0.86 Å and O—H = 0.82 Å and with U_{iso}(H) = 1.2Ueq(C or N) and U_{iso}(H) = 1.5Ueq(O)

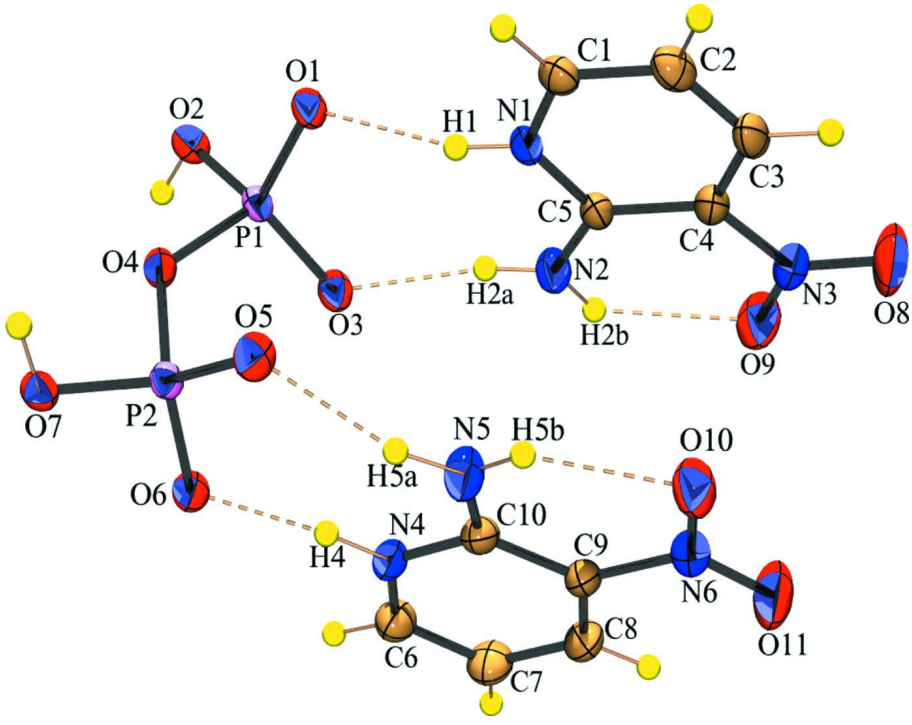

Figure 1

An *ORTEP* view of (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii. Hydrogen bonds are represented as dashed lines.

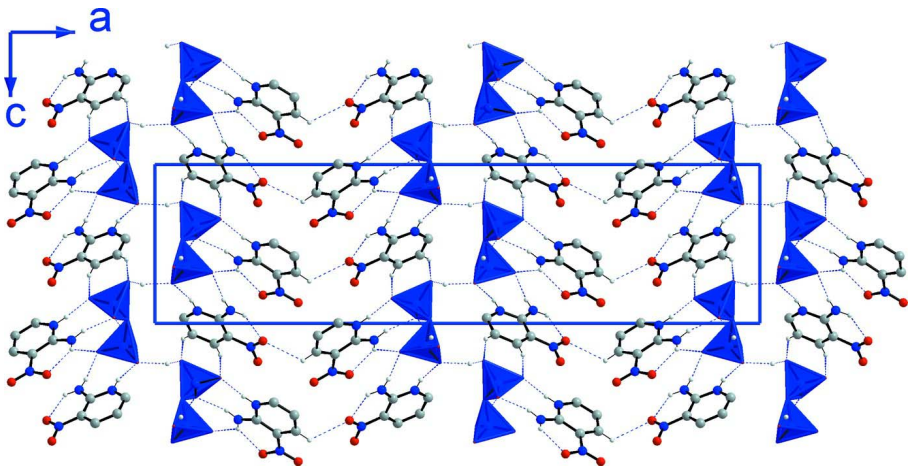

Figure 2

Projection of (I) along the *b* axis. The H-atoms not involved in H-bonding are omitted.

Bis(2-amino-3-nitropyridinium) dihydrogendiphosphate

Crystal data

$2C_5H_6N_3O_2^+\cdot H_2O_7P_2^{2-}$
$M_r = 456.21$
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
$a = 34.250\ (5)$ Å
$b = 5.763\ (2)$ Å
$c = 8.991\ (3)$ Å
$V = 1774.8\ (9)$ Å^3
$Z = 4$
$F(000) = 936$
$D_x = 1.707$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10$–$12°$
$\mu = 0.32$ mm^{-1}
$T = 298$ K
Prism, yellow
0.29 × 0.25 × 0.19 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
non–profiled ω scans
2726 measured reflections
2724 independent reflections
2279 reflections with $I > 2\sigma(I)$
$R_{int} = 0.008$
$\theta_{max} = 30.0°$, $\theta_{min} = 3.3°$
$h = -48\rightarrow0$
$k = 0\rightarrow8$
$l = -12\rightarrow0$
2 standard reflections every 120 min
intensity decay: 3%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.091$
$S = 1.09$
2724 reflections
265 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 0.7964P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0192 (12)
Absolute structure: Flack (1983)
Absolute structure parameter: −0.15 (11)

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}
P1	0.05181 (2)	0.76331 (12)	0.64677 (9)	0.02939 (15)
P2	0.06740 (2)	0.49228 (13)	0.38188 (9)	0.02940 (15)
O1	0.02869 (6)	0.6068 (4)	0.7473 (3)	0.0388 (5)
O2	0.03160 (6)	1.0043 (4)	0.6468 (3)	0.0380 (5)
H2	0.0432	1.0916	0.5898	0.057*
O3	0.09419 (6)	0.7686 (4)	0.6795 (3)	0.0406 (5)
O4	0.04503 (6)	0.6839 (4)	0.4767 (2)	0.0349 (4)
O5	0.06725 (7)	0.2687 (4)	0.4645 (3)	0.0442 (6)
O6	0.10798 (6)	0.5779 (4)	0.3433 (3)	0.0381 (5)
O7	0.04355 (6)	0.4892 (4)	0.2361 (2)	0.0367 (5)
H7	0.0207	0.4592	0.2548	0.055*
O8	0.17007 (11)	0.0987 (8)	1.2413 (5)	0.0996 (14)
O9	0.17848 (8)	0.4036 (7)	1.1115 (4)	0.0796 (12)
O10	0.17870 (9)	−0.0306 (6)	0.8224 (4)	0.0689 (9)
O11	0.23687 (9)	0.0861 (7)	0.8703 (5)	0.0899 (12)
N1	0.07030 (7)	0.3161 (5)	0.9226 (3)	0.0334 (5)
H1	0.0606	0.4078	0.8567	0.040*
N2	0.12502 (8)	0.5449 (5)	0.9194 (3)	0.0445 (7)
H2A	0.1139	0.6299	0.8532	0.053*
H2B	0.1481	0.5788	0.9499	0.053*
N3	0.15874 (9)	0.2373 (7)	1.1479 (5)	0.0578 (9)
N4	0.16725 (8)	0.4967 (5)	0.5130 (4)	0.0396 (6)
H4	0.1465	0.5191	0.4608	0.048*
N5	0.13779 (8)	0.1725 (6)	0.6059 (4)	0.0522 (8)
H5A	0.1184	0.1998	0.5479	0.063*
H5B	0.1374	0.0536	0.6637	0.063*
N6	0.20652 (10)	0.1031 (6)	0.8028 (4)	0.0548 (8)
C1	0.04851 (9)	0.1383 (5)	0.9672 (4)	0.0374 (6)
H1A	0.0236	0.1196	0.9281	0.045*
C2	0.06201 (11)	−0.0169 (6)	1.0689 (4)	0.0450 (8)
H2C	0.0469	−0.1431	1.0978	0.054*
C3	0.09860 (10)	0.0180 (6)	1.1278 (4)	0.0453 (8)
H3	0.1084	−0.0843	1.1986	0.054*
C4	0.12081 (9)	0.2041 (6)	1.0822 (4)	0.0404 (7)
C5	0.10672 (8)	0.3631 (5)	0.9740 (4)	0.0350 (6)

C6	0.19675 (10)	0.6453 (6)	0.4979 (5)	0.0470 (8)
H6	0.1943	0.7678	0.4312	0.056*
C7	0.23056 (10)	0.6223 (7)	0.5778 (5)	0.0550 (10)
H7C	0.2512	0.7255	0.5652	0.066*
C8	0.23302 (9)	0.4406 (7)	0.6779 (4)	0.0511 (9)
H8	0.2554	0.4221	0.7352	0.061*
C9	0.20255 (9)	0.2872 (6)	0.6933 (4)	0.0417 (7)
C10	0.16813 (9)	0.3125 (6)	0.6061 (4)	0.0389 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0326 (3)	0.0309 (3)	0.0247 (3)	−0.0046 (3)	−0.0008 (3)	0.0044 (3)
P2	0.0323 (3)	0.0269 (3)	0.0291 (3)	−0.0007 (3)	0.0004 (3)	0.0045 (3)
O1	0.0377 (10)	0.0429 (12)	0.0357 (11)	−0.0058 (9)	−0.0001 (9)	0.0130 (10)
O2	0.0473 (11)	0.0334 (10)	0.0333 (11)	−0.0004 (9)	0.0047 (10)	0.0004 (11)
O3	0.0373 (10)	0.0474 (12)	0.0371 (13)	−0.0090 (10)	−0.0036 (9)	0.0097 (10)
O4	0.0379 (10)	0.0374 (10)	0.0293 (10)	0.0054 (9)	−0.0045 (9)	0.0000 (9)
O5	0.0461 (13)	0.0321 (11)	0.0544 (15)	−0.0020 (9)	0.0013 (11)	0.0162 (11)
O6	0.0336 (10)	0.0412 (11)	0.0394 (12)	−0.0049 (9)	0.0003 (9)	0.0102 (10)
O7	0.0357 (10)	0.0457 (12)	0.0288 (10)	−0.0050 (10)	−0.0004 (9)	−0.0028 (10)
O8	0.072 (2)	0.126 (3)	0.101 (3)	0.007 (2)	−0.035 (2)	0.058 (3)
O9	0.0414 (14)	0.108 (3)	0.089 (3)	−0.0142 (16)	−0.0172 (16)	0.035 (2)
O10	0.0647 (18)	0.073 (2)	0.069 (2)	−0.0055 (16)	−0.0033 (15)	0.0349 (18)
O11	0.0635 (19)	0.114 (3)	0.092 (3)	0.0031 (19)	−0.025 (2)	0.045 (3)
N1	0.0393 (13)	0.0353 (13)	0.0257 (11)	0.0034 (10)	−0.0001 (9)	0.0036 (10)
N2	0.0426 (14)	0.0462 (16)	0.0447 (17)	−0.0056 (12)	−0.0057 (12)	0.0137 (13)
N3	0.0423 (15)	0.079 (2)	0.0518 (17)	0.0116 (17)	−0.0067 (16)	0.018 (2)
N4	0.0325 (11)	0.0423 (14)	0.0440 (15)	0.0013 (11)	−0.0029 (11)	0.0083 (13)
N5	0.0423 (15)	0.0524 (17)	0.062 (2)	−0.0119 (13)	−0.0101 (15)	0.0222 (16)
N6	0.0492 (16)	0.066 (2)	0.0494 (18)	0.0083 (16)	0.0005 (15)	0.0154 (17)
C1	0.0393 (15)	0.0418 (16)	0.0309 (14)	−0.0026 (13)	0.0037 (13)	−0.0027 (14)
C2	0.0549 (19)	0.0353 (16)	0.0447 (18)	−0.0021 (15)	0.0087 (16)	0.0062 (15)
C3	0.0535 (17)	0.0414 (16)	0.0411 (19)	0.0132 (14)	0.0058 (15)	0.0119 (16)
C4	0.0373 (15)	0.0488 (18)	0.0350 (16)	0.0079 (13)	−0.0004 (13)	0.0054 (15)
C5	0.0372 (14)	0.0390 (16)	0.0288 (13)	0.0054 (12)	0.0018 (12)	0.0035 (13)
C6	0.0419 (17)	0.0463 (18)	0.053 (2)	−0.0023 (14)	0.0041 (15)	0.0086 (17)
C7	0.0374 (17)	0.061 (2)	0.066 (3)	−0.0102 (16)	0.0042 (18)	0.008 (2)
C8	0.0303 (14)	0.072 (2)	0.051 (2)	0.0006 (16)	−0.0028 (15)	0.0070 (19)
C9	0.0329 (13)	0.0520 (18)	0.0404 (15)	0.0050 (13)	0.0030 (12)	0.0089 (16)
C10	0.0345 (14)	0.0408 (16)	0.0412 (16)	0.0024 (13)	0.0042 (13)	0.0041 (13)

Geometric parameters (Å, º)

P1—O3	1.481 (2)	N4—C6	1.331 (4)
P1—O1	1.503 (2)	N4—C10	1.353 (4)
P1—O2	1.552 (2)	N4—H4	0.8600
P1—O4	1.613 (2)	N5—C10	1.316 (4)

P2—O5	1.487 (2)	N5—H5A	0.8600
P2—O6	1.515 (2)	N5—H5B	0.8600
P2—O7	1.545 (2)	N6—C9	1.454 (5)
P2—O4	1.592 (2)	C1—C2	1.360 (5)
O2—H2	0.8200	C1—H1A	0.9300
O7—H7	0.8200	C2—C3	1.375 (5)
O8—N3	1.222 (5)	C2—H2C	0.9300
O9—N3	1.217 (5)	C3—C4	1.377 (5)
O10—N6	1.238 (4)	C3—H3	0.9300
O11—N6	1.208 (4)	C4—C5	1.420 (4)
N1—C1	1.330 (4)	C6—C7	1.369 (5)
N1—C5	1.358 (4)	C6—H6	0.9300
N1—H1	0.8600	C7—C8	1.383 (5)
N2—C5	1.316 (4)	C7—H7C	0.9300
N2—H2A	0.8600	C8—C9	1.375 (5)
N2—H2B	0.8600	C8—H8	0.9300
N3—C4	1.440 (4)	C9—C10	1.423 (5)

O3—P1—O1	114.15 (13)	O10—N6—C9	118.6 (3)
O3—P1—O2	114.74 (13)	N1—C1—C2	121.2 (3)
O1—P1—O2	107.60 (13)	N1—C1—H1A	119.4
O3—P1—O4	109.59 (13)	C2—C1—H1A	119.4
O1—P1—O4	108.93 (14)	C1—C2—C3	118.2 (3)
O2—P1—O4	100.93 (13)	C1—C2—H2C	120.9
O5—P2—O6	113.55 (13)	C3—C2—H2C	120.9
O5—P2—O7	114.34 (15)	C2—C3—C4	120.2 (3)
O6—P2—O7	107.14 (13)	C2—C3—H3	119.9
O5—P2—O4	109.41 (14)	C4—C3—H3	119.9
O6—P2—O4	109.76 (13)	C3—C4—C5	121.2 (3)
O7—P2—O4	101.99 (12)	C3—C4—N3	118.7 (3)
P1—O2—H2	109.5	C5—C4—N3	120.1 (3)
P2—O4—P1	129.43 (14)	N2—C5—N1	118.0 (3)
P2—O7—H7	109.5	N2—C5—C4	127.4 (3)
C1—N1—C5	124.5 (3)	N1—C5—C4	114.6 (3)
C1—N1—H1	117.7	N4—C6—C7	121.7 (4)
C5—N1—H1	117.7	N4—C6—H6	119.1
C5—N2—H2A	120.0	C7—C6—H6	119.1
C5—N2—H2B	120.0	C6—C7—C8	117.8 (3)
H2A—N2—H2B	120.0	C6—C7—H7C	121.1
O9—N3—O8	121.5 (4)	C8—C7—H7C	121.1
O9—N3—C4	119.7 (3)	C9—C8—C7	120.4 (3)
O8—N3—C4	118.8 (4)	C9—C8—H8	119.8
C6—N4—C10	123.4 (3)	C7—C8—H8	119.8
C6—N4—H4	118.3	C8—C9—C10	120.5 (3)
C10—N4—H4	118.3	C8—C9—N6	117.8 (3)
C10—N5—H5A	120.0	C10—C9—N6	121.7 (3)
C10—N5—H5B	120.0	N5—C10—N4	117.6 (3)
H5A—N5—H5B	120.0	N5—C10—C9	126.3 (3)

O11—N6—O10	122.7 (4)	N4—C10—C9	116.1 (3)
O11—N6—C9	118.7 (3)		
O5—P2—O4—P1	53.0 (2)	N3—C4—C5—N2	1.9 (6)
O6—P2—O4—P1	−72.2 (2)	C3—C4—C5—N1	0.4 (5)
O7—P2—O4—P1	174.45 (18)	N3—C4—C5—N1	−178.7 (3)
O3—P1—O4—P2	39.2 (2)	C10—N4—C6—C7	−0.5 (6)
O1—P1—O4—P2	−86.3 (2)	N4—C6—C7—C8	−1.1 (6)
O2—P1—O4—P2	160.61 (18)	C6—C7—C8—C9	1.2 (6)
C5—N1—C1—C2	−1.3 (5)	C7—C8—C9—C10	0.2 (6)
N1—C1—C2—C3	1.6 (5)	C7—C8—C9—N6	−178.6 (4)
C1—C2—C3—C4	−0.9 (5)	O11—N6—C9—C8	−3.4 (6)
C2—C3—C4—C5	−0.1 (5)	O10—N6—C9—C8	177.0 (4)
C2—C3—C4—N3	179.0 (4)	O11—N6—C9—C10	177.8 (4)
O9—N3—C4—C3	−178.4 (4)	O10—N6—C9—C10	−1.8 (5)
O8—N3—C4—C3	0.5 (6)	C6—N4—C10—N5	−176.9 (4)
O9—N3—C4—C5	0.7 (6)	C6—N4—C10—C9	1.9 (5)
O8—N3—C4—C5	179.6 (4)	C8—C9—C10—N5	177.0 (4)
C1—N1—C5—N2	179.7 (3)	N6—C9—C10—N5	−4.2 (6)
C1—N1—C5—C4	0.2 (4)	C8—C9—C10—N4	−1.7 (5)
C3—C4—C5—N2	−179.0 (3)	N6—C9—C10—N4	177.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O5^{i}	0.82	1.73	2.549 (3)	178
O7—H7···O1^{ii}	0.82	1.73	2.537 (3)	166
N1—H1···O1	0.86	1.87	2.706 (3)	165
N2—H2*A*···O3	0.86	1.88	2.726 (4)	168
N2—H2*B*···O9	0.86	2.05	2.645 (4)	126
N4—H4···O6	0.86	1.72	2.582 (4)	174
N5—H5*A*···O5	0.86	1.95	2.786 (4)	165
N5—H5*B*···O10	0.86	2.07	2.669 (5)	126
N5—H5*B*···O3^{iii}	0.86	2.22	2.843 (4)	130
C2—H2*C*···O7^{iv}	0.93	2.46	3.280 (4)	147
C3—H3···O6^{iv}	0.93	2.34	3.208 (4)	155
C8—H8···O9^{v}	0.93	2.52	3.097 (4)	120

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*, −*y*+1, *z*−1/2; (iii) *x*, *y*−1, *z*; (iv) *x*, *y*−1, *z*+1; (v) −*x*+1/2, *y*, *z*−1/2.