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Cyclohexyldimethylammonium tetrahydroxypentaborate

Hui Li, Guo-Ming Wang,* Shu-Yun Xue and Qiang Liang

Department of Chemistry, Teachers College of Qingdao University, Qingdao, Shandong 266071, People's Republic of China
Correspondence e-mail: gmwang_pub@163.com

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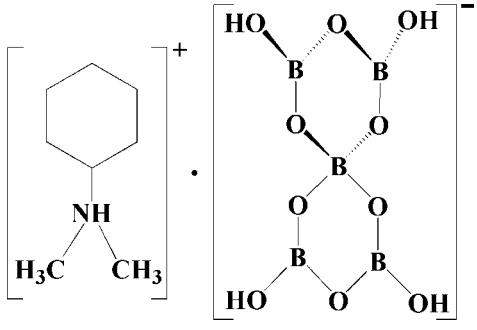
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.120; data-to-parameter ratio = 15.2.

The title compound, $[C_8H_{18}N]^+\cdot[B_5O_6(OH)_4]^-$, has been synthesized under mild solvothermal conditions in the presence of *N*,*N*-dimethylcyclohexylamine acting as a template. The structure consists of pentaborate $[B_5O_6(OH)_4]^-$ anions connected through O—H···O hydrogen bonds into a three-dimensional framework, with large channels along [100], [010] and [001] directions. The $[C_8H_{18}N]^+$ cations reside in the channels, interacting with the framework through N—H···O hydrogen bonds.

Related literature

For related literature, see: Batsanov *et al.* (1982); Burns *et al.* (1995); Chen *et al.* (1995); Grice *et al.* (1999); Liu & Li (2006); Liu *et al.* (2006); Schubert *et al.* (2000); Touboul *et al.* (2003); Wang *et al.* (2004, 2008*a*,*b*)



Experimental

Crystal data

$C_8H_{18}N^+\cdot B_5H_4O_{10}^-$
M_r = 346.32
Triclinic, $P\overline{1}$
a = 8.6971 (4) Å
b = 9.8990 (2) Å
c = 10.2300 (3) Å
α = 74.591 (3)°
β = 74.442 (2)°
γ = 82.190 (5)°
V = 815.98 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 295 (2) K
0.45 × 0.45 × 0.45 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.948, T_{max} = 0.949
6623 measured reflections
3318 independent reflections
2536 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.119
S = 1.08
3318 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

B1—O1	1.350 (2)	B3—O6	1.469 (2)
B1—O5	1.3552 (19)	B3—O7	1.473 (2)
B1—O2	1.377 (2)	B4—O10	1.346 (2)
B2—O3	1.341 (2)	B4—O7	1.3491 (19)
B2—O4	1.357 (2)	B4—O9	1.387 (2)
B2—O2	1.375 (2)	B5—O8	1.343 (2)
B3—O4	1.452 (2)	B5—O6	1.3439 (19)
B3—O5	1.4651 (19)	B5—O9	1.388 (2)
O1—B1—O5	122.22 (15)	O4—B3—O7	108.58 (13)
O1—B1—O2	117.10 (14)	O5—B3—O7	108.76 (12)
O5—B1—O2	120.66 (14)	O6—B3—O7	110.28 (12)
O3—B2—O4	121.91 (16)	O10—B4—O7	118.13 (15)
O3—B2—O2	117.92 (15)	O10—B4—O9	121.04 (14)
O4—B2—O2	120.14 (15)	O7—B4—O9	120.83 (14)
O4—B3—O5	111.21 (12)	O8—B5—O6	123.78 (14)
O4—B3—O6	108.43 (12)	O8—B5—O9	115.84 (14)
O5—B3—O6	109.57 (13)	O6—B5—O9	120.38 (14)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O5^{i}	0.82	1.96	2.7759 (16)	174
O3—H3A···O4^{ii}	0.82	1.99	2.8143 (16)	178
O8—H8A···O6^{iii}	0.82	1.96	2.7816 (15)	179
O10—H10A···O9^{iv}	0.82	2.03	2.8477 (15)	178
N1—H1D···O7	0.91	1.94	2.8368 (18)	169

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT-Plus* (Bruker, 2002); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MG2056).

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Cyclohexyldimethylammonium tetrahydroxypentaborate

Hui Li, Guo-Ming Wang, Shu-Yun Xue and Qiang Liang

S1. Comment

Borate materials have been receiving particular attention due to their fascinating structural diversities and potential applications in mineralogy and industry (Burns *et al.*, 1995; Chen *et al.*, 1995; Grice *et al.*, 1999; Touboul *et al.*, 2003). From a structural point of view, the ability of B to adopt both BO_3 and BO_4 coordination modes, coupled with the tendency of such units to polymerize into a wide range of polyanions, has led to a rapidly growing family of borates. Thus far, numerous inorganic borate materials with alkali metals, alkaline earth metals, rare earths and transition metals have been extensively studied. In contrast, the analogous chemistry of organically templated borates is still relatively undeveloped. To the best of our knowledge, only a few examples with polyanions, such as $[B_4O_5(OH)_4]$ (Batsanov *et al.*, 1982), $[B_5O_6(OH)_4]$ (Wang *et al.*, 2004), $[B_7O_9(OH)_5]$ (Liu & Li, 2006; Liu *et al.*, 2006), $[B_9O_{12}(OH)_6]$ (Schubert *et al.*, 2000) and $[B_{14}O_{20}(OH)_6]$ (Liu *et al.*, 2006), have been reported. The aim of our work is to explore the construction of novel microporous aluminoborates templated by organic agents with different shape and size (Wang *et al.*, 2008a,b). Unexpectedly, the title compound, (I), was isolated, a new organically templated pentaborate.

As shown in Fig. 1, the asymmetric unit of (I) contains one $[B_5O_6(OH)_4]^-$ anion and one $[C_8H_{18}N]^+$ cation. The anionic $[B_5O_6(OH)_4]^-$ polyanion is composed of two common B_3O_3 rings, each containing two BO_3 triangles and one BO_4 tetrahedron. The B—O bond distances lie in the range 1.341 (2)–1.388 (2) Å for the BO_3 triangles (B1, B2, B4 and B5) and 1.452 (2)–1.473 (2) Å for the B(3)O_4 tetrahedron, in good agreement with those reported previously for other borate compounds. The O—B—O bond angles lie in the range 115.8 (2)–123.7 (2) ° for the triangles and 108.4 (2)–111.2 (2) ° for the tetrahedron. The anionic $[B_5O_6(OH)_4]^-$ groups are connected to each other through intermolecular O—H···O hydrogen bonds, forming a three-dimensional framework with large channels along [100], [010] and [001] directions. The $[C_8H_{18}N]^+$ cations reside in these channels, interacting with the framework through N—H···O hydrogen bonds (Fig. 2).

S2. Experimental

A mixture of H_3BO_3 (0.186 g), Al_2O_3 (0.104 g), *N*,*N*-dimethylcyclohexylamine (0.75 ml), pyridine (4.4 ml) and H_2O (0.50 ml) was sealed in a Teflon-lined steel autoclave, heated at 453 K for 8 days, and then cooled to room temperature. The homogeneous product consisting of large colorless block-shaped crystals was separated from the solution by filtration, washed with distilled water, and then dried in air.

S3. Refinement

All H atoms were positioned geometrically and treated as riding atoms: O—H = 0.82 Å, N—H = 0.91 Å and C—H = 0.96–0.98 Å with U_{iso}(H) = 1.2–1.5U_{eq}(parent atoms).

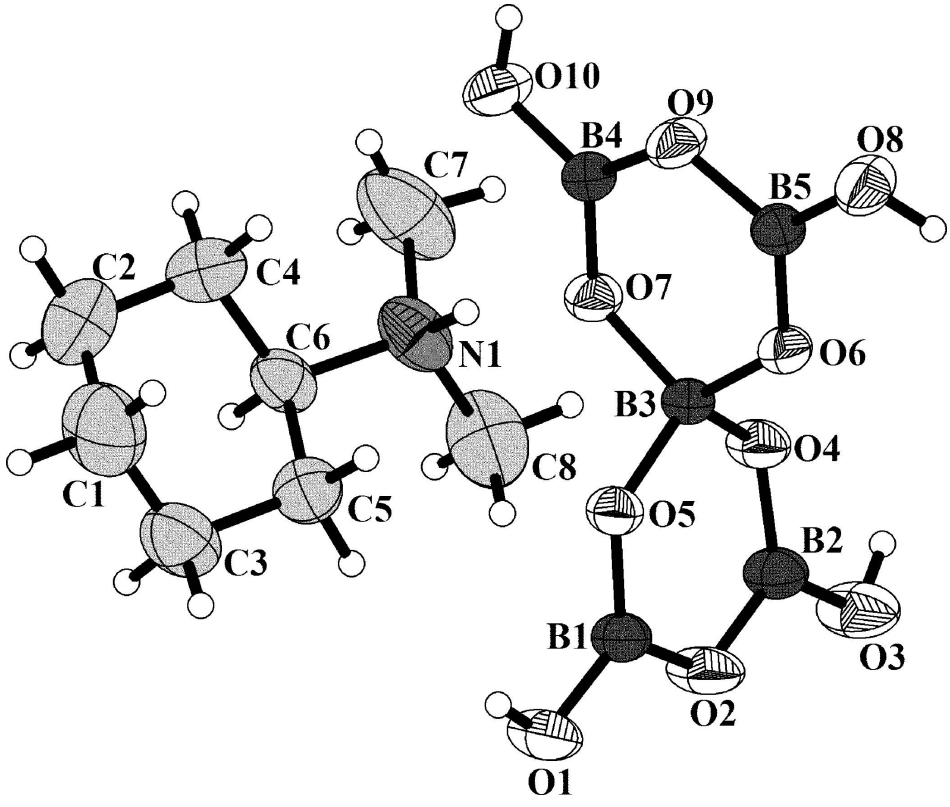

Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level for non-H atoms.

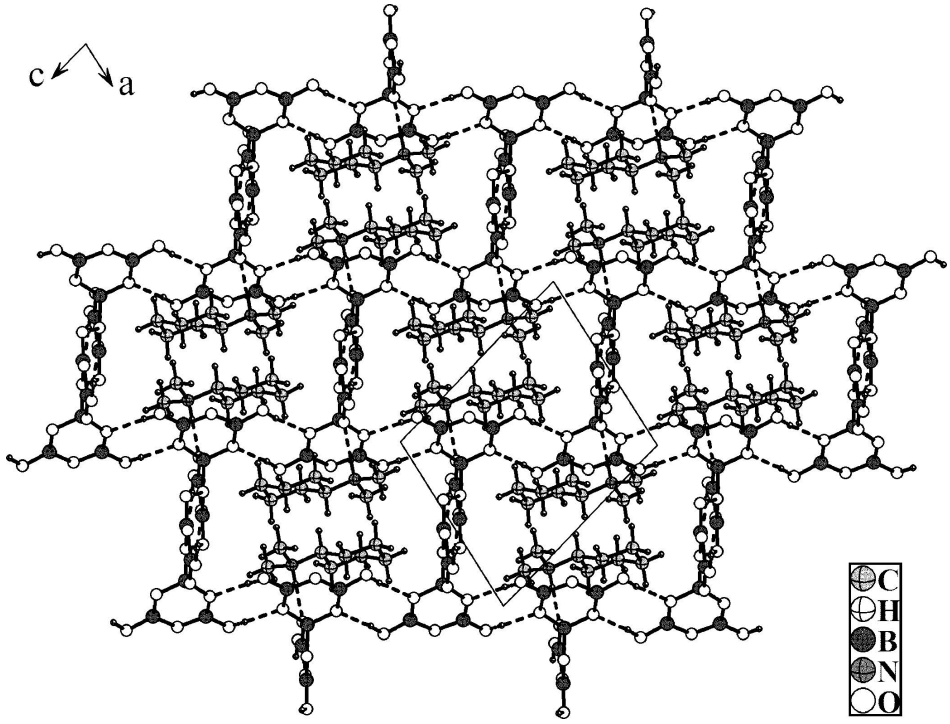

Figure 2

Projection of (I) along b, showing $[B_5O_6(OH)_4]^-$ anions linked into a three-dimensional framework, with $[C_8H_{18}N]^+$ cations occupying channels. Hydrogen bonds are shown as dashed lines.

Cyclohexyldimethylammonium tetrahydroxypentaborate

Crystal data

$C_8H_{18}N^+·B_5H_4O^{10-}$
M_r = 346.32
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.6971 (4) Å
b = 9.8990 (2) Å
c = 10.2300 (3) Å
α = 74.591 (3)°
β = 74.442 (2)°
γ = 82.190 (5)°
V = 815.98 (5) Å^3
Z = 2
$F(000)$ = 364
D_x = 1.410 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6623 reflections
θ = 2.1–26.5°
μ = 0.12 mm^{-1}
T = 295 K
Block, colorless
0.45 × 0.45 × 0.45 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.949, T_{max} = 0.949
6623 measured reflections
3318 independent reflections
2536 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 26.5°, θ_{min} = 2.1°
h = −10→10
k = −12→12
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.119$
$S = 1.08$
3318 reflections
218 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.0744P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.058 (6)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
B1	0.3071 (2)	1.10774 (18)	0.59941 (19)	0.0342 (4)
B2	0.1056 (2)	1.1184 (2)	0.8073 (2)	0.0372 (4)
B3	0.3133 (2)	0.92080 (17)	0.81503 (17)	0.0296 (4)
B4	0.3702 (2)	0.66200 (18)	0.88838 (18)	0.0309 (4)
B5	0.5114 (2)	0.81317 (18)	0.95617 (18)	0.0311 (4)
O1	0.35979 (15)	1.16205 (12)	0.46086 (12)	0.0477 (3)
H1A	0.4376	1.1133	0.4291	0.072*
O2	0.17524 (14)	1.17636 (12)	0.66942 (12)	0.0480 (3)
O3	−0.02096 (16)	1.18988 (13)	0.87215 (13)	0.0555 (4)
H3A	−0.0641	1.1391	0.9470	0.083*
O4	0.16229 (13)	0.99089 (11)	0.87271 (11)	0.0362 (3)
O5	0.37677 (12)	0.98883 (11)	0.66764 (10)	0.0328 (3)
O6	0.42790 (13)	0.92583 (10)	0.89591 (11)	0.0334 (3)
O7	0.28642 (13)	0.77398 (10)	0.82604 (11)	0.0331 (3)
O8	0.61961 (15)	0.82028 (12)	1.02584 (13)	0.0454 (3)
H8A	0.6045	0.8953	1.0486	0.068*
O9	0.48965 (13)	0.67959 (11)	0.94784 (12)	0.0375 (3)
O10	0.33377 (15)	0.53291 (11)	0.89197 (13)	0.0453 (3)
H10A	0.3859	0.4736	0.9386	0.068*
C2	0.2698 (4)	0.5351 (3)	0.4335 (3)	0.0907 (9)
H2A	0.3327	0.4461	0.4360	0.109*
H2B	0.1854	0.5349	0.3880	0.109*
C1	0.3752 (4)	0.6525 (3)	0.3495 (3)	0.0884 (8)

H1B	0.4659	0.6475	0.3892	0.106*
H1C	0.4156	0.6425	0.2542	0.106*
C4	0.1958 (3)	0.5485 (2)	0.5814 (2)	0.0685 (6)
H4A	0.1248	0.4738	0.6301	0.082*
H4B	0.2793	0.5392	0.6304	0.082*
C3	0.2836 (3)	0.7915 (3)	0.3491 (2)	0.0677 (6)
H3B	0.2010	0.8008	0.2990	0.081*
H3C	0.3552	0.8659	0.3005	0.081*
C5	0.2074 (3)	0.8069 (2)	0.4963 (2)	0.0552 (5)
H5A	0.2908	0.8097	0.5421	0.066*
H5B	0.1428	0.8952	0.4922	0.066*
C6	0.1036 (2)	0.6880 (2)	0.58154 (18)	0.0464 (4)
H6A	0.0141	0.6920	0.5391	0.056*
C7	−0.0497 (3)	0.5880 (3)	0.8280 (3)	0.0899 (9)
H7A	−0.0881	0.6078	0.9185	0.135*
H7B	0.0219	0.5050	0.8341	0.135*
H7D	−0.1386	0.5732	0.7956	0.135*
C8	−0.0711 (3)	0.8397 (3)	0.7322 (3)	0.0774 (7)
H8B	−0.1092	0.8485	0.8270	0.116*
H8E	−0.1603	0.8354	0.6953	0.116*
H8C	−0.0124	0.9194	0.6767	0.116*
N1	0.03619 (19)	0.70824 (19)	0.72858 (16)	0.0540 (4)
H1D	0.1208	0.7174	0.7614	0.065*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
B1	0.0377 (10)	0.0291 (9)	0.0329 (9)	0.0001 (8)	−0.0099 (8)	−0.0021 (7)
B2	0.0364 (10)	0.0328 (10)	0.0367 (10)	0.0043 (8)	−0.0081 (8)	−0.0027 (8)
B3	0.0345 (9)	0.0252 (8)	0.0286 (9)	0.0013 (7)	−0.0110 (7)	−0.0038 (7)
B4	0.0346 (9)	0.0268 (9)	0.0308 (9)	−0.0004 (7)	−0.0100 (7)	−0.0050 (7)
B5	0.0318 (9)	0.0298 (9)	0.0316 (9)	0.0026 (7)	−0.0096 (7)	−0.0075 (7)
O1	0.0515 (8)	0.0430 (7)	0.0336 (6)	0.0102 (6)	−0.0047 (5)	0.0038 (5)
O2	0.0495 (8)	0.0379 (7)	0.0381 (7)	0.0151 (5)	−0.0026 (5)	0.0048 (5)
O3	0.0515 (8)	0.0468 (8)	0.0467 (7)	0.0198 (6)	0.0006 (6)	0.0008 (6)
O4	0.0361 (6)	0.0325 (6)	0.0319 (6)	0.0059 (5)	−0.0056 (5)	−0.0010 (5)
O5	0.0364 (6)	0.0296 (6)	0.0284 (6)	0.0036 (4)	−0.0073 (4)	−0.0037 (4)
O6	0.0422 (6)	0.0247 (5)	0.0361 (6)	0.0024 (5)	−0.0179 (5)	−0.0062 (4)
O7	0.0372 (6)	0.0274 (6)	0.0370 (6)	−0.0002 (5)	−0.0177 (5)	−0.0037 (4)
O8	0.0540 (8)	0.0337 (6)	0.0605 (8)	0.0078 (5)	−0.0354 (6)	−0.0155 (5)
O9	0.0439 (7)	0.0248 (6)	0.0496 (7)	0.0050 (5)	−0.0261 (5)	−0.0076 (5)
O10	0.0546 (8)	0.0262 (6)	0.0614 (8)	−0.0016 (5)	−0.0320 (6)	−0.0036 (5)
C2	0.130 (2)	0.0621 (16)	0.0858 (19)	0.0030 (16)	−0.0256 (18)	−0.0321 (14)
C1	0.0910 (19)	0.101 (2)	0.0638 (15)	0.0082 (16)	−0.0015 (14)	−0.0295 (15)
C4	0.0907 (17)	0.0440 (12)	0.0684 (15)	−0.0043 (11)	−0.0254 (13)	−0.0035 (10)
C3	0.0751 (15)	0.0731 (15)	0.0487 (12)	−0.0154 (12)	−0.0111 (11)	−0.0032 (11)
C5	0.0682 (13)	0.0471 (11)	0.0508 (11)	−0.0127 (10)	−0.0154 (10)	−0.0073 (9)
C6	0.0485 (11)	0.0532 (11)	0.0407 (10)	−0.0104 (9)	−0.0183 (8)	−0.0055 (8)

C7	0.0835 (18)	0.125 (2)	0.0532 (14)	−0.0480 (17)	−0.0113 (13)	0.0068 (14)
C8	0.0516 (13)	0.110 (2)	0.0765 (16)	0.0118 (13)	−0.0205 (12)	−0.0362 (15)
N1	0.0436 (9)	0.0767 (12)	0.0442 (9)	−0.0127 (8)	−0.0178 (7)	−0.0071 (8)

Geometric parameters (Å, º)

B1—O1	1.350 (2)	C1—C3	1.492 (4)
B1—O5	1.3552 (19)	C1—H1B	0.9700
B1—O2	1.377 (2)	C1—H1C	0.9700
B2—O3	1.341 (2)	C4—C6	1.500 (3)
B2—O4	1.357 (2)	C4—H4A	0.9700
B2—O2	1.375 (2)	C4—H4B	0.9700
B3—O4	1.452 (2)	C3—C5	1.513 (3)
B3—O5	1.4651 (19)	C3—H3B	0.9700
B3—O6	1.469 (2)	C3—H3C	0.9700
B3—O7	1.473 (2)	C5—C6	1.510 (3)
B4—O10	1.346 (2)	C5—H5A	0.9700
B4—O7	1.3491 (19)	C5—H5B	0.9700
B4—O9	1.387 (2)	C6—N1	1.517 (2)
B5—O8	1.343 (2)	C6—H6A	0.9800
B5—O6	1.3439 (19)	C7—N1	1.484 (3)
B5—O9	1.388 (2)	C7—H7A	0.9600
O1—H1A	0.8200	C7—H7B	0.9600
O3—H3A	0.8200	C7—H7D	0.9600
O8—H8A	0.8200	C8—N1	1.497 (3)
O10—H10A	0.8200	C8—H8B	0.9600
C2—C1	1.506 (4)	C8—H8E	0.9600
C2—C4	1.510 (3)	C8—H8C	0.9600
C2—H2A	0.9700	N1—H1D	0.9100
C2—H2B	0.9700		
O1—B1—O5	122.22 (15)	C6—C4—H4A	109.5
O1—B1—O2	117.10 (14)	C2—C4—H4A	109.5
O5—B1—O2	120.66 (14)	C6—C4—H4B	109.5
O3—B2—O4	121.91 (16)	C2—C4—H4B	109.5
O3—B2—O2	117.92 (15)	H4A—C4—H4B	108.1
O4—B2—O2	120.14 (15)	C1—C3—C5	111.33 (19)
O4—B3—O5	111.21 (12)	C1—C3—H3B	109.4
O4—B3—O6	108.43 (12)	C5—C3—H3B	109.4
O5—B3—O6	109.57 (13)	C1—C3—H3C	109.4
O4—B3—O7	108.58 (13)	C5—C3—H3C	109.4
O5—B3—O7	108.76 (12)	H3B—C3—H3C	108.0
O6—B3—O7	110.28 (12)	C6—C5—C3	112.21 (17)
O10—B4—O7	118.13 (15)	C6—C5—H5A	109.2
O10—B4—O9	121.04 (14)	C3—C5—H5A	109.2
O7—B4—O9	120.83 (14)	C6—C5—H5B	109.2
O8—B5—O6	123.78 (14)	C3—C5—H5B	109.2
O8—B5—O9	115.84 (14)	H5A—C5—H5B	107.9

O6—B5—O9	120.38 (14)	C4—C6—C5	110.93 (18)
B1—O1—H1A	109.5	C4—C6—N1	111.82 (15)
B2—O2—B1	119.89 (13)	C5—C6—N1	109.11 (15)
B2—O3—H3A	109.5	C4—C6—H6A	108.3
B2—O4—B3	123.53 (13)	C5—C6—H6A	108.3
B1—O5—B3	123.25 (13)	N1—C6—H6A	108.3
B5—O6—B3	124.60 (12)	N1—C7—H7A	109.5
B4—O7—B3	123.84 (12)	N1—C7—H7B	109.5
B5—O8—H8A	109.5	H7A—C7—H7B	109.5
B4—O9—B5	119.28 (12)	N1—C7—H7D	109.5
B4—O10—H10A	109.5	H7A—C7—H7D	109.5
C1—C2—C4	112.3 (2)	H7B—C7—H7D	109.5
C1—C2—H2A	109.1	N1—C8—H8B	109.5
C4—C2—H2A	109.1	N1—C8—H8E	109.5
C1—C2—H2B	109.1	H8B—C8—H8E	109.5
C4—C2—H2B	109.1	N1—C8—H8C	109.5
H2A—C2—H2B	107.9	H8B—C8—H8C	109.5
C3—C1—C2	110.5 (2)	H8E—C8—H8C	109.5
C3—C1—H1B	109.6	C7—N1—C8	108.9 (2)
C2—C1—H1B	109.6	C7—N1—C6	114.16 (19)
C3—C1—H1C	109.6	C8—N1—C6	112.63 (16)
C2—C1—H1C	109.6	C7—N1—H1D	106.9
H1B—C1—H1C	108.1	C8—N1—H1D	106.9
C6—C4—C2	110.61 (18)	C6—N1—H1D	106.9

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O5^{i}	0.82	1.96	2.7759 (16)	174
O3—H3*A*···O4^{ii}	0.82	1.99	2.8143 (16)	178
O8—H8*A*···O6^{iii}	0.82	1.96	2.7816 (15)	179
O10—H10*A*···O9^{iv}	0.82	2.03	2.8477 (15)	178
N1—H1*D*···O7	0.91	1.94	2.8368 (18)	169

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