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Hexamethylenetetraminium disalicylatoborate

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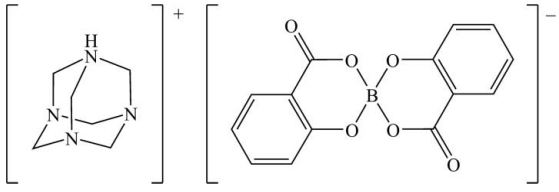
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.046; wR factor = 0.129; data-to-parameter ratio = 12.1.

The title compound, $C_6H_{13}N_4^+\cdot[B(C_7H_4O_3)_2]^-$, contains hexamethylenetetraminium cations and isolated disalicylatoborate anions. The coordination geometry around the B atom is tetrahedral and the dihedral angle between the planes of the benzene rings of the two salicylate ligands is 86.1 (1)°. In addition to electrostatic interactions between the cations and anions, N—H···O hydrogen bonds are formed between the NH group of the cation and the O atoms of one carboxylate group in the anion.

Related literature

For related literature, see: Barthel *et al.* (2000); Chen & Wu (1985); Downard *et al.* (2002); Green *et al.* (2000); Li & Liu (2006); Mori *et al.* (1995); Wu *et al.* (1993); Zhang *et al.* (2005).



Experimental

Crystal data

$C_6H_{13}N_4^+\cdot C_{14}H_8BO_6^-$
M_r = 424.22
Triclinic, $P\overline{1}$
a = 8.697 (4) Å
b = 10.164 (5) Å
c = 12.212 (6) Å
α = 71.111 (7)°
β = 72.765 (6)°
γ = 79.160 (7)°
V = 970.4 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 (2) K
0.41 × 0.29 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.957, T_{max} = 0.987
5112 measured reflections
3382 independent reflections
2132 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.129
S = 1.02
3382 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O5^{i}	0.91	1.91	2.778 (3)	160
N1—H1···O4^{i}	0.91	2.53	3.186 (3)	129

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2234).

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supplementary materials

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Hexamethylenetetraminium disalicylatoborate

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Comment

Inorganic borate compounds have been studied extensively since they can exhibit interesting physical properties, such as nonlinear optical behavior for $CsLiB_6O_{10}$ (Mori *et al.*,1995), CsB_3O_5 (Wu *et al.*,1993) and β-BaB_2O_4(Chen & Wu,1985). By contrast, studies of organic borates have been less extensive (Zhang *et al.*, 2005; Downard *et al.*, 2002; Green *et al.*, 2000, Li & Liu, 2006). To date, alkali-metal bis(salicylato)borates have received the most attention (Zhang *et al.*, 2005; Downard *et al.*, 2002), since lithium organoborates have been considered as electrolytes for lithium batteries (Barthel *et al.*, 2000). Herein, we report the synthesis and crystal structure of the salt of bis(salicylato)borate with the organic hexamethylenetetraminium cation.

The title compound is composed of $[C_6H_{13}N_4]^+$ cations and isolated $[B(C_7H_4O_3)_2]^-$ anions (Fig. 1). In the anion, the sp^3-hybridized B atom is bonded to four O atoms in a tetrahedral geometry, with B—O distances in the range 1.444 (4)–1.480 (4) Å and O—B—O angles in the range 105.7 (2)–113.7 (2)°. Each salicylato ligand is approximately planar, and the ring plaes lie almost perpendicular to each other (dihedral angle 86.1 (1) °). In addition to electrostatic interactions between the cations and anions, N—H···O hydrogen bonds are formed between the N—H group of the cation and the two O atoms of one carboxylate group in the anion.

Experimental

A solution of boric acid (0.337 g) in 5 ml distilled water was added to a stirred solution of salicylic acid (1.394 g) in 10 ml of a mixed ethanol/water (1:1) solvent. The reaction mixture was stirred at 353 K for 20 min, then hexamethylenetetramine (0.725 g) was added slowly. After 4 h continued heating and stirring, the pH of the mixture had changed from 2 to 6, and the clear solution was then allowed to stand for 15 days at room temperature. The title compound was isolated as colorless transparent crystals. Elemental anlalysis calculated: C 56.62, N 13.21, H 5.00%; found C 56.76, N 13.00, H 4.86%.

Refinement

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.97 Å or N—H = 0.91 Å, and with $U_{iso}(H) = 1.2U_{eq}(C/N)$.

Figures

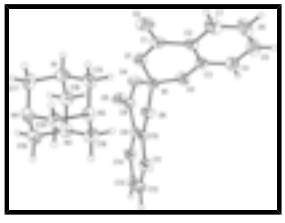


Fig. 1. The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level for non-H atoms.

Hexamethylenetetraminium disalicylatoborate

Crystal data

$C_6H_{13}N_4^+ \cdot C_{14}H_8B_1O_6^-$	$Z = 2$
$M_r = 424.22$	$F_{000} = 444$
Triclinic, $P\overline{1}$	$D_x = 1.452$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.697$ (4) Å	Cell parameters from 1460 reflections
$b = 10.164$ (5) Å	$\theta = 2.4$–23.4º
$c = 12.212$ (6) Å	$\mu = 0.11$ mm^{-1}
$\alpha = 71.111$ (7)º	$T = 298$ (2) K
$\beta = 72.765$ (6)º	Plate, colourless
$\gamma = 79.160$ (7)º	0.41 × 0.29 × 0.12 mm
$V = 970.4$ (8) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3382 independent reflections
Radiation source: fine-focus sealed tube	2132 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.016$
$T = 298$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Bruker, 1999)	$h = -10 \rightarrow 10$
$T_{min} = 0.957$, $T_{max} = 0.987$	$k = -12 \rightarrow 8$
5112 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.046$	H-atom parameters constrained
$wR(F^2) = 0.129$	$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 0.4284P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
3382 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
280 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
N1	0.6656 (3)	0.7669 (2)	0.5102 (2)	0.0535 (6)
H1	0.5596	0.7527	0.5443	0.064*
N2	0.8490 (3)	0.9067 (2)	0.34266 (18)	0.0470 (6)
N3	0.9283 (3)	0.6597 (2)	0.4279 (2)	0.0527 (6)
N4	0.9022 (3)	0.8249 (2)	0.53993 (19)	0.0492 (6)
O1	0.4850 (2)	0.6951 (2)	0.29242 (16)	0.0559 (5)
O2	0.3403 (2)	0.8933 (2)	0.3087 (2)	0.0759 (7)
O3	0.5212 (2)	0.6141 (2)	0.11880 (17)	0.0584 (5)
O4	0.5638 (2)	0.45922 (19)	0.30073 (17)	0.0566 (5)
O5	0.6526 (2)	0.2370 (2)	0.35252 (18)	0.0632 (6)
O6	0.7469 (2)	0.63698 (17)	0.18453 (16)	0.0481 (5)
B1	0.5799 (4)	0.6034 (3)	0.2206 (3)	0.0477 (8)
C1	0.3984 (3)	0.8123 (3)	0.2488 (3)	0.0515 (7)
C2	0.3747 (3)	0.8344 (3)	0.1294 (2)	0.0475 (7)
C3	0.4371 (3)	0.7340 (3)	0.0697 (2)	0.0466 (7)
C4	0.4102 (3)	0.7520 (3)	−0.0412 (3)	0.0609 (8)
H4	0.4525	0.6839	−0.0810	0.073*
C5	0.3218 (4)	0.8695 (4)	−0.0913 (3)	0.0793 (10)
H5	0.3034	0.8810	−0.1653	0.095*
C6	0.2594 (5)	0.9713 (4)	−0.0342 (4)	0.0895 (12)
H6	0.1995	1.0512	−0.0695	0.107*
C7	0.2856 (4)	0.9548 (3)	0.0761 (3)	0.0740 (9)
H7	0.2439	1.0239	0.1148	0.089*
C8	0.6813 (3)	0.3568 (3)	0.2937 (2)	0.0454 (6)
C9	0.8423 (3)	0.3944 (3)	0.2199 (2)	0.0387 (6)
C10	0.8691 (3)	0.5344 (3)	0.1716 (2)	0.0386 (6)
C11	1.0252 (3)	0.5703 (3)	0.1124 (2)	0.0451 (6)
H11	1.0449	0.6638	0.0825	0.054*
C12	1.1496 (3)	0.4677 (3)	0.0983 (2)	0.0494 (7)
H12	1.2537	0.4924	0.0586	0.059*
C13	1.1237 (3)	0.3283 (3)	0.1418 (2)	0.0512 (7)
H13	1.2090	0.2597	0.1297	0.061*
C14	0.9706 (3)	0.2917 (3)	0.2033 (2)	0.0466 (6)

H14	0.9525	0.1979	0.2340	0.056*
C15	0.6829 (3)	0.8848 (3)	0.3955 (2)	0.0543 (7)
H15A	0.6388	0.8623	0.3402	0.065*
H15B	0.6224	0.9697	0.4120	0.065*
C16	0.7608 (3)	0.6371 (3)	0.4823 (3)	0.0552 (7)
H16A	0.7519	0.5605	0.5554	0.066*
H16B	0.7169	0.6119	0.4284	0.066*
C17	0.7364 (4)	0.8026 (3)	0.5945 (2)	0.0602 (8)
H17A	0.6768	0.8864	0.6139	0.072*
H17B	0.7274	0.7269	0.6682	0.072*
C18	0.9388 (3)	0.7771 (3)	0.3193 (2)	0.0581 (8)
H18A	0.8966	0.7536	0.2636	0.070*
H18B	1.0516	0.7923	0.2819	0.070*
C19	0.9915 (4)	0.6990 (3)	0.5116 (3)	0.0616 (8)
H19A	0.9846	0.6228	0.5848	0.074*
H19B	1.1047	0.7142	0.4762	0.074*
C20	0.9137 (3)	0.9386 (3)	0.4284 (2)	0.0529 (7)
H20A	1.0262	0.9558	0.3923	0.063*
H20B	0.8544	1.0232	0.4463	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0462 (13)	0.0528 (14)	0.0587 (14)	−0.0155 (11)	−0.0064 (11)	−0.0128 (12)
N2	0.0548 (14)	0.0414 (13)	0.0469 (13)	−0.0137 (11)	−0.0184 (10)	−0.0054 (10)
N3	0.0558 (14)	0.0398 (13)	0.0622 (15)	−0.0049 (11)	−0.0133 (11)	−0.0152 (12)
N4	0.0609 (15)	0.0421 (13)	0.0519 (13)	−0.0069 (11)	−0.0258 (11)	−0.0118 (11)
O1	0.0525 (11)	0.0609 (13)	0.0593 (12)	0.0089 (10)	−0.0192 (9)	−0.0274 (10)
O2	0.0596 (13)	0.0812 (16)	0.0983 (16)	0.0059 (11)	−0.0110 (11)	−0.0560 (14)
O3	0.0576 (12)	0.0595 (13)	0.0687 (13)	0.0102 (10)	−0.0274 (10)	−0.0314 (11)
O4	0.0387 (10)	0.0484 (12)	0.0714 (13)	−0.0031 (9)	−0.0071 (9)	−0.0089 (10)
O5	0.0564 (12)	0.0436 (12)	0.0716 (13)	−0.0113 (9)	−0.0012 (10)	−0.0028 (10)
O6	0.0428 (10)	0.0386 (10)	0.0615 (11)	−0.0017 (8)	−0.0136 (8)	−0.0133 (9)
B1	0.0408 (17)	0.0463 (19)	0.0586 (19)	0.0062 (14)	−0.0179 (15)	−0.0194 (16)
C1	0.0338 (15)	0.0531 (18)	0.0683 (19)	−0.0066 (13)	−0.0033 (13)	−0.0260 (16)
C2	0.0363 (14)	0.0405 (16)	0.0623 (17)	−0.0061 (12)	−0.0107 (12)	−0.0106 (14)
C3	0.0369 (14)	0.0477 (17)	0.0543 (17)	−0.0115 (12)	−0.0118 (12)	−0.0091 (14)
C4	0.0569 (18)	0.067 (2)	0.0607 (19)	−0.0179 (16)	−0.0176 (15)	−0.0121 (16)
C5	0.085 (3)	0.076 (3)	0.072 (2)	−0.023 (2)	−0.0296 (19)	0.002 (2)
C6	0.089 (3)	0.065 (3)	0.096 (3)	−0.003 (2)	−0.044 (2)	0.018 (2)
C7	0.072 (2)	0.0458 (19)	0.096 (3)	−0.0008 (16)	−0.0225 (19)	−0.0111 (18)
C8	0.0453 (15)	0.0425 (16)	0.0464 (15)	−0.0067 (13)	−0.0117 (12)	−0.0085 (13)
C9	0.0399 (14)	0.0406 (15)	0.0339 (13)	−0.0042 (11)	−0.0094 (11)	−0.0082 (11)
C10	0.0403 (14)	0.0413 (15)	0.0361 (13)	−0.0035 (11)	−0.0128 (11)	−0.0110 (12)
C11	0.0509 (16)	0.0434 (15)	0.0425 (14)	−0.0133 (13)	−0.0071 (12)	−0.0138 (12)
C12	0.0410 (15)	0.0607 (19)	0.0465 (15)	−0.0104 (13)	−0.0026 (12)	−0.0200 (14)
C13	0.0451 (16)	0.0522 (18)	0.0523 (16)	0.0035 (13)	−0.0082 (13)	−0.0182 (14)
C14	0.0525 (17)	0.0382 (15)	0.0449 (15)	−0.0039 (13)	−0.0123 (13)	−0.0066 (12)

C15	0.0504 (17)	0.0540 (18)	0.0580 (17)	−0.0048 (13)	−0.0236 (14)	−0.0065 (15)
C16	0.0667 (19)	0.0416 (16)	0.0596 (17)	−0.0136 (14)	−0.0147 (14)	−0.0141 (14)
C17	0.074 (2)	0.062 (2)	0.0469 (16)	−0.0067 (16)	−0.0154 (15)	−0.0184 (15)
C18	0.0597 (18)	0.0584 (19)	0.0549 (17)	−0.0112 (15)	−0.0038 (14)	−0.0211 (15)
C19	0.0613 (19)	0.0535 (19)	0.071 (2)	0.0036 (15)	−0.0311 (16)	−0.0114 (16)
C20	0.0615 (18)	0.0426 (16)	0.0614 (17)	−0.0148 (13)	−0.0249 (14)	−0.0102 (14)

Geometric parameters (Å, °)

N1—C16	1.502 (3)	C5—C6	1.372 (5)
N1—C17	1.507 (3)	C5—H5	0.930
N1—C15	1.510 (3)	C6—C7	1.384 (5)
N1—H1	0.910	C6—H6	0.930
N2—C15	1.424 (3)	C7—H7	0.930
N2—C18	1.467 (3)	C8—C9	1.466 (3)
N2—C20	1.468 (3)	C9—C10	1.388 (3)
N3—C16	1.439 (3)	C9—C14	1.393 (3)
N3—C18	1.461 (3)	C10—C11	1.391 (3)
N3—C19	1.479 (3)	C11—C12	1.367 (3)
N4—C17	1.425 (3)	C11—H11	0.930
N4—C19	1.454 (3)	C12—C13	1.379 (4)
N4—C20	1.464 (3)	C12—H12	0.930
O1—C1	1.326 (3)	C13—C14	1.374 (4)
O1—B1	1.460 (3)	C13—H13	0.930
O2—C1	1.217 (3)	C14—H14	0.930
O3—C3	1.353 (3)	C15—H15A	0.970
O3—B1	1.444 (4)	C15—H15B	0.970
O4—C8	1.320 (3)	C16—H16A	0.970
O4—B1	1.480 (4)	C16—H16B	0.970
O5—C8	1.226 (3)	C17—H17A	0.970
O6—C10	1.354 (3)	C17—H17B	0.970
O6—B1	1.460 (3)	C18—H18A	0.970
C1—C2	1.473 (4)	C18—H18B	0.970
C2—C3	1.380 (4)	C19—H19A	0.970
C2—C7	1.395 (4)	C19—H19B	0.970
C3—C4	1.390 (4)	C20—H20A	0.970
C4—C5	1.361 (4)	C20—H20B	0.970
C4—H4	0.930		
C16—N1—C17	108.2 (2)	O6—C10—C9	121.3 (2)
C16—N1—C15	108.6 (2)	O6—C10—C11	119.2 (2)
C17—N1—C15	109.0 (2)	C9—C10—C11	119.5 (2)
C16—N1—H1	110.4	C12—C11—C10	119.7 (2)
C17—N1—H1	110.4	C12—C11—H11	120.1
C15—N1—H1	110.4	C10—C11—H11	120.1
C15—N2—C18	108.9 (2)	C11—C12—C13	121.3 (2)
C15—N2—C20	108.7 (2)	C11—C12—H12	119.3
C18—N2—C20	107.8 (2)	C13—C12—H12	119.3
C16—N3—C18	108.7 (2)	C14—C13—C12	119.3 (3)
C16—N3—C19	108.4 (2)	C14—C13—H13	120.4

C18—N3—C19	107.9 (2)	C12—C13—H13	120.4
C17—N4—C19	109.7 (2)	C13—C14—C9	120.4 (2)
C17—N4—C20	109.0 (2)	C13—C14—H14	119.8
C19—N4—C20	108.4 (2)	C9—C14—H14	119.8
C1—O1—B1	123.2 (2)	N2—C15—N1	110.1 (2)
C3—O3—B1	119.7 (2)	N2—C15—H15A	109.6
C8—O4—B1	122.7 (2)	N1—C15—H15A	109.6
C10—O6—B1	119.2 (2)	N2—C15—H15B	109.6
O3—B1—O6	111.8 (2)	N1—C15—H15B	109.6
O3—B1—O1	113.7 (2)	H15A—C15—H15B	108.1
O6—B1—O1	106.8 (2)	N3—C16—N1	110.4 (2)
O3—B1—O4	107.4 (2)	N3—C16—H16A	109.6
O6—B1—O4	111.4 (2)	N1—C16—H16A	109.6
O1—B1—O4	105.7 (2)	N3—C16—H16B	109.6
O2—C1—O1	119.7 (3)	N1—C16—H16B	109.6
O2—C1—C2	123.6 (3)	H16A—C16—H16B	108.1
O1—C1—C2	116.7 (2)	N4—C17—N1	109.7 (2)
C3—C2—C7	119.0 (3)	N4—C17—H17A	109.7
C3—C2—C1	120.2 (2)	N1—C17—H17A	109.7
C7—C2—C1	120.8 (3)	N4—C17—H17B	109.7
O3—C3—C2	121.1 (2)	N1—C17—H17B	109.7
O3—C3—C4	118.3 (3)	H17A—C17—H17B	108.2
C2—C3—C4	120.5 (3)	N3—C18—N2	112.8 (2)
C5—C4—C3	119.8 (3)	N3—C18—H18A	109.0
C5—C4—H4	120.1	N2—C18—H18A	109.0
C3—C4—H4	120.1	N3—C18—H18B	109.0
C4—C5—C6	120.9 (3)	N2—C18—H18B	109.0
C4—C5—H5	119.6	H18A—C18—H18B	107.8
C6—C5—H5	119.6	N4—C19—N3	111.9 (2)
C5—C6—C7	119.9 (3)	N4—C19—H19A	109.2
C5—C6—H6	120.0	N3—C19—H19A	109.2
C7—C6—H6	120.0	N4—C19—H19B	109.2
C6—C7—C2	120.0 (3)	N3—C19—H19B	109.2
C6—C7—H7	120.0	H19A—C19—H19B	107.9
C2—C7—H7	120.0	N4—C20—N2	112.3 (2)
O5—C8—O4	118.9 (2)	N4—C20—H20A	109.1
O5—C8—C9	123.5 (2)	N2—C20—H20A	109.1
O4—C8—C9	117.6 (2)	N4—C20—H20B	109.1
C10—C9—C14	119.6 (2)	N2—C20—H20B	109.1
C10—C9—C8	119.3 (2)	H20A—C20—H20B	107.9
C14—C9—C8	120.9 (2)		
C3—O3—B1—O6	−94.9 (3)	B1—O6—C10—C9	−16.5 (3)
C3—O3—B1—O1	26.1 (3)	B1—O6—C10—C11	165.7 (2)
C3—O3—B1—O4	142.7 (2)	C14—C9—C10—O6	179.1 (2)
C10—O6—B1—O3	−87.8 (3)	C8—C9—C10—O6	−4.6 (3)
C10—O6—B1—O1	147.3 (2)	C14—C9—C10—C11	−3.2 (3)
C10—O6—B1—O4	32.4 (3)	C8—C9—C10—C11	173.2 (2)
C1—O1—B1—O3	−25.2 (4)	O6—C10—C11—C12	−179.7 (2)
C1—O1—B1—O6	98.5 (3)	C9—C10—C11—C12	2.5 (4)

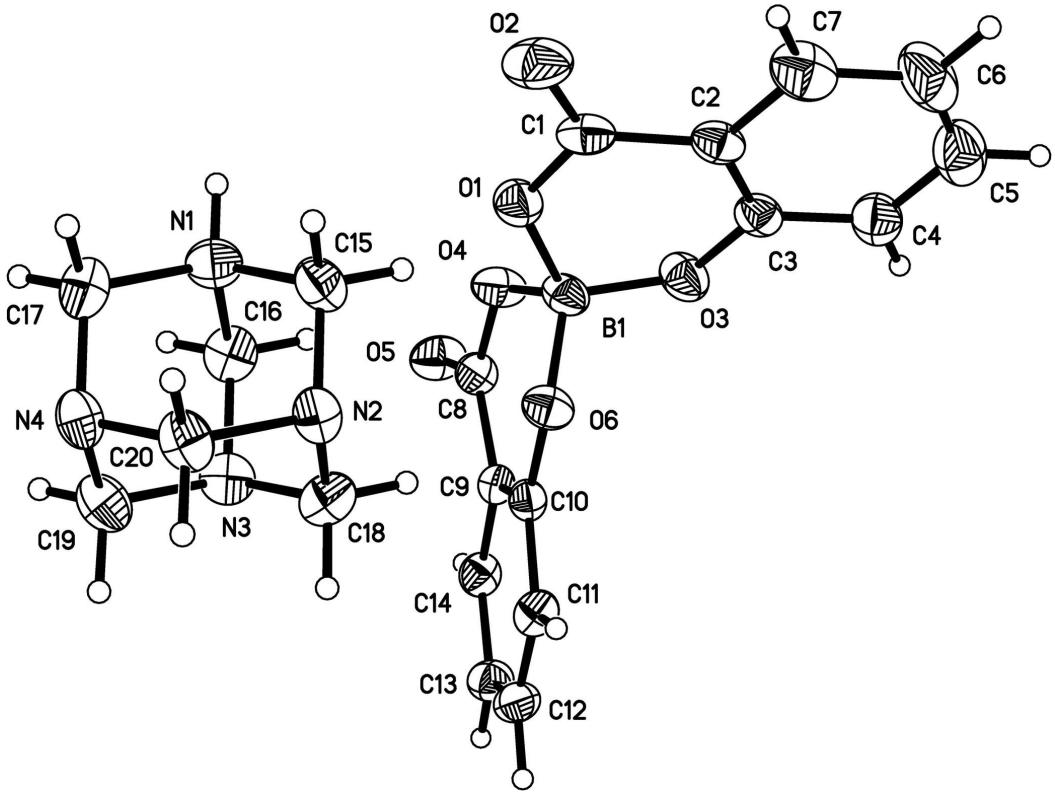
C1—O1—B1—O4	−142.8 (2)	C10—C11—C12—C13	0.0 (4)
C8—O4—B1—O3	91.8 (3)	C11—C12—C13—C14	−1.7 (4)
C8—O4—B1—O6	−30.9 (3)	C12—C13—C14—C9	1.0 (4)
C8—O4—B1—O1	−146.5 (2)	C10—C9—C14—C13	1.4 (4)
B1—O1—C1—O2	−170.0 (2)	C8—C9—C14—C13	−174.8 (2)
B1—O1—C1—C2	11.6 (4)	C18—N2—C15—N1	58.8 (3)
O2—C1—C2—C3	−176.4 (2)	C20—N2—C15—N1	−58.5 (3)
O1—C1—C2—C3	1.9 (3)	C16—N1—C15—N2	−59.0 (3)
O2—C1—C2—C7	1.9 (4)	C17—N1—C15—N2	58.6 (3)
O1—C1—C2—C7	−179.8 (2)	C18—N3—C16—N1	−58.2 (3)
B1—O3—C3—C2	−14.7 (4)	C19—N3—C16—N1	58.8 (3)
B1—O3—C3—C4	167.4 (2)	C17—N1—C16—N3	−59.5 (3)
C7—C2—C3—O3	−178.5 (2)	C15—N1—C16—N3	58.6 (3)
C1—C2—C3—O3	−0.2 (4)	C19—N4—C17—N1	−59.7 (3)
C7—C2—C3—C4	−0.6 (4)	C20—N4—C17—N1	58.9 (3)
C1—C2—C3—C4	177.7 (2)	C16—N1—C17—N4	59.3 (3)
O3—C3—C4—C5	178.0 (3)	C15—N1—C17—N4	−58.5 (3)
C2—C3—C4—C5	0.0 (4)	C16—N3—C18—N2	59.2 (3)
C3—C4—C5—C6	0.4 (5)	C19—N3—C18—N2	−58.1 (3)
C4—C5—C6—C7	−0.2 (5)	C15—N2—C18—N3	−59.9 (3)
C5—C6—C7—C2	−0.3 (5)	C20—N2—C18—N3	57.9 (3)
C3—C2—C7—C6	0.8 (4)	C17—N4—C19—N3	60.2 (3)
C1—C2—C7—C6	−177.5 (3)	C20—N4—C19—N3	−58.8 (3)
B1—O4—C8—O5	−170.9 (2)	C16—N3—C19—N4	−59.2 (3)
B1—O4—C8—C9	12.1 (4)	C18—N3—C19—N4	58.3 (3)
O5—C8—C9—C10	−169.9 (2)	C17—N4—C20—N2	−60.5 (3)
O4—C8—C9—C10	6.9 (3)	C19—N4—C20—N2	58.8 (3)
O5—C8—C9—C14	6.4 (4)	C15—N2—C20—N4	60.1 (3)
O4—C8—C9—C14	−176.8 (2)	C18—N2—C20—N4	−57.7 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O5^{i}	0.91	1.91	2.778 (3)	160
N1—H1···O4^{i}	0.91	2.53	3.186 (3)	129

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

Fig. 1


O2
C7
C6
C2
C1
C5
O1
N1
C15
C4
O4
C3
C17
C16
B1
O3
O5
C8
N4
N2
O6
C20
C9
C10
N3
C18
C19
C14
C11
C13
C12