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(2*S*,N*S*)-*N*-Allyl-*N*-benzyl-1-hydroxy-3-(4-hydroxyphenyl)-*N*-methylpropan-2-aminium bromide

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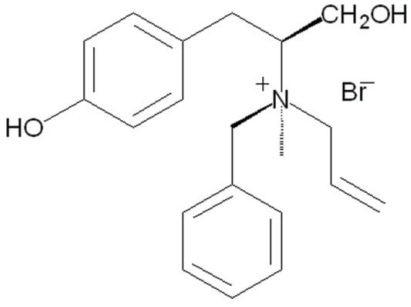
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.011 Å; disorder in main residue; R factor = 0.055; wR factor = 0.211; data-to-parameter ratio = 20.1.

The title compound, $C_{20}H_{26}NO_2^+\cdot Br^-$, is an *N*-chiral quaternary ammonium salt synthesized from (2*S**)-*N*-benzyl-*N*-methyltyrosine methyl ester. The dihedral angle between the phenyl ring and the benzene ring is 11.61 (19)°. In the crystal structure, the allyl group is disordered over two positions with site occupancy factors of *ca* 0.8 and 0.2. The bromide anion links to the quaternary ammonium cations *via* O—H···Br hydrogen bonding. An intramolecular O—H···Br hydrogen bond is also observed.

Related literature

For general background, see: Maruoka & Ooi (2003); Ooi & Maruoka (2007). For a related structure, see: Tayama & Tanaka (2007). For synthesis, see: White & Konopelski (2005).



Experimental

Crystal data

$C_{20}H_{26}NO_2^+\cdot Br^-$
M_r = 392.33
Orthorhombic, $P2_12_12_1$
a = 10.3716 (10) Å
b = 12.1566 (10) Å
c = 15.6790 (16) Å
V = 1976.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.09 mm^{-1}
T = 293 (2) K
0.45 × 0.43 × 0.40 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.406, T_{max} = 0.433
18872 measured reflections
4524 independent reflections
2606 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.211
S = 1.00
4524 reflections
225 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.89 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}
Absolute structure: Flack (1983), with 1949 Friedel pairs
Flack parameter: 0.009 (19)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···Br1	0.82	2.43	3.231 (4)	167
O2—H2O···Br1^{i}	0.82	2.38	3.192 (5)	171

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

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2435).

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supporting information

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(2*S*,N*S*)-*N*-Allyl-*N*-benzyl-1-hydroxy-3-(4-hydroxyphenyl)-*N*-methylpropan-2-aminium bromide

Hua-Fang Wu, Ying-Gang Luo, Kai-Bei Yu, Guo-Lin Zhang and Xin-Fu Pan

S1. Comment

As an important class of asymmetric catalysts of phase-transfer catalysts, chiral quaternary ammonium salts show great application in asymmetric organic synthesis (Maruoka & Ooi, 2003; Ooi & Maruoka, 2007). The title compound is a N-chiral quaternary ammonium salt (N-CQAS), we present here its structure.

The molecular structure is shown in Fig. 1. The quaternary ammonium cation displays an extended structure, the C14—N1—C8—C7 torsion angle is 179.3 (5)°. The terminal C1-benzene and C15-phenyl rings are nearly parallel to each other [dihedral angle 11.61 (19)°], and approximately perpendicular to the central C7/C6/N1/C14 mean plane with dihedral angles of 85.1 (3) and 88.8 (4)°, respectively. Bond lengths and angles agree with those found in a reported N-chiral quaternary ammonium salt (Tayama & Tanaka, 2007).

In the crystal structure the Br^- anion links with the quaternary ammonium cations *via* O—H···Br hydrogen bonding (Table 1), to form the one dimensional supra-molecular structure along the *b* axis (Fig. 2).

S2. Experimental

(2*S**)-*N*-Benzyl-*N*-methyltyrosine methyl ester (White & Konopelski, 2005) (1 mmol) was reduced by lithium aluminium hydride (1 mmol) to afford (2*S**)-*N*-Benzyl-*N*-methyl-2-amino-3-(4-hydroxyphenyl)propan-1-ol, which was then dissolved in absolute acetonitrile (5 ml), and allyl bromide (2 mmol) was added. The mixture was heated to reflux for 42 h. After being cooled to room temperature, the excess allyl bromide and acetonitrile were removed under reduced pressure. The residue was purified by flash chromatography eluted with ethyl acetate/methanol (8:1) to afford the diastereomeric mixture of the N-CQAS with yields (90%). The mixture was recrystallized from ethanol to afford the single crystals of the title compound. Yield (41%).

S3. Refinement

H atoms were placed in calculated positions with C—H = 0.93–0.98 Å, O—H = 0.82 Å, and refined in riding mode with U_{iso}(H) = 1.2U_{eq}(C,O). The terminal carbon (C13) atom of the allyl group is disordered over two sites, occupancies were refined and converged to 0.778:0.222.

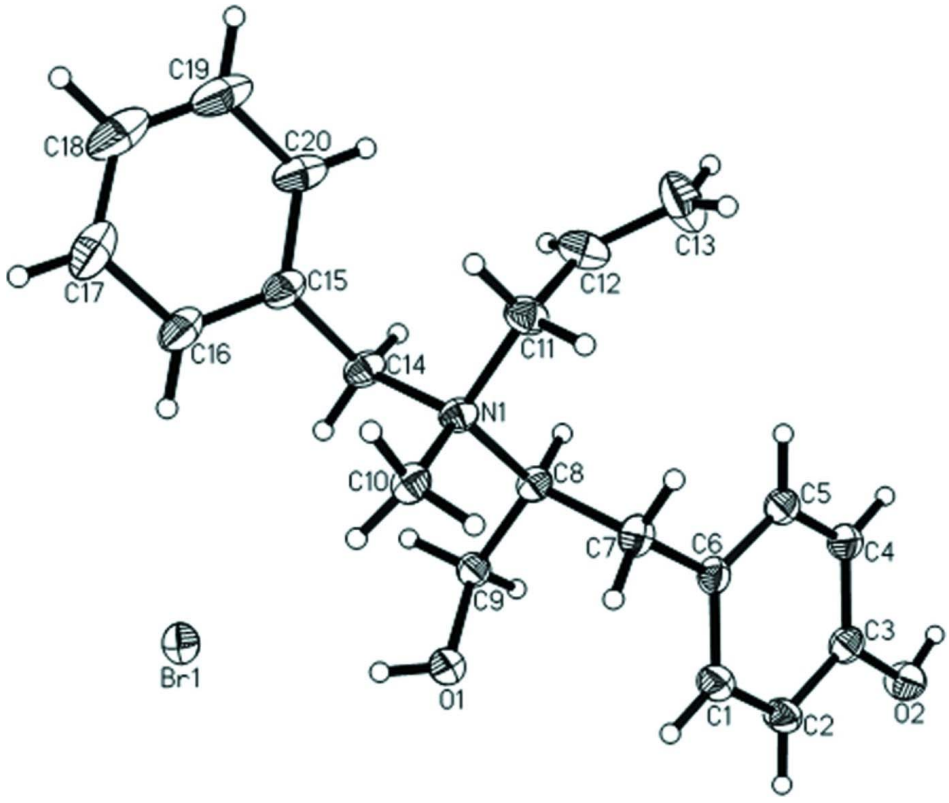

Figure 1

The molecular structure of the title compound, displacement ellipsoids are drawn at the 30% probability level. The minor disordered component has been omitted for clarity.

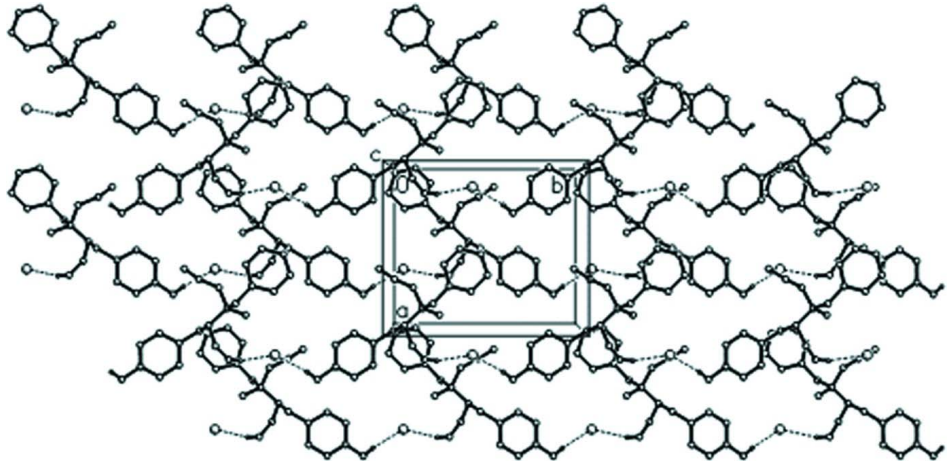

Figure 2

The unit cell packing diagram of the title compound. Dashed lines indicate hydrogen bonding.

(2*S,N*S**)-*N*-Allyl-*N*-benzyl-1-hydroxy-3- (4-hydroxyphenyl)-*N*-methylpropan-2-aminium bromide**

Crystal data

$C_{20}H_{26}NO_2^+ \cdot Br^-$
$M_r = 392.33$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 10.3716\ (10)$ Å
$b = 12.1566\ (10)$ Å
$c = 15.6790\ (16)$ Å
$V = 1976.9\ (3)$ Å^3
$Z = 4$
$F(000) = 816$
$D_x = 1.318$ Mg m^{-3}
Melting point: 449(5) K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 10762 reflections
$\theta = 3.1–27.4°$
$\mu = 2.09$ mm^{-1}
$T = 293$ K
Block, colourless
0.45 × 0.43 × 0.40 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: Rotating anode
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.406$, $T_{max} = 0.434$
18872 measured reflections
4524 independent reflections
2606 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -13 \rightarrow 13$
$k = -15 \rightarrow 15$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.211$
$S = 1.00$
4524 reflections
225 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.128P)^2 + 0.338P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.89$ e Å^{-3}
$\Delta\rho_{min} = -0.69$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.058 (6)
Absolute structure: Flack (1983), with 1949 Friedel pairs
Absolute structure parameter: 0.009 (19)

Special details

Experimental. IR (KBr): 3297, 3034, 1612, 1515, 1464, 1264, 1058, 850 (cm^{-1}); ^{13}CNMR (150 MHz, DMSO-d$_6$, δ, p.p.m.): 156.8, 133.7, 130.8, 129.4, 128.5, 127.4, 126.9, 126.8, 116.0, 73.9, 63.7, 62.9, 56.6, 47.0, 29.6.

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1	0.63828 (7)	0.06624 (5)	0.31732 (5)	0.0766 (3)	
O1	0.6728 (4)	0.3120 (4)	0.3923 (3)	0.0748 (12)	
H1O	0.6764	0.2479	0.3762	0.090*	
O2	0.7918 (4)	0.8588 (4)	0.3897 (4)	0.0863 (14)	
H2O	0.7452	0.9091	0.3736	0.104*	
N1	0.3651 (4)	0.3213 (4)	0.4017 (3)	0.0552 (10)	
C1	0.7120 (6)	0.5784 (6)	0.4504 (5)	0.0739 (17)	
H1	0.7557	0.5151	0.4668	0.089*	
C2	0.7823 (6)	0.6731 (5)	0.4309 (5)	0.0739 (18)	
H2	0.8718	0.6726	0.4334	0.089*	
C3	0.7171 (6)	0.7673 (5)	0.4080 (4)	0.0680 (16)	
C4	0.5853 (6)	0.7668 (5)	0.4011 (4)	0.0696 (16)	
H4	0.5420	0.8296	0.3830	0.083*	
C5	0.5173 (6)	0.6733 (5)	0.4210 (5)	0.0667 (16)	
H5	0.4278	0.6747	0.4178	0.080*	
C6	0.5784 (5)	0.5767 (5)	0.4459 (4)	0.0595 (13)	
C7	0.5053 (7)	0.4747 (5)	0.4658 (4)	0.0666 (15)	
H7A	0.4282	0.4936	0.4976	0.080*	
H7B	0.5578	0.4271	0.5013	0.080*	
C8	0.4670 (5)	0.4131 (4)	0.3849 (4)	0.0538 (12)	
H8	0.4261	0.4670	0.3471	0.065*	
C9	0.5867 (5)	0.3719 (5)	0.3389 (4)	0.0576 (13)	
H9A	0.5603	0.3251	0.2919	0.069*	
H9B	0.6322	0.4345	0.3149	0.069*	
C10	0.4099 (6)	0.2377 (5)	0.4638 (4)	0.0606 (13)	
H10A	0.3393	0.1905	0.4790	0.073*	
H10B	0.4419	0.2738	0.5140	0.073*	
H10C	0.4775	0.1947	0.4386	0.073*	
C11	0.2426 (6)	0.3716 (6)	0.4391 (4)	0.0707 (16)	
H11A	0.1774	0.3147	0.4435	0.085*	
H11B	0.2611	0.3974	0.4964	0.085*	
C12	0.1902 (7)	0.4635 (6)	0.3892 (5)	0.092 (2)	0.778 (18)
H12	0.1973	0.4594	0.3302	0.111*	0.778 (18)
C13	0.1339 (16)	0.5511 (10)	0.4216 (8)	0.132 (6)	0.778 (18)
H13A	0.1250	0.5581	0.4804	0.158*	0.778 (18)
H13B	0.1030	0.6060	0.3857	0.158*	0.778 (18)
C12′	0.1902 (7)	0.4635 (6)	0.3892 (5)	0.092 (2)	0.222 (18)
H12′	0.2394	0.5064	0.3525	0.111*	0.222 (18)
C13′	0.0657 (12)	0.479 (5)	0.402 (3)	0.132 (6)	0.222 (18)
H13C	0.0212	0.4331	0.4396	0.158*	0.222 (18)
H13D	0.0225	0.5346	0.3736	0.158*	0.222 (18)
C14	0.3330 (5)	0.2665 (5)	0.3165 (4)	0.0644 (14)	
H14A	0.3090	0.3235	0.2762	0.077*	
H14B	0.4106	0.2317	0.2950	0.077*	
C15	0.2279 (6)	0.1823 (6)	0.3179 (5)	0.0728 (17)	

C16	0.2603 (7)	0.0727 (7)	0.3287 (5)	0.086 (2)
H16	0.3459	0.0529	0.3372	0.103*
C17	0.1623 (10)	−0.0099 (9)	0.3266 (6)	0.111 (3)
H17	0.1820	−0.0839	0.3346	0.133*
C18	0.0386 (10)	0.0242 (12)	0.3125 (7)	0.121 (4)
H18	−0.0263	−0.0285	0.3114	0.145*
C19	0.0055 (9)	0.1317 (14)	0.3001 (7)	0.119 (4)
H19	−0.0799	0.1514	0.2902	0.143*
C20	0.1000 (6)	0.2092 (8)	0.3026 (5)	0.093 (2)
H20	0.0781	0.2826	0.2938	0.112*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0760 (4)	0.0657 (4)	0.0881 (5)	0.0026 (3)	−0.0014 (4)	−0.0123 (3)
O1	0.066 (2)	0.060 (2)	0.098 (3)	0.004 (2)	−0.012 (2)	−0.007 (2)
O2	0.069 (3)	0.062 (2)	0.127 (4)	−0.015 (2)	0.000 (3)	0.015 (3)
N1	0.048 (2)	0.066 (3)	0.051 (2)	−0.006 (2)	0.003 (2)	0.0028 (19)
C1	0.068 (4)	0.060 (4)	0.093 (5)	0.006 (3)	−0.008 (3)	0.002 (4)
C2	0.061 (3)	0.055 (3)	0.105 (5)	0.001 (3)	−0.007 (3)	0.008 (3)
C3	0.066 (3)	0.057 (3)	0.081 (4)	−0.014 (3)	0.001 (3)	−0.001 (3)
C4	0.068 (3)	0.057 (3)	0.083 (4)	−0.001 (3)	−0.008 (3)	0.000 (3)
C5	0.061 (3)	0.059 (3)	0.081 (4)	−0.007 (3)	0.002 (3)	−0.004 (3)
C6	0.065 (3)	0.048 (3)	0.065 (3)	−0.005 (3)	0.002 (3)	−0.004 (3)
C7	0.076 (4)	0.059 (3)	0.065 (4)	−0.007 (3)	0.002 (3)	−0.002 (3)
C8	0.055 (3)	0.053 (3)	0.054 (3)	−0.009 (2)	0.001 (2)	0.007 (2)
C9	0.055 (3)	0.054 (3)	0.064 (3)	−0.002 (2)	0.003 (2)	0.001 (2)
C10	0.067 (3)	0.055 (3)	0.060 (3)	−0.012 (3)	−0.001 (3)	0.012 (2)
C11	0.060 (3)	0.087 (4)	0.065 (4)	0.011 (3)	0.009 (3)	−0.003 (3)
C12	0.063 (4)	0.115 (7)	0.099 (5)	0.019 (4)	0.010 (4)	0.011 (5)
C13	0.178 (14)	0.128 (11)	0.089 (7)	0.077 (12)	−0.012 (8)	−0.028 (7)
C12′	0.063 (4)	0.115 (7)	0.099 (5)	0.019 (4)	0.010 (4)	0.011 (5)
C13′	0.178 (14)	0.128 (11)	0.089 (7)	0.077 (12)	−0.012 (8)	−0.028 (7)
C14	0.057 (3)	0.086 (4)	0.050 (3)	−0.013 (3)	0.000 (3)	−0.004 (3)
C15	0.059 (3)	0.097 (5)	0.062 (3)	−0.020 (3)	0.007 (3)	−0.014 (4)
C16	0.071 (4)	0.100 (5)	0.086 (5)	−0.031 (4)	0.010 (3)	−0.024 (5)
C17	0.122 (8)	0.113 (7)	0.097 (6)	−0.055 (6)	0.026 (5)	−0.032 (5)
C18	0.093 (6)	0.193 (12)	0.076 (5)	−0.070 (7)	0.017 (5)	−0.032 (7)
C19	0.066 (5)	0.203 (11)	0.089 (7)	−0.037 (6)	−0.002 (4)	−0.040 (8)
C20	0.059 (3)	0.139 (7)	0.080 (5)	−0.018 (4)	−0.012 (3)	−0.003 (5)

Geometric parameters (Å, º)

O1—C9	1.425 (7)	C10—H10A	0.9600
O1—H1O	0.8200	C10—H10B	0.9600
O2—C3	1.385 (7)	C10—H10C	0.9600
O2—H2O	0.8200	C11—C12	1.468 (10)
N1—C10	1.482 (7)	C11—H11A	0.9700

N1—C11	1.527 (7)	C11—H11B	0.9700
N1—C14	1.531 (7)	C12—C13	1.317 (3)
N1—C8	1.560 (6)	C12—H12	0.9300
C1—C6	1.387 (9)	C13—H13A	0.9300
C1—C2	1.396 (10)	C13—H13B	0.9300
C1—H1	0.9300	C13′—H13C	0.9300
C2—C3	1.377 (9)	C13′—H13D	0.9300
C2—H2	0.9300	C14—C15	1.495 (8)
C3—C4	1.372 (9)	C14—H14A	0.9700
C4—C5	1.373 (9)	C14—H14B	0.9700
C4—H4	0.9300	C15—C16	1.384 (11)
C5—C6	1.391 (9)	C15—C20	1.388 (10)
C5—H5	0.9300	C16—C17	1.429 (10)
C6—C7	1.487 (8)	C16—H16	0.9300
C7—C8	1.525 (8)	C17—C18	1.367 (17)
C7—H7A	0.9700	C17—H17	0.9300
C7—H7B	0.9700	C18—C19	1.365 (17)
C8—C9	1.520 (8)	C18—H18	0.9300
C8—H8	0.9800	C19—C20	1.361 (13)
C9—H9A	0.9700	C19—H19	0.9300
C9—H9B	0.9700	C20—H20	0.9300

C9—O1—H1O	109.5	N1—C10—H10A	109.5
C3—O2—H2O	109.5	N1—C10—H10B	109.5
C10—N1—C11	106.5 (4)	H10A—C10—H10B	109.5
C10—N1—C14	110.1 (5)	N1—C10—H10C	109.5
C11—N1—C14	109.2 (4)	H10A—C10—H10C	109.5
C10—N1—C8	112.9 (4)	H10B—C10—H10C	109.5
C11—N1—C8	110.0 (4)	C12—C11—N1	114.1 (5)
C14—N1—C8	108.1 (4)	C12—C11—H11A	108.7
C6—C1—C2	121.5 (7)	N1—C11—H11A	108.7
C6—C1—H1	119.2	C12—C11—H11B	108.7
C2—C1—H1	119.2	N1—C11—H11B	108.7
C3—C2—C1	119.1 (6)	H11A—C11—H11B	107.6
C3—C2—H2	120.5	C13—C12—C11	125.0 (9)
C1—C2—H2	120.5	C13—C12—H12	117.5
C4—C3—C2	120.4 (6)	C11—C12—H12	117.5
C4—C3—O2	123.0 (6)	C12—C13—H13A	120.0
C2—C3—O2	116.5 (6)	C12—C13—H13B	120.0
C3—C4—C5	119.8 (6)	H13A—C13—H13B	120.0
C3—C4—H4	120.1	H13C—C13′—H13D	120.0
C5—C4—H4	120.1	C15—C14—N1	116.3 (5)
C4—C5—C6	121.9 (6)	C15—C14—H14A	108.2
C4—C5—H5	119.0	N1—C14—H14A	108.2
C6—C5—H5	119.0	C15—C14—H14B	108.2
C1—C6—C5	117.1 (6)	N1—C14—H14B	108.2
C1—C6—C7	120.8 (6)	H14A—C14—H14B	107.4
C5—C6—C7	122.1 (5)	C16—C15—C20	118.7 (7)

C6—C7—C8	111.6 (5)	C16—C15—C14	118.9 (6)
C6—C7—H7A	109.3	C20—C15—C14	122.2 (7)
C8—C7—H7A	109.3	C15—C16—C17	120.1 (8)
C6—C7—H7B	109.3	C15—C16—H16	120.0
C8—C7—H7B	109.3	C17—C16—H16	120.0
H7A—C7—H7B	108.0	C18—C17—C16	117.2 (10)
C9—C8—C7	110.1 (5)	C18—C17—H17	121.4
C9—C8—N1	113.5 (4)	C16—C17—H17	121.4
C7—C8—N1	112.8 (4)	C19—C18—C17	123.4 (9)
C9—C8—H8	106.7	C19—C18—H18	118.3
C7—C8—H8	106.7	C17—C18—H18	118.3
N1—C8—H8	106.7	C20—C19—C18	118.5 (10)
O1—C9—C8	113.6 (5)	C20—C19—H19	120.7
O1—C9—H9A	108.8	C18—C19—H19	120.7
C8—C9—H9A	108.8	C19—C20—C15	122.0 (10)
O1—C9—H9B	108.8	C19—C20—H20	119.0
C8—C9—H9B	108.8	C15—C20—H20	119.0
H9A—C9—H9B	107.7		

C6—C1—C2—C3	1.0 (12)	C7—C8—C9—O1	51.2 (6)
C1—C2—C3—C4	−2.6 (12)	N1—C8—C9—O1	−76.3 (6)
C1—C2—C3—O2	179.8 (7)	C10—N1—C11—C12	175.1 (6)
C2—C3—C4—C5	3.1 (12)	C14—N1—C11—C12	−66.1 (7)
O2—C3—C4—C5	−179.5 (6)	C8—N1—C11—C12	52.5 (7)
C3—C4—C5—C6	−2.0 (11)	N1—C11—C12—C13	−144.3 (12)
C2—C1—C6—C5	0.1 (11)	C10—N1—C14—C15	61.4 (6)
C2—C1—C6—C7	179.2 (6)	C11—N1—C14—C15	−55.1 (7)
C4—C5—C6—C1	0.4 (10)	C8—N1—C14—C15	−174.8 (5)
C4—C5—C6—C7	−178.7 (6)	N1—C14—C15—C16	−93.4 (8)
C1—C6—C7—C8	−98.8 (8)	N1—C14—C15—C20	91.5 (9)
C5—C6—C7—C8	80.4 (8)	C20—C15—C16—C17	−2.0 (12)
C6—C7—C8—C9	65.0 (6)	C14—C15—C16—C17	−177.3 (7)
C6—C7—C8—N1	−167.1 (5)	C15—C16—C17—C18	1.0 (13)
C10—N1—C8—C9	67.4 (6)	C16—C17—C18—C19	0.4 (17)
C11—N1—C8—C9	−173.9 (4)	C17—C18—C19—C20	−0.6 (18)
C14—N1—C8—C9	−54.6 (6)	C18—C19—C20—C15	−0.5 (16)
C10—N1—C8—C7	−58.7 (6)	C16—C15—C20—C19	1.7 (14)
C11—N1—C8—C7	60.0 (6)	C14—C15—C20—C19	176.9 (8)
C14—N1—C8—C7	179.3 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···Br1	0.82	2.43	3.231 (4)	167
O2—H2*O*···Br1^{i}	0.82	2.38	3.192 (5)	171

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