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3*H*-2,1-Benzoxaborole-1-spiro-4′-(5-oxa-3a-aza-4-borapyrene)

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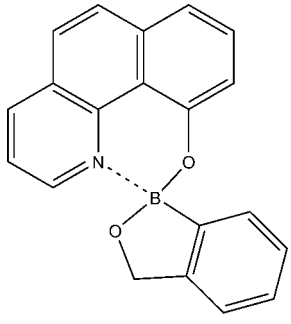
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.008 Å; R factor = 0.068; wR factor = 0.093; data-to-parameter ratio = 8.2.

In the title compound, $C_{20}H_{14}BNO_2$, the B atom has a tetrahedral geometry with two short B—O and two long B—C and B—N bonds, revealing a significant difference between C_{ar}—O—B and C_{alkyl}—O—B bond distances. Intermolecular Ar—H···O hydrogen bonds and strong π–π interactions (3.368 Å) between aromatic cores of neighbouring molecules result in hexagonal channels along the crystallographic c axis, which are potentially accessible for small molecules.

Related literature

For the general synthesis and applications of benzoboroxoles, see: Nicolaou *et al.* (1998, 1999); Tan *et al.* (2001); Benkovic *et al.* (2005); Baker *et al.* (2006); Alexander *et al.* (1999). For the crystal structures of benzoboroxoles, see: Tan *et al.* (2001); Sporzynski *et al.* (2005); Coghlan *et al.* (2005); Arcus *et al.* (1993); Murafuji *et al.* (1999); Zhdankin *et al.* (1999); Yamamoto *et al.* (2005); Gunasekera *et al.* (2007).

For related literature, see: Allen (2002); Prince (1982); Watkin (1994).



Experimental

Crystal data

$C_{20}H_{14}BNO_2$
M_r = 311.13
Trigonal, $R\overline{3}$
a = 33.079 (5) Å
c = 7.358 (5) Å
V = 6973 (5) Å^3
Z = 18
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 K
0.58 × 0.12 × 0.07 mm

Data collection

Rigaku AFC-7*R* diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.96, T_{max} = 0.99
3564 measured reflections
3564 independent reflections
1558 reflections with $I > 2.0\sigma(I)$
3 standard reflections
every 150 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.093
S = 1.07
1779 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected bond lengths (Å).

B1—O2	1.479 (6)	B1—O1	1.432 (6)
B1—N1	1.646 (6)	B1—C1	1.602 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H16···O2^{i}	0.93	2.59	3.490 (8)	163

Symmetry code: (i) $x-y+\frac{1}{3}, x-\frac{1}{3}, -z+\frac{2}{3}$.

Data collection: *AFC-7R Diffractometer Control Software* (Rigaku/MSC, 1997); cell refinement: *WinAFC* (Rigaku/MSC, 2000); data reduction: *TEXSAN* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *CRYSTALS*.

Generous support from the Department of Chemistry and Biochemistry, University of Minnesota Duluth, is greatly appreciated. X-ray data were collected at the University of Minnesota Duluth X-ray crystallography facility.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EM2005).

References

Alexander, C., Smith, C. R., Whitcombe, M. J. & Vulfson, E. N. (1999). *J. Am. Chem. Soc.* **121**, 6640–6651.
Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Altomare, A., Cascarano, G., Giacovazzo, G., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Arcus, V. L., Main, L. & Nicholson, B. K. (1993). *J. Organomet. Chem.* **460**, 139–147.

  doi:10.1107/S1600536807066731

Baker, S. J., Zhang, Y. K., Akama, T., Lau, A., Zhou, H., Hernandez, V., Mao, W., Alley, M. R. K., Sanders, V. & Plattner, J. J. (2006). *J. Med. Chem.* **49**, 4447–4450.
Benkovic, S. J., Baker, S. J., Alley, M. R. K., Woo, Y. H., Zhang, Y. K., Akama, T., Mao, W., Baboval, J., Rajagopalan, P. T. R., Wall, M., Kahng, L. S., Tavassoli, A. & Shapiro, L. (2005). *J. Med. Chem.* **48**, 7468–7476.
Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
Coghlan, S. W., Giles, R. L., Howard, J. A. K., Patrick, L. G. F., Probert, M. R., Smith, G. E. & Whiting, A. (2005). *J. Organomet. Chem.* **690**, 4784–4794.
Gunasekera, D. S., Gerold, D. J., Aalderks, N. S., Chandra, J. S., Maanu, C. A., Kiprof, P., Zhdankin, V. V. & Reddy, M. V. R. (2007). *Tetrahedron*, **63**, 9401–9405.
Murafuji, T., Sugihara, Y., Moriya, T., Mikata, Y. & Yano, S. (1999). *New J. Chem.* **23**, 683–685.
Nicolaou, K. C., Li, H., Boody, C. N. C., Ramanjulu, J. M., Yue, T. Y., Natarajan, S., Chu, X. J., Brase, S. & Rubsam, F. (1999). *Chem. Eur. J.* **5**, 2584–2601.
Nicolaou, K. C., Natarajan, S., Li, H., Jain, N. F., Hughes, R., Solomon, M. E., Ramanjulu, J. M., Boddy, C. N. C. & Takayanagi, M. (1998). *Angew. Chem. Int. Ed.* **37**, 2708–2714.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Prince, E. (1982). *Mathematical Techniques in Crystallography and Materials Science*. New York: Springer-Verlag.
Rigaku/MSC (1997). *AFC-7R Diffractometer Control Software*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Rigaku/MSC (2000). *WinAFC*. Version 1.0.2. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Rigaku/MSC (2004). *TEXSAN*. Version 10.3b. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sporzynski, A., Lewandowski, R., Rogowska, P. & Cyranski, M. K. (2005). *Appl. Organomet. Chem.* **19**, 1202–1203.
Tan, Y. L., White, A. J. P., Widdowson, D. A., Wilhelm, R. & Williams, D. J. (2001). *J. Chem. Soc. Perkin Trans. 1*, pp. 3269–3280.
Watkin, D. (1994). *Acta Cryst.* A**50**, 411–437.
Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.
Yamamoto, Y., Ishii, J., Nishiyama, H. & Itoh, K. (2005). *J. Am. Chem. Soc.* **127**, 9625–9631.
Zhdankin, V. V., Persichini, P. J. III, Zhang, L., Fix, S. & Kiprof, P. (1999). *Tetrahedron Lett.* **40**, 6705–6708.

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S1. Comment

Benzoboroxoles are useful synthons for cross-coupling reactions (Nicolaou *et al.*, 1998; Nicolaou *et al.*, 1999; Tan *et al.*, 2001) and are utilized in a wide variety of applications in medicinal (Benkovic *et al.*, 2005; Baker *et al.*, 2006) and materials (Alexander *et al.*, 1999) chemistry.

The number of known structures of boroxoles and their adducts with a tetrahedral boron atom is very small (CSD 2007; Tan *et al.* 2001; Sporzynski *et al.*, 2005; Coghlan *et al.*, 2005; Arcus *et al.*, 1993; Murafuji *et al.*, 1999; Zhdankin *et al.*, 1999; Yamamoto *et al.*, 2005; Gunasekera *et al.*, 2007). 10-(benzo[*c*][1,2]oxaborol-1(*3H*)-yloxy)benzo[*h*]quinoline, **I**, (Fig. 1) is the first known structure of a boroxole derivative in which the boron atom is coordinated to two oxygen, one carbon, and one nitrogen atoms and has a tetrahedral geometry. The B1—O1 and B1—O2 distances, in spite of their similar nature, are quite different (Table 1) and, probably reflect the difference in the electron density on the phenolic and benzylic type oxygen atoms. The B1—C1 and B1—N1 bond distances are significantly longer than boron-oxygen bond distances with B1—N1 being the longest.

The molecules of **I** are linked together into two-dimensional polymeric units by weak C(ar)—H···O hydrogen bonds (Table 2) formed between the H16 aryl hydrogen atom and the phenolic oxygen O2 of a neighboring molecule at (*x*-*y* + *1/3, x* - *1/3, -z* + *2/3*), generated by a translation along threefold screw axis (Fig. 2). This two-dimensional polymeric chain forms small hexagonal channels oriented along the *c* axis.The hexagonal channels are further stabilized by strongπ-π interactions between molecules related by inversion with the shortest C···C contacts being between C10 and C20^{ii} (3.368 Å; symmetry operator ii = 1 - *x*, 1 - *y*, 1 - *z*).

S2. Experimental

The title compound was prepared by the reaction between equivalent amounts of benzoboroxole and 10-hydroxy-benzo[*h*]quinoline in dry hexane under an argon atmosphere. Crystals suitable for X-ray analysis were grown by slow diffusion of pentane into a methylenechloride solution of **I**. Selected data for title compound: Analysis calculated for $C_{20}H_{14}BNO_2$; C, 77.20%; H, 4.54%; N, 4.5%. Found C, 73.41%; H, 4.59%; N, 4.19% (Note: %C found is low because of the formation of highly stable boron carbide during the combustion process). ^{1}H NMR ($CDCl_3$): δ 5.2 (d, 2H), 5.3 (d, 2H). ^{11}B NMR ($CDCl_3$): δ 11.14. ^{13}C NMR ($CDCl_3$) δ 159, 155.9, 148.8, 42.3, 139.6, 134.5, 132.8, 130.6, 128.4, 127.8, 126.5, 123.4, 121.5, 120.8, 117.9, 116.9, 72.3. A bsorption λ_{max} = 248, 303, and 413 nm.

S3. Refinement

In the absence of significant anomalous scattering, Friedel pairs were merged. All H atoms were placed in calculated positions with C—H distances of 0.93 (aromatic) and 0.98 Å (alkyl). All hydrogen atoms were refined with U_{iso}(H) = 1.3U_{eq} of their respective carrier atom using riding constraints.

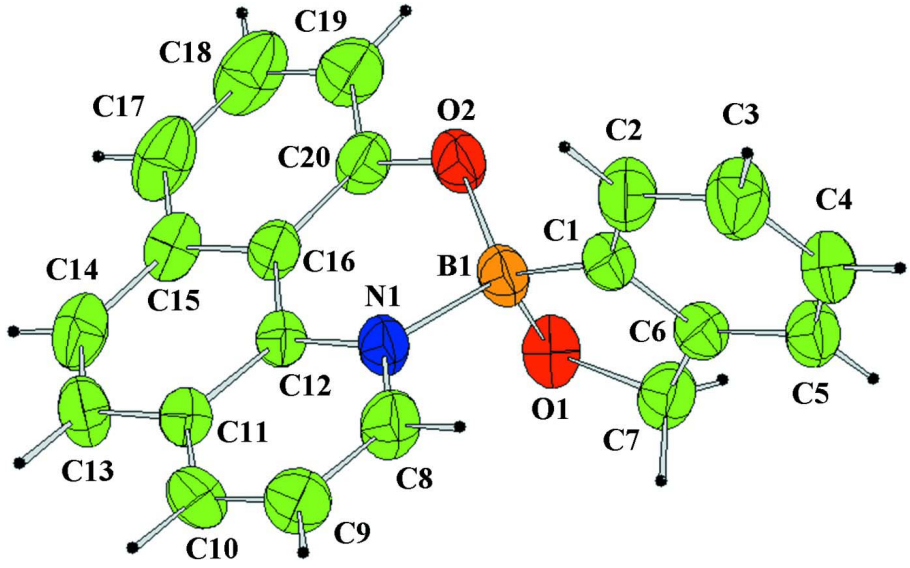

Figure 1

The title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitary radius.

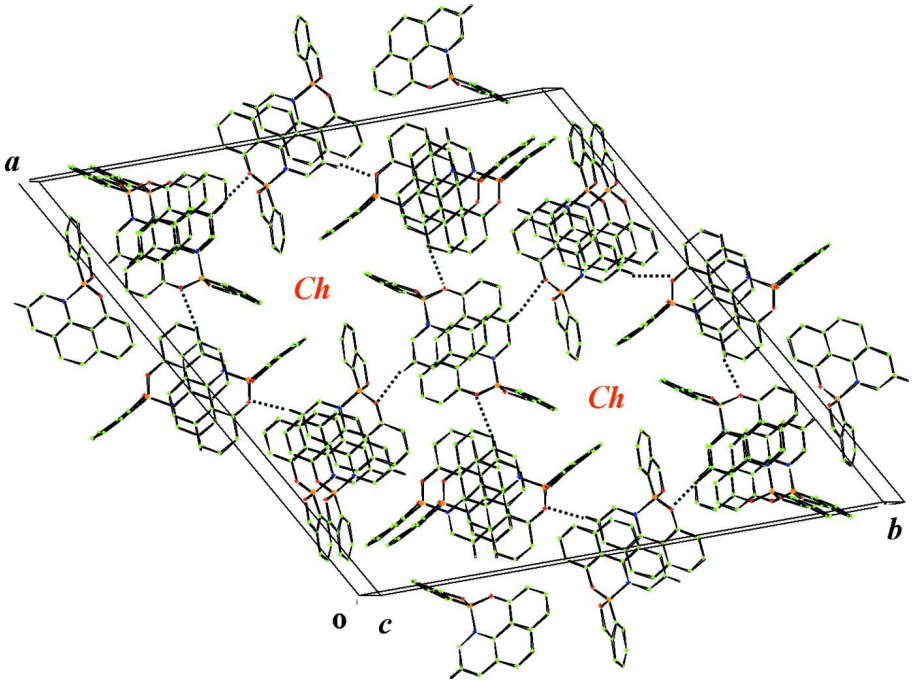

Figure 2

Unit cell representation showing the small hexagonal channels along *c* axis. Hexagonal channels are labeled in red with 'Ch'.

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Crystal data

$C_{20}H_{14}BNO_2$
$M_r = 311.13$
Trigonal, $R\bar{3}$
Hall symbol: -R 3
$a = 33.079$ (5) Å
$c = 7.358$ (5) Å
$V = 6973$ (5) Å^3
$Z = 18$
$F(000) = 2916$
$D_x = 1.334$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 15$–18°
$\mu = 0.09$ mm^{-1}
$T = 295$ K
Needle, yellow
0.58 × 0.12 × 0.07 mm

Data collection

Serial diffractometer
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.96$, $T_{max} = 0.99$
3564 measured reflections
3564 independent reflections
1558 reflections with $I > 2.0\sigma(I)$
$R_{int} = 0.000$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.9°$
$h = 0 \rightarrow 42$
$k = -36 \rightarrow 36$
$l = 0 \rightarrow 9$
3 standard reflections every 150 reflections
intensity decay: 0.0%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.093$
$S = 1.07$
1779 reflections
218 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
Method, part 1, Chebychev polynomial, (Watkin, 1994, *P*rince, 1982) [*w*eight] = 1.0/[A_0*T_0(x) + A_1*T_1(x) ··· + A_{n-1}]*T_{n-1}(x)] where A_i are the Chebychev coefficients listed below and x = *F* /*F*max Method = Robust Weighting (*P*rince, 1982) W = [*w*eight] * [1-(delta*F*/6*sigma*F*)^2]^2 A_i are: 6.52 6.79 1.78
$(\Delta/\sigma)_{max} = 0.000267$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
Extinction correction: Larson (1970), Equation 22
Extinction coefficient: 269 (15)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
B1	0.60386 (17)	0.50314 (19)	0.3431 (8)	0.0461
N1	0.54645 (12)	0.47492 (12)	0.3338 (5)	0.0441
O1	0.61889 (10)	0.50681 (11)	0.1583 (4)	0.0556
O2	0.61678 (10)	0.54880 (11)	0.4258 (5)	0.0557
C1	0.62617 (15)	0.47612 (16)	0.4450 (7)	0.0470
C2	0.62919 (18)	0.46446 (19)	0.6229 (7)	0.0641
C3	0.65528 (19)	0.4431 (2)	0.6641 (8)	0.0738
C4	0.67847 (17)	0.43392 (18)	0.5313 (8)	0.0612
C5	0.67633 (15)	0.44539 (16)	0.3534 (7)	0.0536
C6	0.64948 (15)	0.46632 (15)	0.3118 (7)	0.0453

C7	0.64298 (16)	0.48142 (17)	0.1297 (7)	0.0549
C8	0.52178 (17)	0.42836 (16)	0.3387 (7)	0.0556
C9	0.47493 (17)	0.40339 (17)	0.2966 (7)	0.0615
C10	0.45304 (16)	0.42688 (17)	0.2430 (7)	0.0568
C11	0.47733 (16)	0.47560 (17)	0.2342 (7)	0.0465
C12	0.52458 (15)	0.49909 (15)	0.2852 (6)	0.0420
C13	0.45737 (18)	0.5029 (2)	0.1721 (7)	0.0611
C14	0.48327 (19)	0.5502 (2)	0.1649 (7)	0.0603
C15	0.53031 (18)	0.57485 (17)	0.2257 (7)	0.0524
C16	0.55138 (15)	0.54933 (15)	0.2865 (6)	0.0441
C17	0.5559 (2)	0.62379 (19)	0.2316 (8)	0.0699
C18	0.5997 (2)	0.64575 (19)	0.3060 (9)	0.0767
C19	0.62077 (18)	0.62144 (17)	0.3711 (8)	0.0655
C20	0.59680 (16)	0.57271 (16)	0.3584 (7)	0.0492
H11	0.6135	0.4706	0.7139	0.0862*
H12	0.6569	0.4352	0.7841	0.1024*
H13	0.6955	0.4194	0.5614	0.0794*
H14	0.6922	0.4396	0.2624	0.0612*
H15	0.5372	0.4125	0.3718	0.0623*
H16	0.4586	0.3710	0.3045	0.0698*
H17	0.4215	0.4107	0.2128	0.0625*
H71	0.6732	0.5015	0.0712	0.0750*
H72	0.6242	0.4541	0.0528	0.0750*
H131	0.4263	0.4879	0.1352	0.0773*
H141	0.4698	0.5669	0.1193	0.0818*
H171	0.5430	0.6412	0.1877	0.0923*
H181	0.6162	0.6782	0.3100	0.0853*
H191	0.6501	0.6370	0.4249	0.0712*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
B1	0.033 (3)	0.048 (3)	0.056 (4)	0.020 (3)	0.000 (3)	0.000 (3)
N1	0.033 (2)	0.039 (2)	0.060 (3)	0.0174 (18)	0.0013 (19)	−0.0006 (19)
O1	0.049 (2)	0.060 (2)	0.063 (2)	0.0316 (19)	0.0060 (18)	0.0093 (18)
O2	0.0365 (18)	0.046 (2)	0.083 (3)	0.0192 (16)	−0.0066 (17)	−0.0093 (18)
C1	0.034 (3)	0.048 (3)	0.057 (3)	0.019 (2)	−0.002 (2)	−0.007 (2)
C2	0.060 (3)	0.086 (4)	0.061 (4)	0.048 (3)	0.000 (3)	0.000 (3)
C3	0.077 (4)	0.105 (5)	0.063 (4)	0.062 (4)	−0.002 (3)	0.007 (3)
C4	0.053 (3)	0.072 (4)	0.071 (4)	0.041 (3)	−0.006 (3)	−0.002 (3)
C5	0.039 (3)	0.054 (3)	0.068 (4)	0.024 (3)	0.004 (3)	−0.002 (3)
C6	0.035 (3)	0.042 (3)	0.054 (3)	0.016 (2)	0.002 (2)	−0.004 (2)
C7	0.050 (3)	0.056 (3)	0.063 (4)	0.030 (3)	0.009 (3)	−0.001 (3)
C8	0.048 (3)	0.038 (3)	0.080 (4)	0.022 (2)	0.006 (3)	0.003 (3)
C9	0.047 (3)	0.041 (3)	0.084 (4)	0.012 (3)	0.004 (3)	−0.007 (3)
C10	0.034 (3)	0.055 (3)	0.069 (4)	0.013 (3)	−0.003 (3)	−0.010 (3)
C11	0.039 (3)	0.051 (3)	0.051 (3)	0.024 (2)	0.001 (2)	−0.006 (2)
C12	0.036 (3)	0.044 (3)	0.048 (3)	0.021 (2)	0.001 (2)	−0.004 (2)

C13	0.045 (3)	0.081 (4)	0.067 (4)	0.039 (3)	−0.005 (3)	−0.005 (3)
C14	0.068 (4)	0.072 (4)	0.063 (4)	0.052 (3)	0.007 (3)	0.007 (3)
C15	0.056 (3)	0.056 (3)	0.055 (3)	0.036 (3)	0.010 (3)	0.005 (3)
C16	0.040 (3)	0.040 (3)	0.055 (3)	0.021 (2)	0.006 (2)	−0.002 (2)
C17	0.079 (4)	0.054 (4)	0.093 (5)	0.045 (3)	0.023 (4)	0.015 (3)
C18	0.081 (4)	0.041 (3)	0.110 (5)	0.032 (3)	0.031 (4)	0.010 (3)
C19	0.048 (3)	0.043 (3)	0.092 (5)	0.013 (3)	0.014 (3)	−0.009 (3)
C20	0.043 (3)	0.040 (3)	0.065 (3)	0.022 (2)	0.007 (2)	−0.004 (2)

Geometric parameters (Å, º)

O2—C20	1.354 (5)	C3—H12	0.930
B1—O2	1.479 (6)	C4—C5	1.374 (7)
C20—C16	1.405 (6)	C4—H13	0.930
C20—C19	1.399 (6)	C5—H14	0.930
C16—C12	1.440 (6)	C8—C9	1.378 (6)
C16—C15	1.410 (6)	C8—H15	0.930
C12—N1	1.367 (5)	C9—C10	1.359 (6)
C12—C11	1.405 (6)	C9—H16	0.930
B1—N1	1.646 (6)	C10—C11	1.397 (6)
N1—C8	1.335 (5)	C10—H17	0.930
B1—O1	1.432 (6)	C11—C13	1.434 (6)
B1—C1	1.602 (7)	C13—C14	1.358 (7)
O1—C7	1.433 (5)	C13—H131	0.930
C7—C6	1.482 (6)	C14—C15	1.420 (7)
C7—H71	0.980	C14—H141	0.930
C7—H72	0.980	C15—C17	1.403 (7)
C6—C1	1.382 (6)	C17—C18	1.368 (7)
C6—C5	1.406 (6)	C17—H171	0.930
C1—C2	1.382 (6)	C18—C19	1.387 (7)
C2—C3	1.396 (7)	C18—H181	0.930
C2—H11	0.930	C19—H191	0.930
C3—C4	1.366 (7)		

C20—O2—B1	118.0 (4)	C4—C3—H12	120.0
O2—C20—C16	121.1 (4)	C3—C4—C5	120.5 (5)
O2—C20—C19	119.2 (5)	C3—C4—H13	119.7
C16—C20—C19	119.6 (5)	C5—C4—H13	119.8
C20—C16—C12	120.6 (4)	C6—C5—C4	118.4 (5)
C20—C16—C15	120.2 (4)	C6—C5—H14	120.5
C12—C16—C15	119.1 (4)	C4—C5—H14	121.1
C16—C12—N1	118.2 (4)	N1—C8—C9	122.8 (5)
C16—C12—C11	120.8 (4)	N1—C8—H15	117.9
N1—C12—C11	120.9 (4)	C9—C8—H15	119.3
C12—N1—B1	118.5 (4)	C8—C9—C10	118.9 (5)
C12—N1—C8	119.0 (4)	C8—C9—H16	120.6
B1—N1—C8	121.3 (4)	C10—C9—H16	120.5
N1—B1—O2	105.0 (4)	C9—C10—C11	120.6 (4)

N1—B1—O1	105.2 (4)	C9—C10—H17	120.3
O2—B1—O1	113.1 (4)	C11—C10—H17	119.0
N1—B1—C1	115.2 (4)	C12—C11—C10	117.7 (4)
O2—B1—C1	113.5 (4)	C12—C11—C13	118.2 (5)
O1—B1—C1	104.7 (4)	C10—C11—C13	124.1 (5)
B1—O1—C7	111.2 (4)	C11—C13—C14	120.9 (5)
O1—C7—C6	106.4 (4)	C11—C13—H131	119.4
O1—C7—H71	110.0	C14—C13—H131	119.7
C6—C7—H71	110.8	C13—C14—C15	121.9 (5)
O1—C7—H72	110.0	C13—C14—H141	119.0
C6—C7—H72	110.1	C15—C14—H141	119.1
H71—C7—H72	109.5	C14—C15—C16	118.9 (5)
C7—C6—C1	111.7 (4)	C14—C15—C17	121.9 (5)
C7—C6—C5	126.6 (4)	C16—C15—C17	119.1 (5)
C1—C6—C5	121.6 (5)	C15—C17—C18	119.6 (5)
B1—C1—C6	105.4 (4)	C15—C17—H171	120.2
B1—C1—C2	135.8 (5)	C18—C17—H171	120.2
C6—C1—C2	118.7 (4)	C17—C18—C19	122.4 (5)
C1—C2—C3	119.8 (5)	C17—C18—H181	118.6
C1—C2—H11	119.6	C19—C18—H181	119.0
C3—C2—H11	120.6	C20—C19—C18	119.0 (5)
C2—C3—C4	121.0 (5)	C20—C19—H191	120.0
C2—C3—H12	119.0	C18—C19—H191	120.9

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H16···O2^{i}	0.93	2.59	3.490 (8)	163

Symmetry code: (i) $x-y+1/3, x-1/3, -z+2/3$.