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Bis[(*m*-phenylenedimethylene)-diammonium] tetradecaborate

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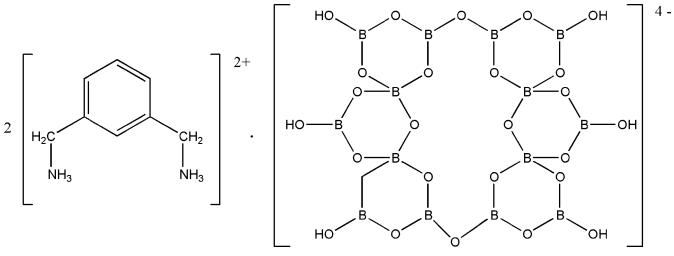
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; R factor = 0.035; wR factor = 0.128; data-to-parameter ratio = 11.1.

The title compound $2C_8H_{14}N_2^{2+}\cdot[B_{14}O_{20}(OH)_6]^{4-}$, contains diprotonated $C_8H_{14}N_2^{2+}$ cations and centrosymmetric tetradecaborate anions. The crystal structure is stabilized by O—H···O and N—H···O hydrogen bonds.

Related literature

For background on the importance of borate compounds, see: Chen *et al.* (1995); Grice *et al.* (1999). For previous work on boron oxoanions, see: Liu *et al.* (2006); Pan *et al.* (2007); Grice *et al.* (1999); Schubert *et al.* (2000); Touboul *et al.* (2003); Burns (1995).



Experimental

Crystal data

$2C_8H_{14}N_2^{2+}\cdot B_{14}H_6O_{26}^{4-}$
M_r = 849.81
Triclinic, $P\overline{1}$
a = 9.1025 (18) Å
b = 10.293 (2) Å
c = 10.942 (2) Å
α = 109.68 (3)°
β = 108.24 (3)°
γ = 102.19 (3)°
V = 857.4 (5) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 295 (2) K
0.34 × 0.26 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.964, T_{max} = 0.973
6803 measured reflections
3009 independent reflections
2002 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.128
S = 1.24
3009 reflections
272 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O10—H10A···O2^{i}	0.82	1.98	2.784 (2)	168
O11—H11A···O3^{ii}	0.82	1.84	2.659 (2)	179
O13—H13A···O11^{iii}	0.82	2.00	2.815 (2)	173
N1—H1A···O7	0.89	2.08	2.863 (2)	146
N1—H1B···O13^{iv}	0.89	1.98	2.850 (2)	166
N1—H1C···O6^{v}	0.89	2.20	2.916 (2)	137
N1—H1C···O1^{v}	0.89	2.54	3.394 (2)	161
N2—H2A···O4^{vi}	0.89	1.97	2.822 (2)	159
N2—H2B···O1^{v}	0.89	1.99	2.877 (2)	173
N2—H2B···O9^{v}	0.89	2.55	3.052 (2)	116
N2—H2C···O12^{vii}	0.89	2.19	3.067 (2)	168

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976); 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: BT2801).

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supplementary materials

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Bis[(*m*-phenylenedimethylene)diammonium] tetradecaborate

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Comment

Borate compounds have considerable mineralogical and industrial importance (Chen *et al.*, 1995; Grice *et al.*, 1999). Boron atoms form strong bonds with oxygen atoms not only in trigonal planar BO_3, but also in tetrahedral BO_4 groups. These BO_3 and BO_4 groups may be linked together by sharing common oxygen to form isolated rings and cages or extended chains, sheets, and networks. So far, a number of isolated boron oxoanions have been found in mineral and synthetic borates, such as $[B(OH)_4]^-$, $[B_2O(OH)_6]^{2-}$, $[B_3O_3(OH)_4]^-$, $[B_4O_5(OH)_4]^{2-}$, $[B_5O_6(OH)_4]^-$, $[B_6O_7(OH)_6]^{2-}$ (Grice *et al.*, 1999; Touboul *et al.*, 2003), $[B_7O_9(OH)_5]^{2-}$ (Liu *et al.*, 2006; Pan *et al.*, 2007), $[B_9O_{12}(OH)_6]^{3-}$ (Schubert *et al.*, 2000), and $[B_{14}O_{20}(OH)_6]^{4-}$ (Liu *et al.*, 2006; Pan *et al.*, 2007). Compared with metal borates, the synthesis of organically modified nonmetal borates was less well explored in the past decades. Herein, we describe the synthesis and crystal structure of a new nonmetal borate with $[B_{14}O_{20}(OH)_6]^{4-}$ as polyanions.

As shown in Fig. 1, the title compound consists of isolated $[B_{14}O_{20}(OH)_6]^{4-}$ polyborate anions and $[C_8H_{14}N_2]^{2+}$ cations. The $[B_{14}O_{20}(OH)_6]^{4-}$ borate anion is composed of four BO_4, four BO_3, and six $BO_2(OH)$ groups (Burns, 1995). It can also be seen as two $[B_7O_9(OH)_5]^{2-}$ clusters combined with each other through the dehydration of four hydroxyl groups. Each $[B_7O_9(OH)_5]^{2-}$ group contains three B_3O_3 cycles held together *via* two common BO_4 tetrahedra. The B—O bond lengths and O—B—O bond angles are in the range of 1.332 (4)–1.509 (4) Å and 105.9 (3)–124.5 (3)° (Table 1), which are in good agreement with other borates reported previously (Liu *et al.*, 2006; Pan *et al.*, 2007).

In the present instance, the isolated tetradecaborates anions are linked together through hydrogen bonds: O10—H10A···O2, O11—H11A···O3 (Fig. 2), forming a two-dimensional sheetlike structure. The adjacent borate sheets are further linked together by strong H-bonding interactions [O13—H13A···O11] to form a three-dimensional network (Fig. 3). The hydrogen bonds are listed in Table 2.

Experimental

The title compound was obtained by the reaction of H_3BO_3 and 1,3-Bis(aminomethyl)benzene under mild solvothermal conditions. Typically, a mixture of H_3BO_3 (0.9882 g), 1,3-Bis(aminomethyl)benzene (3 ml) was stirred at room temperature. The final mixture was sealed in a Teflon-lined autoclave, heated to 443 K at a rate of 10 K/h, kept at 443 K for 4 days and then cooled to room temperature at a rate of 5 K/h. Colorless transparent block-like crystals were collected and dried in air.

Refinement

All H atoms were positioned geometrically and refined as riding model [O—H = 0.82 Å, N—H = 0.89 Å, C—$H_{aromatic}$ = 0.93 Å, C—H_2 = 0.97 Å, and with U_{iso}(H) = 1.5U_{eq}(O), U_{iso}(H) = 1.5U_{eq}(N), U_{iso}(H) = 1.2U_{eq}(C)].

Figures

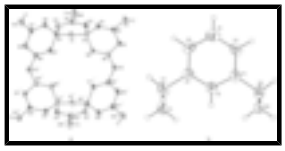

Fig. 1. The crystal structure of $[(C_8H_{14}N_2)]_2[B_{14}O_{20}(OH)_6]$: (*a*) $[B_{14}O_{20}(OH)_6]^{4-}$; (*b*) $[(C_8H_{14}N_2)]^{2+}$, drawn at the 50% probability level. [Symmetry codes: (i) -*x*+1, -*y*+1, -*z*+1.]

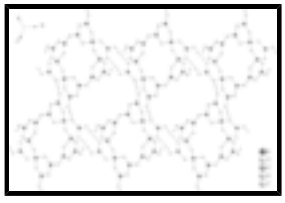

Fig. 2. Formation of the two-dimensional sheet from the $[B_{14}O_{20}(OH)_6]^{4-}$ polyanions. Hydrogen bonds are indicated by dashed lines.

Fig. 3. View of the diprotonated of organic amines in the inorganic borate network along *a* axis.

Bis[(m-phenylenedimethylene)diammonium] tetradecaborate

Crystal data

$2C_8H_{14}N_2^{2+}\cdot B_{14}H_6O_{26}^{4-}$	$Z = 1$
$M_r = 849.81$	$F_{000} = 436$
Triclinic, $P\overline{1}$	$D_x = 1.646$ Mg m^{-3}
Hall symbol: -P1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.1025$ (18) Å	Cell parameters from 4940 reflections
$b = 10.293$ (2) Å	$\theta = 6.7$–54.9°
$c = 10.942$ (2) Å	$\mu = 0.14$ mm^{-1}
$\alpha = 109.68$ (3)°	$T = 295$ (2) K
$\beta = 108.24$ (3)°	Block, colourless
$\gamma = 102.19$ (3)°	0.34 × 0.26 × 0.18 mm
$V = 857.4$ (5) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	3009 independent reflections
Radiation source: fine-focus sealed tube	2002 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 295$(2) K	$\theta_{max} = 25.0^\circ$
ω scans	$\theta_{min} = 3.4^\circ$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -10\rightarrow10$
$T_{min} = 0.964$, $T_{max} = 0.973$	$k = -12\rightarrow12$
6803 measured reflections	$l = -12\rightarrow12$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.035$	$w = 1/[\sigma^2(F_o^2) + (0.0299P)^2 + 1.2547P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.128$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.24$	$\Delta\rho_{max} = 0.42$ e Å^{-3}
3009 reflections	$\Delta\rho_{min} = -0.46$ e Å^{-3}
272 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.012 (2)
Secondary atom site location: difference Fourier map	

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	0.6460 (5)	0.4668 (4)	0.7888 (4)	0.0240 (8)
B2	0.7413 (4)	0.3345 (4)	0.6060 (4)	0.0222 (8)
B3	0.5338 (4)	0.1936 (4)	0.6602 (4)	0.0247 (8)
B4	0.6535 (4)	0.6248 (4)	1.0187 (4)	0.0209 (7)
B5	0.4617 (5)	0.6104 (4)	0.8040 (4)	0.0233 (8)
B6	0.7437 (4)	0.3478 (4)	0.3829 (4)	0.0225 (8)
B7	0.9709 (5)	0.3173 (4)	0.5343 (4)	0.0252 (8)
O1	0.7649 (3)	0.4597 (2)	0.7304 (2)	0.0238 (5)
O2	0.6220 (3)	0.1961 (2)	0.5811 (2)	0.0279 (5)
O3	0.5410 (3)	0.3195 (2)	0.7601 (2)	0.0266 (5)
O4	0.7324 (3)	0.5555 (2)	0.9474 (2)	0.0231 (5)
O5	0.5160 (3)	0.6519 (2)	0.9489 (2)	0.0259 (5)
O6	0.5330 (3)	0.5377 (2)	0.7283 (2)	0.0248 (5)
O7	0.6718 (3)	0.3576 (2)	0.4736 (2)	0.0263 (5)
O8	0.8946 (3)	0.3301 (3)	0.4095 (2)	0.0297 (6)
O9	0.9009 (3)	0.3166 (2)	0.6244 (2)	0.0260 (5)

O10	0.4275 (3)	0.0652 (3)	0.6413 (3)	0.0447 (7)
H10A	0.4225	−0.0042	0.5733	0.067*
O11	0.7074 (3)	0.6690 (2)	1.1630 (2)	0.0269 (5)
H11A	0.6297	0.6722	1.1852	0.040*
O12	0.3292 (3)	0.6490 (3)	0.7475 (2)	0.0284 (5)
O13	1.1239 (3)	0.3064 (3)	0.5617 (2)	0.0374 (6)
H13A	1.1659	0.3147	0.6433	0.056*
N1	0.3291 (3)	0.3057 (3)	0.4112 (3)	0.0329 (7)
H1A	0.4353	0.3287	0.4654	0.049*
H1B	0.2747	0.3228	0.4662	0.049*
H1C	0.3203	0.3605	0.3633	0.049*
N2	−0.1153 (3)	0.4082 (3)	0.0950 (3)	0.0320 (7)
H2A	−0.1372	0.4667	0.0531	0.048*
H2B	−0.0078	0.4427	0.1513	0.048*
H2C	−0.1730	0.4060	0.1471	0.048*
C1	0.0788 (4)	0.1079 (4)	0.2176 (4)	0.0316 (8)
C2	0.0378 (4)	0.1765 (4)	0.1291 (4)	0.0313 (8)
H2D	0.1214	0.2350	0.1185	0.038*
C3	−0.1245 (4)	0.1600 (4)	0.0564 (4)	0.0310 (8)
C4	−0.2492 (4)	0.0650 (4)	0.0667 (4)	0.0380 (9)
H4A	−0.3593	0.0505	0.0165	0.046*
C5	−0.2107 (5)	−0.0074 (4)	0.1508 (4)	0.0452 (10)
H5A	−0.2949	−0.0713	0.1563	0.054*
C6	−0.0475 (5)	0.0143 (4)	0.2272 (4)	0.0387 (9)
H6A	−0.0220	−0.0337	0.2850	0.046*
C7	0.2573 (5)	0.1467 (4)	0.3083 (4)	0.0413 (9)
H7A	0.2681	0.0865	0.3600	0.050*
H7B	0.3166	0.1274	0.2483	0.050*
C8	−0.1624 (5)	0.2555 (4)	−0.0168 (4)	0.0373 (9)
H8A	−0.2794	0.2172	−0.0789	0.045*
H8B	−0.1006	0.2570	−0.0744	0.045*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
B1	0.0293 (19)	0.027 (2)	0.0191 (19)	0.0131 (16)	0.0134 (16)	0.0092 (16)
B2	0.0212 (18)	0.025 (2)	0.0231 (19)	0.0095 (15)	0.0124 (16)	0.0104 (16)
B3	0.0267 (19)	0.024 (2)	0.024 (2)	0.0084 (16)	0.0132 (16)	0.0098 (17)
B4	0.0219 (18)	0.0198 (18)	0.0207 (19)	0.0057 (14)	0.0104 (15)	0.0081 (15)
B5	0.0287 (19)	0.0248 (19)	0.0197 (19)	0.0128 (16)	0.0115 (16)	0.0101 (16)
B6	0.0245 (19)	0.0242 (19)	0.0179 (18)	0.0128 (15)	0.0081 (15)	0.0060 (15)
B7	0.0265 (19)	0.032 (2)	0.0162 (18)	0.0142 (17)	0.0085 (16)	0.0072 (16)
O1	0.0236 (11)	0.0247 (12)	0.0230 (12)	0.0071 (9)	0.0145 (10)	0.0067 (10)
O2	0.0325 (12)	0.0254 (12)	0.0273 (13)	0.0089 (10)	0.0197 (11)	0.0073 (10)
O3	0.0327 (13)	0.0219 (12)	0.0295 (13)	0.0083 (10)	0.0211 (11)	0.0095 (10)
O4	0.0253 (11)	0.0272 (12)	0.0160 (11)	0.0119 (9)	0.0086 (9)	0.0071 (10)
O5	0.0291 (12)	0.0354 (13)	0.0188 (12)	0.0186 (10)	0.0117 (10)	0.0119 (10)
O6	0.0292 (12)	0.0320 (13)	0.0190 (11)	0.0182 (10)	0.0119 (10)	0.0113 (10)

O7	0.0251 (12)	0.0394 (14)	0.0243 (12)	0.0182 (10)	0.0145 (10)	0.0168 (11)
O8	0.0280 (12)	0.0458 (15)	0.0253 (13)	0.0196 (11)	0.0161 (10)	0.0183 (11)
O9	0.0248 (12)	0.0392 (14)	0.0237 (12)	0.0175 (10)	0.0153 (10)	0.0157 (11)
O10	0.0624 (17)	0.0251 (14)	0.0473 (16)	0.0051 (12)	0.0399 (15)	0.0069 (12)
O11	0.0280 (12)	0.0377 (14)	0.0196 (12)	0.0158 (10)	0.0130 (10)	0.0123 (10)
O12	0.0315 (13)	0.0418 (14)	0.0240 (12)	0.0234 (11)	0.0155 (10)	0.0178 (11)
O13	0.0271 (13)	0.0688 (18)	0.0272 (13)	0.0275 (13)	0.0146 (11)	0.0238 (13)
N1	0.0276 (15)	0.0430 (18)	0.0291 (16)	0.0123 (13)	0.0137 (13)	0.0152 (14)
N2	0.0338 (16)	0.0351 (17)	0.0316 (16)	0.0160 (13)	0.0139 (13)	0.0170 (14)
C1	0.0338 (19)	0.0238 (18)	0.0276 (19)	0.0091 (15)	0.0082 (15)	0.0054 (15)
C2	0.0323 (19)	0.0286 (19)	0.0274 (19)	0.0091 (15)	0.0107 (16)	0.0085 (15)
C3	0.0325 (19)	0.0279 (19)	0.0270 (19)	0.0117 (15)	0.0102 (16)	0.0072 (15)
C4	0.0290 (19)	0.029 (2)	0.045 (2)	0.0075 (16)	0.0120 (17)	0.0087 (18)
C5	0.044 (2)	0.033 (2)	0.054 (3)	0.0065 (18)	0.024 (2)	0.014 (2)
C6	0.050 (2)	0.028 (2)	0.043 (2)	0.0132 (17)	0.0213 (19)	0.0194 (18)
C7	0.041 (2)	0.037 (2)	0.038 (2)	0.0188 (18)	0.0109 (18)	0.0096 (18)
C8	0.041 (2)	0.038 (2)	0.0250 (19)	0.0164 (17)	0.0063 (16)	0.0113 (17)

Geometric parameters (Å, °)

B1—O1	1.421 (4)	O13—H13A	0.8200
B1—O3	1.480 (4)	N1—C7	1.489 (5)
B1—O4	1.496 (4)	N1—H1A	0.8900
B1—O6	1.499 (4)	N1—H1B	0.8900
B2—O1	1.442 (4)	N1—H1C	0.8900
B2—O9	1.463 (4)	N2—C8	1.497 (4)
B2—O2	1.477 (4)	N2—H2A	0.8900
B2—O7	1.509 (4)	N2—H2B	0.8900
B3—O2	1.354 (4)	N2—H2C	0.8900
B3—O3	1.358 (4)	C1—C2	1.385 (5)
B3—O10	1.370 (4)	C1—C6	1.391 (5)
B4—O4	1.351 (4)	C1—C7	1.495 (5)
B4—O11	1.370 (4)	C2—C3	1.383 (5)
B4—O5	1.386 (4)	C2—H2D	0.9300
B5—O6	1.338 (4)	C3—C4	1.394 (5)
B5—O12	1.377 (4)	C3—C8	1.492 (5)
B5—O5	1.380 (4)	C4—C5	1.377 (6)
B6—O7	1.338 (4)	C4—H4A	0.9300
B6—O8	1.377 (4)	C5—C6	1.383 (5)
B6—O12^{i}	1.388 (4)	C5—H5A	0.9300
B7—O9	1.332 (4)	C6—H6A	0.9300
B7—O13	1.368 (4)	C7—H7A	0.9700
B7—O8	1.388 (4)	C7—H7B	0.9700
O10—H10A	0.8200	C8—H8A	0.9700
O11—H11A	0.8200	C8—H8B	0.9700
O12—B6^{i}	1.388 (4)		
O1—B1—O3	112.6 (3)	C7—N1—H1B	109.5
O1—B1—O4	109.6 (3)	H1A—N1—H1B	109.5

O3—B1—O4	107.5 (2)	C7—N1—H1C	109.5
O1—B1—O6	111.1 (3)	H1A—N1—H1C	109.5
O3—B1—O6	107.2 (3)	H1B—N1—H1C	109.5
O4—B1—O6	108.6 (2)	C8—N2—H2A	109.5
O1—B2—O9	108.6 (3)	C8—N2—H2B	109.5
O1—B2—O2	112.9 (2)	H2A—N2—H2B	109.5
O9—B2—O2	109.0 (3)	C8—N2—H2C	109.5
O1—B2—O7	110.2 (3)	H2A—N2—H2C	109.5
O9—B2—O7	110.1 (2)	H2B—N2—H2C	109.5
O2—B2—O7	105.9 (3)	C2—C1—C6	118.9 (3)
O2—B3—O3	121.8 (3)	C2—C1—C7	118.6 (3)
O2—B3—O10	122.5 (3)	C6—C1—C7	122.2 (3)
O3—B3—O10	115.7 (3)	C3—C2—C1	121.5 (3)
O4—B4—O11	120.4 (3)	C3—C2—H2D	119.2
O4—B4—O5	121.5 (3)	C1—C2—H2D	119.2
O11—B4—O5	118.1 (3)	C2—C3—C4	118.6 (3)
O6—B5—O12	124.5 (3)	C2—C3—C8	120.2 (3)
O6—B5—O5	121.6 (3)	C4—C3—C8	120.9 (3)
O12—B5—O5	113.8 (3)	C5—C4—C3	120.5 (3)
O7—B6—O8	122.9 (3)	C5—C4—H4A	119.8
O7—B6—O12^{i}	122.9 (3)	C3—C4—H4A	119.8
O8—B6—O12^{i}	114.2 (3)	C4—C5—C6	120.3 (4)
O9—B7—O13	120.9 (3)	C4—C5—H5A	119.8
O9—B7—O8	122.5 (3)	C6—C5—H5A	119.8
O13—B7—O8	116.6 (3)	C5—C6—C1	120.1 (3)
B1—O1—B2	123.5 (3)	C5—C6—H6A	120.0
B3—O2—B2	122.1 (3)	C1—C6—H6A	120.0
B3—O3—B1	121.8 (2)	N1—C7—C1	109.5 (3)
B4—O4—B1	119.7 (3)	N1—C7—H7A	109.8
B5—O5—B4	118.9 (2)	C1—C7—H7A	109.8
B5—O6—B1	120.7 (2)	N1—C7—H7B	109.8
B6—O7—B2	122.4 (2)	C1—C7—H7B	109.8
B6—O8—B7	117.6 (3)	H7A—C7—H7B	108.2
B7—O9—B2	124.2 (3)	C3—C8—N2	108.3 (3)
B3—O10—H10A	109.5	C3—C8—H8A	110.0
B4—O11—H11A	109.5	N2—C8—H8A	110.0
B5—O12—B6^{i}	132.5 (3)	C3—C8—H8B	110.0
B7—O13—H13A	109.5	N2—C8—H8B	110.0
C7—N1—H1A	109.5	H8A—C8—H8B	108.4

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O10—H10A···O2^{ii}	0.82	1.98	2.784 (2)	168
O11—H11A···O3^{iii}	0.82	1.84	2.659 (2)	179
O13—H13A···O11^{iv}	0.82	2.00	2.815 (2)	173
N1—H1A···O7	0.89	2.08	2.863 (2)	146

N1—H1B···O13^{v}	0.89	1.98	2.850 (2)	166
N1—H1C···O6^{i}	0.89	2.20	2.916 (2)	137
N1—H1C···O1^{i}	0.89	2.54	3.394 (2)	161
N2—H2A···O4^{vi}	0.89	1.97	2.822 (2)	159
N2—H2B···O1^{i}	0.89	1.99	2.877 (2)	173
N2—H2B···O9^{i}	0.89	2.55	3.052 (2)	116
N2—H2C···O12^{vii}	0.89	2.19	3.067 (2)	168

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

Fig. 1

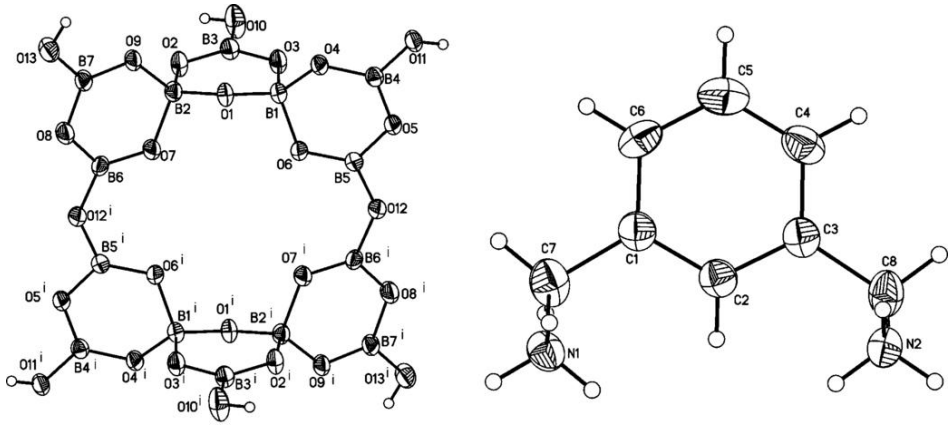
O10
B3
O13
B7
O9
O2
O3
O4
O11
B4
B2
O1
B1
O8
O7
O6
O5
B6
B5
O12
O12i
B5i
O6i
O7i
B6i
O5i
O8i
B1i
O1i
B2i
B7i
O11i
B4i
O4i
O3i
B3i
O2i
O9i
O13i
O10i
a
C5
C6
C4
C7
C1
C3
C8
C2
N1
N2
b

Fig. 2

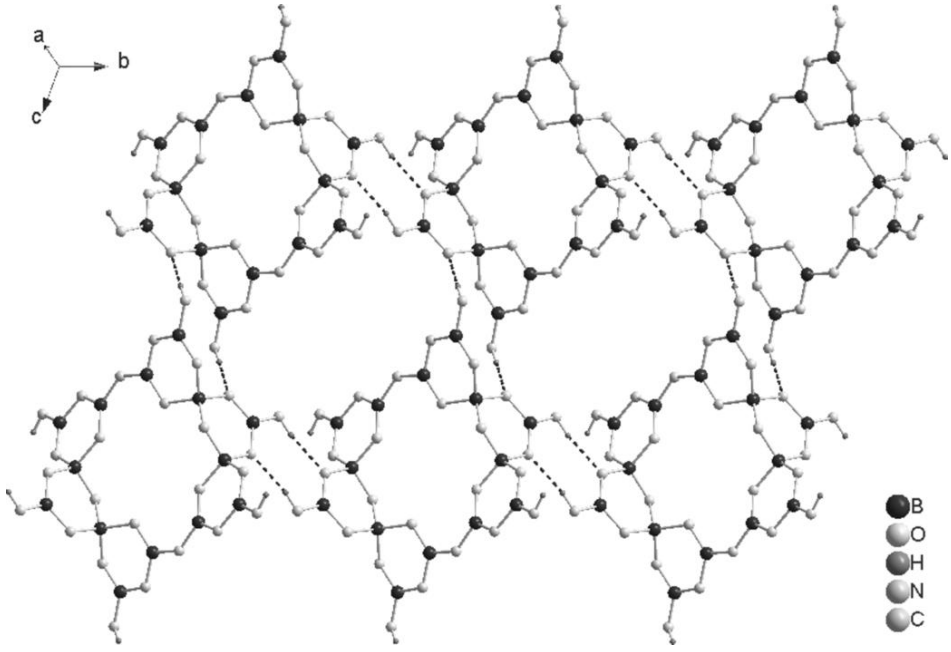

Fig. 3