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Bis(benzylammonium) dihydrogen diphosphate

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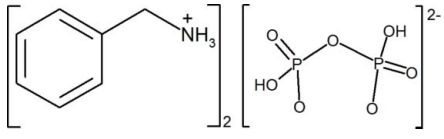
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.127; data-to-parameter ratio = 32.2.

The asymmetric unit of the title salt, $2C_6H_5CH_2NH_3^+\cdot H_2P_2O_7^{2-}$, contains two independent benzylammonium cations and a dihydrogen diphosphate dianion. In the crystal, O—H···O and N—H···O hydrogen bonds link the cations and anions, forming a two-dimensional network parallel to (010). Within this network, weak C—H···O hydrogen bonds are observed.

Related literature

For the chemistry of diphosphate materials, see: Ernester (1992); Lipscomb & Strater (1996); Centi *et al.* (1988); Chen & Munson (2002); Ballarini *et al.* (2006). For details of hydrogen bonds, see: Desiraju (1991); Steiner (2002). For related structures, see: Akriche & Rzaigui (2005, 2008); Ahmed *et al.* (2006); Elboulali *et al.* (2013).



Experimental

Crystal data

$2C_7H_{10}N^+\cdot H_2P_2O_7^{2-}$
M_r = 392.27
Monoclinic, $P2_1/c$
a = 8.1337 (2) Å
b = 28.9015 (9) Å
c = 8.4727 (2) Å
β = 113.449 (1)°
V = 1827.24 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 293 K
0.3 × 0.2 × 0.1 mm

Data collection

Nonius KappaCCD diffractometer
27919 measured reflections
7410 independent reflections
5946 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.127
S = 1.06
7410 reflections
230 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O1*···O6^{i}	0.82	1.90	2.7208 (13)	174
O5—H5*O5*···O3^{ii}	0.82	1.83	2.6061 (13)	158
N1—H1*N1*···O2	0.89	2.07	2.9292 (13)	162
N1—H2*N1*···O6^{iii}	0.89	2.10	2.9698 (15)	166
N1—H2*N1*···O4^{iii}	0.89	2.53	3.1493 (13)	127
N1—H3*N1*···O7^{iv}	0.89	1.88	2.7645 (15)	169
N2—H1*N2*···O3^{ii}	0.89	1.94	2.7956 (15)	160
N2—H2*N2*···O2	0.89	1.98	2.8637 (15)	169
N2—H3*N2*···O6^{iii}	0.89	1.99	2.8053 (14)	152
C1—H1*B*···O5^{ii}	0.97	2.52	3.3333 (19)	141
C8—H8*B*···O7	0.97	2.40	3.1558 (17)	135

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

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DIRAX/LSQ* (Duisenberg *et al.*, 2000); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); 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, 2012) and *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 2012).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5670).

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Acta Cryst. (2014). E**70**, o3 [https://doi.org/10.1107/S1600536813032455]

Bis(benzylammonium) dihydrogen diphosphate

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S1. Comment

There is current interest in the chemistry of diphosphate materials. They are involved in a variety of bioenergetic (Ernester, 1992; Lipscomb & Strater, 1996) and catalytic processes (Centi *et al.*, 1988; Chen *et al.*, 2002; Ballarini *et al.*, 2006). Considering their relevance in several application areas, we are interested in this type of anion in building new hybrid materials associated to organic cations. We report here, the synthesis and the crystal structure of the title compound (I).

The asymmetric unit of (I) shown in Fig. 1, contains one diphosphate $[H_2P_2O_7]^{2-}$ anion and two crystallographically independent benzylammonium cations. The two PO_4 tetrahedral groups are bridged *via* the O4 bridging oxygen atom with P1—O4—P2 = 133.33 (6)° so as to form the diphosphate anion with a bent configurtation. The conformation is eclipsed evidenced by the psuedo-torsion angle O3—P1···P2—O7 = -6.9°. In the diphosphate group, the longest P—O distances correspond to the bridging oxygen atom with average value d(P—O4) = 1.6104 (8) Å, the intermediate distances are the P—OH bonding [*d*(P1—O1) = 1.5693 (9) Å, d(P2—O5) = 1.5607 (10) Å], whereas the shortest distances, ranging between 1.4762 (9) Å and 1.4987 (8) Å are related to the terminal oxygen atoms. The average value of the O—P—O angles is 109.25 (5)°. These geometrical features are in same magnitude as observed for diphosphate groups (Akriche *et al.*, 2005; Ahmed *et al.*, 2006; Akriche *et al.*, 2008; Elboulali *et al.*, 2013).

In the crystal, O—H···O and N—H···O hydrogen bonds link the cations and anions forming a two-dimensional network parallel to (010) (Table 1 and Fig. 2). Within this network, weak C—H···O hydrogen bonds are observed (Desiraju, 1991; Steiner 2002).

S2. Experimental

Prismatic 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 benzylamine (4 mmol, 0.44 ml). The diphosphoric acid was produced from $Na_4P_2O_7$ by using a cation-exchange resin (Amberlite IR 120).

S3. Refinement

All H atoms were placed in calculated positions and treated as riding, with C—H = 0.93 and 0.97 Å respectively for benzene rings and CH_2 groups, N—H = 0.89 Å and O—H = 0.82 Å with U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(N,*O*).

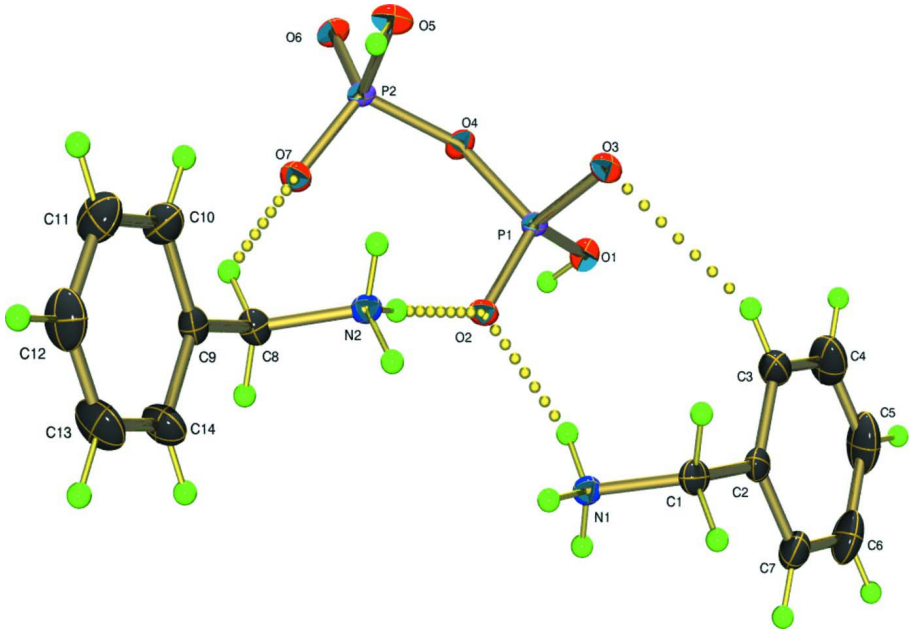

Figure 1

An *ORTEP* (Farrugia, 2012) view of (I) with 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.

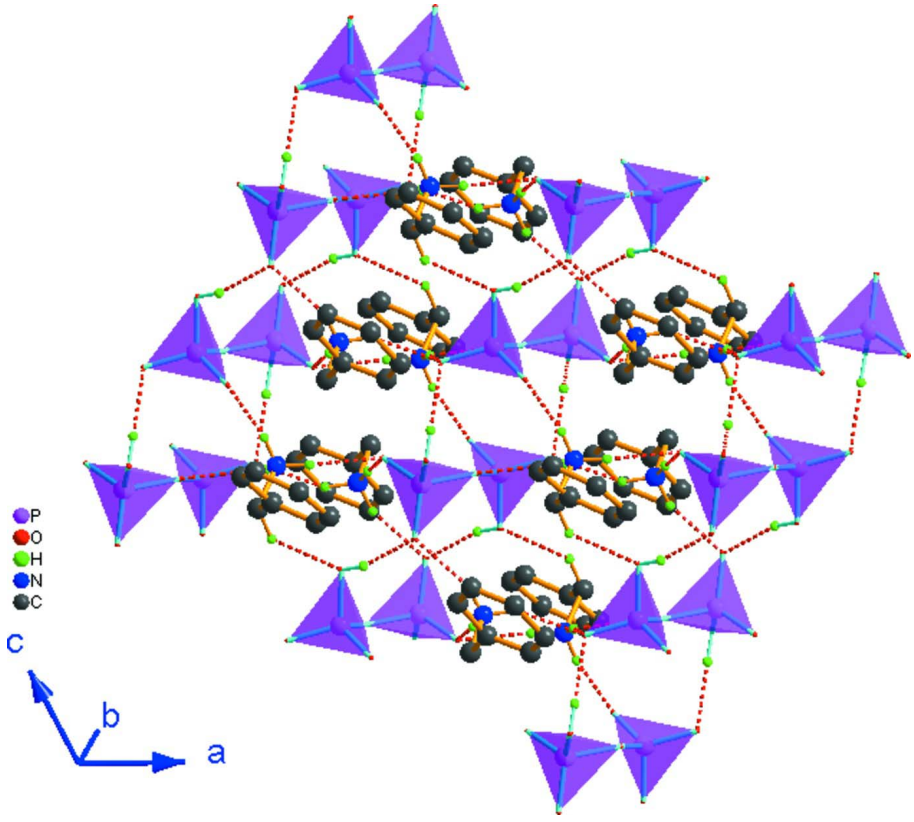

Figure 2

Part of the crystal structure of (I) with hydrogen bonds represented as red dashed lines. The H-atoms not involved in H-bonds are omitted.

Bis(benzylammonium) dihydrogen diphosphate

Crystal data

$2C_7H_{10}N^+\cdot H_2P_2O_7^{2-}$
$M_r = 392.27$
Monoclinic, $P2_1/c$
$a = 8.1337$ (2) Å
$b = 28.9015$ (9) Å
$c = 8.4727$ (2) Å
$\beta = 113.449$ (1)°
$V = 1827.24$ (9) Å^3
$Z = 4$
$F(000) = 824$
$D_x = 1.426$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9$–11°
$\mu = 0.28$ mm^{-1}
$T = 293$ K
Prism, colourless
0.3 × 0.2 × 0.1 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 9 pixels mm^{-1}
CCD rotation images, thick slices scans
27919 measured reflections
7410 independent reflections
5946 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 34.3°$, $\theta_{min} = 2.7°$
$h = -12\rightarrow11$
$k = -45\rightarrow45$
$l = -13\rightarrow12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.127$
$S = 1.06$
7410 reflections
230 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0651P)^2 + 0.3854P]$ 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 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
P1	0.16846 (4)	0.04396 (2)	0.78619 (4)	0.02353 (7)
P2	0.35638 (4)	−0.03781 (2)	0.72893 (4)	0.02459 (8)
O1	0.27096 (13)	0.08328 (3)	0.91571 (12)	0.0351 (2)
H1O1	0.3218	0.0723	1.0123	0.053*
O2	0.05569 (11)	0.01565 (3)	0.85084 (12)	0.03180 (19)
O3	0.07455 (11)	0.06475 (3)	0.61148 (11)	0.03265 (19)
O4	0.33579 (11)	0.01439 (3)	0.78719 (13)	0.03276 (19)
O5	0.25728 (13)	−0.03691 (4)	0.52889 (12)	0.0401 (2)
H5O5	0.1642	−0.0519	0.4998	0.060*
O6	0.55388 (11)	−0.04139 (3)	0.77466 (12)	0.0332 (2)
O7	0.27351 (13)	−0.07023 (4)	0.81039 (13)	0.0367 (2)
N1	−0.27361 (14)	0.05080 (4)	0.87008 (14)	0.0304 (2)
H1N1	−0.1667	0.0467	0.8665	0.046*
H2N1	−0.3407	0.0258	0.8287	0.046*
H3N1	−0.2600	0.0554	0.9784	0.046*
N2	−0.16351 (14)	−0.06105 (4)	0.67481 (15)	0.0320 (2)
H1N2	−0.1638	−0.0614	0.5697	0.048*
H2N2	−0.0859	−0.0399	0.7386	0.048*
H3N2	−0.2727	−0.0541	0.6681	0.048*
C1	−0.36307 (19)	0.09184 (5)	0.76385 (18)	0.0384 (3)
H1A	−0.4815	0.0955	0.7640	0.046*
H1B	−0.3769	0.0869	0.6460	0.046*
C2	−0.25602 (19)	0.13517 (5)	0.83218 (19)	0.0372 (3)
C3	−0.1281 (3)	0.14896 (6)	0.7728 (3)	0.0544 (4)
H3	−0.1092	0.1318	0.6887	0.065*
C4	−0.0272 (3)	0.18878 (8)	0.8397 (4)	0.0820 (8)
H4	0.0598	0.1978	0.8008	0.098*
C5	−0.0551 (4)	0.21432 (8)	0.9606 (4)	0.0865 (8)
H5	0.0111	0.2411	1.0026	0.104*
C6	−0.1804 (3)	0.20080 (7)	1.0213 (3)	0.0717 (6)

H6	−0.1980	0.2183	1.1055	0.086*
C7	−0.2814 (2)	0.16112 (6)	0.9578 (2)	0.0498 (4)
H7	−0.3662	0.1520	0.9996	0.060*
C8	−0.11012 (18)	−0.10755 (5)	0.75535 (19)	0.0381 (3)
H8A	−0.1077	−0.1069	0.8707	0.046*
H8B	0.0098	−0.1148	0.7643	0.046*
C9	−0.23714 (18)	−0.14468 (5)	0.65266 (18)	0.0367 (3)
C10	−0.2192 (2)	−0.16351 (7)	0.5112 (2)	0.0522 (4)
H10	−0.1301	−0.1526	0.4781	0.063*
C11	−0.3324 (3)	−0.19860 (8)	0.4172 (3)	0.0655 (5)
H11	−0.3191	−0.2111	0.3219	0.079*
C12	−0.4640 (3)	−0.21471 (7)	0.4657 (3)	0.0689 (6)
H12	−0.5382	−0.2388	0.4050	0.083*
C13	−0.4863 (3)	−0.19547 (8)	0.6032 (3)	0.0708 (6)
H13	−0.5781	−0.2058	0.6334	0.085*
C14	−0.3720 (3)	−0.16037 (7)	0.6985 (3)	0.0563 (4)
H14	−0.3868	−0.1476	0.7928	0.068*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.01799 (12)	0.03007 (15)	0.02214 (13)	0.00091 (9)	0.00756 (9)	0.00035 (10)
P2	0.01780 (12)	0.03298 (16)	0.02239 (13)	0.00009 (9)	0.00736 (9)	−0.00164 (10)
O1	0.0328 (4)	0.0354 (5)	0.0301 (4)	0.0006 (4)	0.0051 (3)	−0.0056 (3)
O2	0.0255 (4)	0.0393 (5)	0.0350 (4)	0.0009 (3)	0.0167 (3)	0.0055 (4)
O3	0.0284 (4)	0.0423 (5)	0.0243 (4)	0.0000 (3)	0.0073 (3)	0.0042 (3)
O4	0.0219 (4)	0.0333 (5)	0.0454 (5)	−0.0004 (3)	0.0159 (3)	−0.0050 (4)
O5	0.0276 (4)	0.0650 (7)	0.0250 (4)	−0.0070 (4)	0.0076 (3)	−0.0027 (4)
O6	0.0191 (3)	0.0444 (5)	0.0345 (4)	0.0029 (3)	0.0089 (3)	−0.0056 (4)
O7	0.0382 (5)	0.0374 (5)	0.0379 (5)	−0.0049 (4)	0.0187 (4)	0.0000 (4)
N1	0.0269 (4)	0.0310 (5)	0.0351 (5)	−0.0003 (4)	0.0143 (4)	−0.0008 (4)
N2	0.0294 (5)	0.0337 (6)	0.0367 (5)	−0.0035 (4)	0.0174 (4)	−0.0033 (4)
C1	0.0359 (6)	0.0401 (7)	0.0359 (6)	0.0054 (5)	0.0109 (5)	0.0047 (5)
C2	0.0370 (6)	0.0323 (6)	0.0423 (7)	0.0083 (5)	0.0158 (5)	0.0087 (5)
C3	0.0575 (9)	0.0460 (9)	0.0719 (11)	0.0067 (7)	0.0387 (9)	0.0124 (8)
C4	0.0679 (13)	0.0560 (13)	0.132 (2)	−0.0072 (10)	0.0504 (15)	0.0200 (14)
C5	0.0729 (14)	0.0381 (10)	0.127 (2)	−0.0086 (10)	0.0175 (15)	0.0029 (12)
C6	0.0788 (14)	0.0419 (10)	0.0772 (14)	0.0134 (9)	0.0128 (11)	−0.0112 (9)
C7	0.0545 (9)	0.0426 (8)	0.0528 (9)	0.0113 (7)	0.0217 (7)	0.0000 (7)
C8	0.0315 (6)	0.0387 (7)	0.0395 (6)	−0.0033 (5)	0.0093 (5)	0.0023 (5)
C9	0.0324 (6)	0.0309 (6)	0.0426 (7)	−0.0009 (5)	0.0106 (5)	0.0053 (5)
C10	0.0475 (8)	0.0508 (9)	0.0612 (10)	−0.0059 (7)	0.0247 (8)	−0.0099 (8)
C11	0.0687 (12)	0.0545 (11)	0.0703 (12)	−0.0080 (9)	0.0244 (10)	−0.0220 (9)
C12	0.0640 (12)	0.0480 (10)	0.0782 (14)	−0.0195 (9)	0.0110 (10)	−0.0093 (10)
C13	0.0656 (12)	0.0685 (13)	0.0795 (14)	−0.0334 (10)	0.0301 (11)	−0.0005 (11)
C14	0.0568 (10)	0.0588 (11)	0.0584 (10)	−0.0203 (8)	0.0283 (8)	−0.0006 (8)

Geometric parameters (Å, º)

P1—O2	1.4869 (9)	C3—C4	1.396 (3)
P1—O3	1.4953 (9)	C3—H3	0.9300
P1—O1	1.5693 (9)	C4—C5	1.353 (4)
P1—O4	1.6042 (9)	C4—H4	0.9300
P2—O7	1.4762 (10)	C5—C6	1.369 (4)
P2—O6	1.4987 (9)	C5—H5	0.9300
P2—O5	1.5607 (10)	C6—C7	1.388 (3)
P2—O4	1.6166 (10)	C6—H6	0.9300
O1—H1O1	0.8200	C7—H7	0.9300
O5—H5O5	0.8200	C8—C9	1.5035 (19)
N1—C1	1.4917 (17)	C8—H8A	0.9700
N1—H1N1	0.8900	C8—H8B	0.9700
N1—H2N1	0.8900	C9—C10	1.376 (2)
N1—H3N1	0.8900	C9—C14	1.378 (2)
N2—C8	1.4914 (18)	C10—C11	1.388 (3)
N2—H1N2	0.8900	C10—H10	0.9300
N2—H2N2	0.8900	C11—C12	1.372 (3)
N2—H3N2	0.8900	C11—H11	0.9300
C1—C2	1.504 (2)	C12—C13	1.366 (3)
C1—H1A	0.9700	C12—H12	0.9300
C1—H1B	0.9700	C13—C14	1.396 (3)
C2—C3	1.382 (2)	C13—H13	0.9300
C2—C7	1.383 (2)	C14—H14	0.9300
O2—P1—O3	116.03 (5)	C4—C3—H3	120.1
O2—P1—O1	112.01 (6)	C5—C4—C3	120.6 (2)
O3—P1—O1	108.73 (5)	C5—C4—H4	119.7
O2—P1—O4	110.57 (5)	C3—C4—H4	119.7
O3—P1—O4	108.51 (5)	C4—C5—C6	120.2 (2)
O1—P1—O4	99.70 (5)	C4—C5—H5	119.9
O7—P2—O6	118.50 (6)	C6—C5—H5	119.9
O7—P2—O5	112.56 (6)	C5—C6—C7	120.3 (2)
O6—P2—O5	108.61 (5)	C5—C6—H6	119.9
O7—P2—O4	109.12 (5)	C7—C6—H6	119.9
O6—P2—O4	102.49 (5)	C2—C7—C6	119.97 (19)
O5—P2—O4	104.16 (6)	C2—C7—H7	120.0
P1—O1—H1O1	109.5	C6—C7—H7	120.0
P1—O4—P2	133.33 (6)	N2—C8—C9	111.74 (11)
P2—O5—H5O5	109.5	N2—C8—H8A	109.3
C1—N1—H1N1	109.5	C9—C8—H8A	109.3
C1—N1—H2N1	109.5	N2—C8—H8B	109.3
H1N1—N1—H2N1	109.5	C9—C8—H8B	109.3
C1—N1—H3N1	109.5	H8A—C8—H8B	107.9
H1N1—N1—H3N1	109.5	C10—C9—C14	119.20 (15)
H2N1—N1—H3N1	109.5	C10—C9—C8	119.97 (14)
C8—N2—H1N2	109.5	C14—C9—C8	120.83 (15)

C8—N2—H2N2	109.5	C9—C10—C11	120.81 (18)
H1N2—N2—H2N2	109.5	C9—C10—H10	119.6
C8—N2—H3N2	109.5	C11—C10—H10	119.6
H1N2—N2—H3N2	109.5	C12—C11—C10	119.7 (2)
H2N2—N2—H3N2	109.5	C12—C11—H11	120.2
N1—C1—C2	111.18 (11)	C10—C11—H11	120.2
N1—C1—H1A	109.4	C13—C12—C11	120.08 (18)
C2—C1—H1A	109.4	C13—C12—H12	120.0
N1—C1—H1B	109.4	C11—C12—H12	120.0
C2—C1—H1B	109.4	C12—C13—C14	120.38 (19)
H1A—C1—H1B	108.0	C12—C13—H13	119.8
C3—C2—C7	119.23 (16)	C14—C13—H13	119.8
C3—C2—C1	120.29 (15)	C9—C14—C13	119.82 (19)
C7—C2—C1	120.46 (14)	C9—C14—H14	120.1
C2—C3—C4	119.7 (2)	C13—C14—H14	120.1
C2—C3—H3	120.1		

O2—P1—O4—P2	44.21 (10)	C3—C2—C7—C6	0.7 (2)
O3—P1—O4—P2	−84.10 (10)	C1—C2—C7—C6	179.28 (15)
O1—P1—O4—P2	162.27 (9)	C5—C6—C7—C2	−0.2 (3)
O7—P2—O4—P1	−51.43 (10)	N2—C8—C9—C10	81.81 (18)
O6—P2—O4—P1	−177.87 (9)	N2—C8—C9—C14	−98.38 (17)
O5—P2—O4—P1	68.98 (10)	C14—C9—C10—C11	−1.4 (3)
N1—C1—C2—C3	90.66 (17)	C8—C9—C10—C11	178.43 (17)
N1—C1—C2—C7	−87.87 (16)	C9—C10—C11—C12	0.1 (3)
C7—C2—C3—C4	−0.2 (3)	C10—C11—C12—C13	1.7 (4)
C1—C2—C3—C4	−178.79 (18)	C11—C12—C13—C14	−2.0 (4)
C2—C3—C4—C5	−0.8 (4)	C10—C9—C14—C13	1.0 (3)
C3—C4—C5—C6	1.3 (4)	C8—C9—C14—C13	−178.81 (18)
C4—C5—C6—C7	−0.8 (4)	C12—C13—C14—C9	0.7 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*1···O6^{i}	0.82	1.90	2.7208 (13)	174
O5—H5*O*5···O3^{ii}	0.82	1.83	2.6061 (13)	158
N1—H1*N*1···O2	0.89	2.07	2.9292 (13)	162
N1—H2*N*1···O6^{iii}	0.89	2.10	2.9698 (15)	166
N1—H2*N*1···O4^{iii}	0.89	2.53	3.1493 (13)	127
N1—H3*N*1···O7^{iv}	0.89	1.88	2.7645 (15)	169
N2—H1*N*2···O3^{ii}	0.89	1.94	2.7956 (15)	160
N2—H2*N*2···O2	0.89	1.98	2.8637 (15)	169
N2—H3*N*2···O6^{iii}	0.89	1.99	2.8053 (14)	152
C1—H1*B*···O5^{ii}	0.97	2.52	3.3333 (19)	141
C8—H8*B*···O7	0.97	2.40	3.1558 (17)	135

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