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# A monoclinic polymorph of (*R*,*R*)-4,4′-dibromo-2,2′-[cyclohexane-1,2-diylbis(nitrilomethanylylidene)]diphenol

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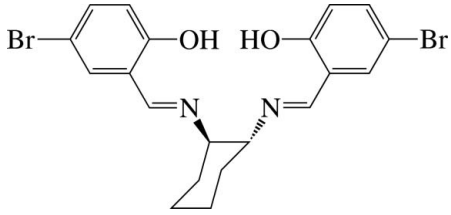
Key indicators: single-crystal X-ray study; $T$ = 200 K; mean $\sigma$(C–C) = 0.009 Å; $R$ factor = 0.039; $wR$ factor = 0.108; data-to-parameter ratio = 16.5.

The title compound, $C_{20}H_{20}Br_2N_2O_2$, a tetradentate Schiff base, is the enantiomerically pure *R*,*R*-diastereomer of four possible stereoisomers. The molecular structure reveals two strong intramolecular O—H···N hydrogen bonds between the hydroxy O atom and the imino N atom, which each generate *S*(6) rings. In the crystal, molecules are stacked in columns along the *a* axis; when viewed down the *b* axis, successive columns are stacked in the opposite direction. The structure reported herein is the monoclinic polymorph of the previously reported orthorhombic form [Yi & Hu (2009). *Acta Cryst.* E**65**, o2643], in which the complete molecule is generated by a crystallographic twofold axis.

## Related literature

For the orthorhombic polymorph, see: Yi & Hu (2009).




## Experimental

### Crystal data

$C_{20}H_{20}Br_2N_2O_2$ $M_r$ = 480.20
Monoclinic, $P2_1$
$a$ = 5.9082 (5) Å
$b$ = 18.8626 (15) Å
$c$ = 9.0088 (7) Å
$\beta$ = 91.867 (2)°
$V$ = 1003.44 (14) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 4.06 mm$^{-1}$
$T$ = 200 K
0.31 × 0.17 × 0.16 mm

### Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.786, $T_{max}$ = 1.000
7343 measured reflections
3868 independent reflections
2484 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.108
$S$ = 1.03
3868 reflections
235 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.88 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.47 e Å$^{-3}$
Absolute structure: Flack (1983), 1331 Friedel pairs
Flack parameter: −0.010 (16)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1*O*···N1 | 0.84 | 1.82 | 2.581 (7) | 150 |
| O2—H2*O*···N2 | 0.84 | 1.87 | 2.626 (7) | 149 |

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); 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: HB6734).

## References

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Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
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Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Yi, J. & Hu, S. (2009). *Acta Cryst.* E**65**, o2643.

# supporting information

*Acta Cryst.* (2012). E**68**, o1449 [doi:10.1107/S1600536812016376]

# A monoclinic polymorph of (*R*,*R*)-4,4′-dibromo-2,2′-[cyclohexane-1,2-diylbis(nitrilomethanylylidene)]diphenol

**Kwang Ha**

## S1. Comment

The crystal structure of the title compound, $C_{20}H_{20}Br_2N_2O_2$, was previously reported in the orthorhombic space group $P2_12_12$ (Yi & Hu, 2009). The structure presented herein is essentially the same as the published structure and represents a monoclinic polymorph.

The title compound is a tetradentate Schiff base (Fig. 1), which can act as a dibasic ligand, *i.e.* the N and O donor atoms can coordinate one metal ion. The compound has two chiral C centres and is one of four possible stereoisomers. Crystallographically, the absolute configuration has been established by anomalous dispersion effects, and the *R* configuration of the asymmetric C atoms (C1 and C6) could be assigned. The Schiff base reveals strong intramolecular O—H···N hydrogen bonds between the hydroxy O atom and the imino N atom, with O···N distances of 2.581 (7) and 2.626 (7) Å, forming nearly planar six-membered rings (Fig. 2, Table 1). In the crystal structure, the benzene rings are not parallel: the dihedral angle between the benzene rings is 67.20 (15)°. The N—C bond lengths and the C—N—C bond angles indicate that the imino N atoms are $sp^2$-hybridized [N1═C7 = 1.274 (8) Å, N1—C1 = 1.461 (8) Å, <C7—N1—C1 = 118.7 (6)°; N2═C14 = 1.280 (8) Å, N2—C6 = 1.474 (8) Å, <C14—N2—C6 = 118.3 (6)°]. The molecules are stacked in columns along the *a* axis. When viewed down the *b* axis, the successive compounds are stacked in the opposite direction. In the columns, the shortest centroid-centroid distance between aromatic rings is 4.709 (3) Å.

## S2. Experimental

1,2-Diaminocyclohexane (0.8007 g, 7.012 mmol) and 5-bromosalicylaldehyde (2.8204 g, 14.031 mmol) in EtOH (20 ml) were stirred for 1 h at room temperature. After addition of pentane (30 ml) to the reaction mixture, the formed precipitate was separated by filtration, washed with ether, and dried at 323 K, to give a yellow powder (1.7660 g). Yellow blocks were obtained by slow evaporation from a $CH_3CN$ solution at room temperature. The previous polymorph (Yi & Hu, 2009) was crystallised from methanol.

## S3. Refinement

Carbon-bound H atoms were positioned geometrically and allowed to ride on their respective parent atoms: C—H = 0.95–1.00 Å with $U_{iso}$(H) = 1.2$U_{eq}$(C). The hydroxy H atoms were located from the difference Fourier map then allowed to ride on their parent atoms in the final cycles of refinement with O—H = 0.84 Å and $U_{iso}$(H) = 1.5 $U_{eq}$(O). The highest peak (0.88 e Å$^{-3}$) and the deepest hole (-0.47 e Å$^{-3}$) in the difference Fourier map are located 1.34 Å and 0.86 Å, respectively, from the atoms Br1 and Br2. The absolute configuration was established by anomalous dispersion effects *via* diffraction measurements on the crystal. The Flack parameter is -0.010 (16) in the final cycles of refinement.

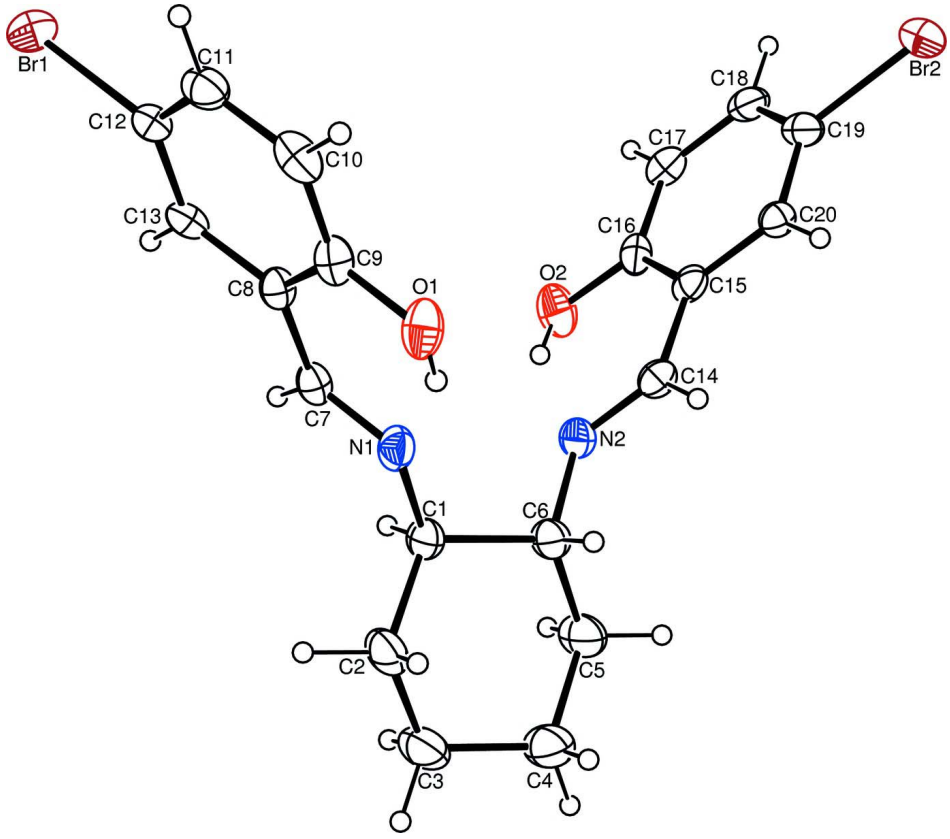


**Figure 1**

A structure detail of the title compound, with atom numbering. Displacement ellipsoids are drawn at the 30% probability level for non-H atoms.

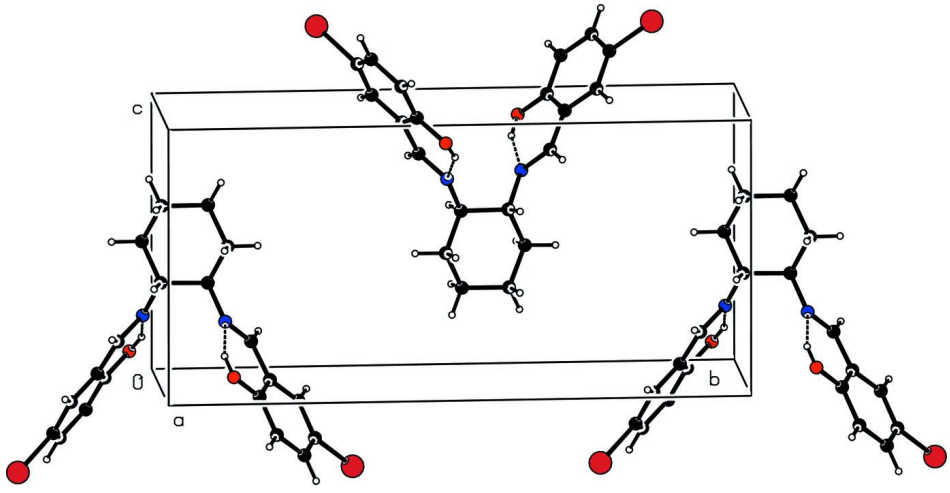


**Figure 2**

A view of the unit-cell contents of the title compound. Intramolecular O—H···N hydrogen-bond interactions are drawn with dashed lines.

**(*R*,*R*)-4,4′-dibromo-2,2′- [cyclohexane-1,2-diylbis(nitrilomethanylylidene)]diphenol**

*Crystal data*

$C_{20}H_{20}Br_2N_2O_2$
$M_r = 480.20$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 5.9082$ (5) Å
$b = 18.8626$ (15) Å
$c = 9.0088$ (7) Å
$\beta = 91.867$ (2)°
$V = 1003.44$ (14) Å$^3$
$Z = 2$
$F(000) = 480$
$D_x = 1.589$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2758 reflections
$\theta = 2.5$–$25.8°$
$\mu = 4.06$ mm$^{-1}$
$T = 200$ K
Block, yellow
0.31 × 0.17 × 0.16 mm

*Data collection*

Bruker SMART 1000 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.786$, $T_{max} = 1.000$
7343 measured reflections
3868 independent reflections
2484 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.2°$
$h = -7 \rightarrow 7$
$k = -20 \rightarrow 25$
$l = -11 \rightarrow 11$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.108$
$S = 1.03$
3868 reflections
235 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.88$ e Å$^{-3}$
$\Delta\rho_{min} = -0.47$ e Å$^{-3}$
Absolute structure: Flack (1983), 1331 Friedel pairs
Absolute structure parameter: −0.010 (16)

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.25215 (12) | 0.33723 (3) | −0.33161 (7) | 0.0600 (3) |
| Br2 | 0.27364 (11) | −0.23777 (3) | −0.33104 (7) | 0.0551 (2) |
| O1 | 0.7141 (7) | 0.1204 (3) | 0.0604 (6) | 0.0539 (13) |

| | | | | |
|---|---|---|---|---|
| H1O | 0.6245 | 0.1070 | 0.1252 | 0.081* |
| O2 | −0.2482 (8) | −0.0312 (3) | 0.0322 (6) | 0.0587 (14) |
| H2O | −0.1588 | −0.0127 | 0.0955 | 0.088* |
| N1 | 0.3538 (9) | 0.1159 (3) | 0.2147 (5) | 0.0428 (12) |
| N2 | 0.1109 (9) | −0.0185 (2) | 0.2097 (5) | 0.0427 (12) |
| C1 | 0.2247 (11) | 0.0899 (5) | 0.3390 (7) | 0.0414 (18) |
| H1 | 0.0634 | 0.1054 | 0.3257 | 0.050* |
| C2 | 0.3242 (15) | 0.1210 (4) | 0.4830 (7) | 0.0601 (19) |
| H2A | 0.4888 | 0.1111 | 0.4893 | 0.072* |
| H2B | 0.3038 | 0.1731 | 0.4816 | 0.072* |
| C3 | 0.2143 (15) | 0.0908 (5) | 0.6200 (10) | 0.068 (2) |
| H3A | 0.2893 | 0.1107 | 0.7106 | 0.081* |
| H3B | 0.0525 | 0.1045 | 0.6194 | 0.081* |
| C4 | 0.2344 (16) | 0.0103 (5) | 0.6219 (10) | 0.071 (3) |
| H4A | 0.1588 | −0.0089 | 0.7097 | 0.086* |
| H4B | 0.3961 | −0.0035 | 0.6288 | 0.086* |
| C5 | 0.1241 (15) | −0.0204 (4) | 0.4802 (7) | 0.061 (2) |
| H5A | 0.1385 | −0.0727 | 0.4818 | 0.073* |
| H5B | −0.0392 | −0.0085 | 0.4763 | 0.073* |
| C6 | 0.2343 (11) | 0.0086 (5) | 0.3428 (8) | 0.0452 (19) |
| H6 | 0.3957 | −0.0073 | 0.3416 | 0.054* |
| C7 | 0.2650 (10) | 0.1629 (4) | 0.1295 (7) | 0.0373 (15) |
| H7 | 0.1164 | 0.1795 | 0.1471 | 0.045* |
| C8 | 0.3885 (9) | 0.1916 (3) | 0.0051 (6) | 0.0344 (12) |
| C9 | 0.6051 (10) | 0.1676 (3) | −0.0268 (7) | 0.0439 (14) |
| C10 | 0.7125 (11) | 0.1940 (5) | −0.1518 (7) | 0.0477 (19) |
| H10 | 0.8586 | 0.1771 | −0.1751 | 0.057* |
| C11 | 0.6082 (11) | 0.2443 (3) | −0.2412 (6) | 0.0459 (15) |
| H11 | 0.6819 | 0.2623 | −0.3255 | 0.055* |
| C12 | 0.3947 (9) | 0.2685 (3) | −0.2071 (5) | 0.0406 (12) |
| C13 | 0.2877 (10) | 0.2432 (3) | −0.0852 (7) | 0.0381 (16) |
| H13 | 0.1428 | 0.2612 | −0.0622 | 0.046* |
| C14 | 0.2091 (10) | −0.0645 (4) | 0.1293 (7) | 0.0378 (15) |
| H14 | 0.3597 | −0.0784 | 0.1555 | 0.045* |
| C15 | 0.0974 (10) | −0.0959 (3) | −0.0004 (6) | 0.0366 (13) |
| C16 | −0.1247 (10) | −0.0773 (3) | −0.0454 (6) | 0.0387 (13) |
| C17 | −0.2241 (12) | −0.1068 (4) | −0.1734 (7) | 0.0443 (18) |
| H17 | −0.3742 | −0.0939 | −0.2032 | 0.053* |
| C18 | −0.1054 (10) | −0.1550 (3) | −0.2579 (6) | 0.0443 (14) |
| H18 | −0.1728 | −0.1752 | −0.3452 | 0.053* |
| C19 | 0.1098 (10) | −0.1725 (3) | −0.2129 (5) | 0.0416 (13) |
| C20 | 0.2136 (9) | −0.1450 (3) | −0.0861 (6) | 0.0333 (14) |
| H20 | 0.3628 | −0.1592 | −0.0572 | 0.040* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0820 (6) | 0.0589 (6) | 0.0384 (4) | 0.0047 (4) | −0.0070 (3) | 0.0073 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| Br2 | 0.0668 (5) | 0.0587 (6) | 0.0400 (4) | 0.0071 (4) | 0.0051 (3) | −0.0076 (4) |
| O1 | 0.042 (3) | 0.041 (3) | 0.080 (4) | 0.010 (2) | 0.004 (2) | 0.005 (3) |
| O2 | 0.044 (3) | 0.050 (3) | 0.082 (4) | 0.010 (2) | 0.003 (3) | −0.012 (3) |
| N1 | 0.049 (3) | 0.030 (3) | 0.049 (3) | −0.004 (2) | 0.000 (2) | 0.002 (2) |
| N2 | 0.056 (3) | 0.031 (3) | 0.042 (3) | −0.007 (2) | 0.003 (2) | 0.000 (2) |
| C1 | 0.049 (4) | 0.033 (4) | 0.042 (5) | −0.007 (3) | 0.004 (3) | 0.000 (3) |
| C2 | 0.089 (6) | 0.039 (4) | 0.053 (4) | −0.013 (4) | 0.007 (4) | −0.013 (3) |
| C3 | 0.100 (7) | 0.058 (6) | 0.046 (5) | −0.023 (5) | 0.006 (4) | −0.014 (5) |
| C4 | 0.111 (7) | 0.056 (6) | 0.046 (5) | −0.022 (5) | −0.001 (4) | 0.003 (5) |
| C5 | 0.086 (6) | 0.047 (4) | 0.049 (4) | −0.026 (4) | 0.003 (4) | −0.004 (3) |
| C6 | 0.060 (5) | 0.035 (5) | 0.041 (5) | −0.012 (3) | −0.001 (4) | −0.002 (3) |
| C7 | 0.036 (3) | 0.030 (4) | 0.045 (4) | −0.001 (3) | −0.002 (3) | −0.007 (3) |
| C8 | 0.031 (3) | 0.030 (3) | 0.041 (3) | 0.000 (2) | −0.002 (2) | −0.003 (2) |
| C9 | 0.041 (3) | 0.035 (3) | 0.056 (4) | 0.004 (3) | 0.000 (3) | −0.004 (3) |
| C10 | 0.038 (3) | 0.048 (5) | 0.058 (4) | −0.008 (3) | 0.011 (3) | −0.018 (3) |
| C11 | 0.051 (4) | 0.047 (4) | 0.040 (3) | −0.011 (3) | 0.007 (3) | −0.007 (3) |
| C12 | 0.054 (3) | 0.036 (3) | 0.031 (3) | 0.000 (3) | −0.001 (2) | −0.006 (3) |
| C13 | 0.040 (3) | 0.043 (4) | 0.031 (3) | 0.000 (3) | −0.001 (2) | −0.012 (3) |
| C14 | 0.038 (3) | 0.038 (4) | 0.038 (3) | −0.003 (3) | 0.003 (3) | 0.007 (3) |
| C15 | 0.042 (3) | 0.029 (3) | 0.038 (3) | −0.006 (2) | 0.001 (2) | 0.009 (2) |
| C16 | 0.039 (3) | 0.029 (3) | 0.049 (3) | 0.004 (2) | 0.006 (3) | 0.004 (3) |
| C17 | 0.044 (4) | 0.044 (4) | 0.044 (4) | −0.003 (3) | −0.003 (3) | 0.012 (3) |
| C18 | 0.056 (4) | 0.044 (4) | 0.032 (3) | −0.007 (3) | −0.005 (2) | 0.007 (3) |
| C19 | 0.047 (3) | 0.047 (4) | 0.031 (3) | −0.002 (3) | 0.002 (2) | 0.000 (3) |
| C20 | 0.029 (3) | 0.037 (4) | 0.033 (3) | 0.002 (2) | 0.001 (2) | 0.003 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—C12 | 1.894 (6) | C5—H5B | 0.9900 |
| Br2—C19 | 1.912 (6) | C6—H6 | 1.0000 |
| O1—C9 | 1.337 (7) | C7—C8 | 1.461 (8) |
| O1—H1O | 0.8400 | C7—H7 | 0.9500 |
| O2—C16 | 1.345 (7) | C8—C13 | 1.391 (8) |
| O2—H2O | 0.8400 | C8—C9 | 1.396 (8) |
| N1—C7 | 1.274 (8) | C9—C10 | 1.403 (9) |
| N1—C1 | 1.461 (8) | C10—C11 | 1.377 (10) |
| N2—C14 | 1.280 (8) | C10—H10 | 0.9500 |
| N2—C6 | 1.474 (8) | C11—C12 | 1.385 (8) |
| C1—C2 | 1.524 (10) | C11—H11 | 0.9500 |
| C1—C6 | 1.534 (7) | C12—C13 | 1.370 (8) |
| C1—H1 | 1.0000 | C13—H13 | 0.9500 |
| C2—C3 | 1.523 (10) | C14—C15 | 1.451 (9) |
| C2—H2A | 0.9900 | C14—H14 | 0.9500 |
| C2—H2B | 0.9900 | C15—C20 | 1.398 (8) |
| C3—C4 | 1.522 (8) | C15—C16 | 1.405 (8) |
| C3—H3A | 0.9900 | C16—C17 | 1.393 (9) |
| C3—H3B | 0.9900 | C17—C18 | 1.390 (9) |
| C4—C5 | 1.528 (11) | C17—H17 | 0.9500 |

| | | | |
|---|---|---|---|
| C4—H4A | 0.9900 | C18—C19 | 1.363 (8) |
| C4—H4B | 0.9900 | C18—H18 | 0.9500 |
| C5—C6 | 1.520 (10) | C19—C20 | 1.380 (8) |
| C5—H5A | 0.9900 | C20—H20 | 0.9500 |
| | | | |
| C9—O1—H1O | 107.9 | N1—C7—H7 | 119.6 |
| C16—O2—H2O | 106.3 | C8—C7—H7 | 119.6 |
| C7—N1—C1 | 118.7 (6) | C13—C8—C9 | 119.0 (5) |
| C14—N2—C6 | 118.3 (6) | C13—C8—C7 | 119.6 (5) |
| N1—C1—C2 | 109.1 (6) | C9—C8—C7 | 121.5 (5) |
| N1—C1—C6 | 109.5 (7) | O1—C9—C8 | 121.4 (5) |
| C2—C1—C6 | 110.6 (7) | O1—C9—C10 | 119.1 (6) |
| N1—C1—H1 | 109.2 | C8—C9—C10 | 119.4 (6) |
| C2—C1—H1 | 109.2 | C11—C10—C9 | 120.6 (6) |
| C6—C1—H1 | 109.2 | C11—C10—H10 | 119.7 |
| C3—C2—C1 | 112.5 (7) | C9—C10—H10 | 119.7 |
| C3—C2—H2A | 109.1 | C10—C11—C12 | 119.4 (6) |
| C1—C2—H2A | 109.1 | C10—C11—H11 | 120.3 |
| C3—C2—H2B | 109.1 | C12—C11—H11 | 120.3 |
| C1—C2—H2B | 109.1 | C13—C12—C11 | 120.7 (5) |
| H2A—C2—H2B | 107.8 | C13—C12—Br1 | 120.3 (4) |
| C4—C3—C2 | 110.3 (8) | C11—C12—Br1 | 119.0 (4) |
| C4—C3—H3A | 109.6 | C12—C13—C8 | 120.9 (5) |
| C2—C3—H3A | 109.6 | C12—C13—H13 | 119.6 |
| C4—C3—H3B | 109.6 | C8—C13—H13 | 119.6 |
| C2—C3—H3B | 109.6 | N2—C14—C15 | 122.0 (6) |
| H3A—C3—H3B | 108.1 | N2—C14—H14 | 119.0 |
| C3—C4—C5 | 109.8 (9) | C15—C14—H14 | 119.0 |
| C3—C4—H4A | 109.7 | C20—C15—C16 | 118.5 (5) |
| C5—C4—H4A | 109.7 | C20—C15—C14 | 119.8 (5) |
| C3—C4—H4B | 109.7 | C16—C15—C14 | 121.7 (5) |
| C5—C4—H4B | 109.7 | O2—C16—C17 | 117.8 (6) |
| H4A—C4—H4B | 108.2 | O2—C16—C15 | 122.0 (5) |
| C6—C5—C4 | 111.2 (6) | C17—C16—C15 | 120.2 (6) |
| C6—C5—H5A | 109.4 | C18—C17—C16 | 120.5 (6) |
| C4—C5—H5A | 109.4 | C18—C17—H17 | 119.7 |
| C6—C5—H5B | 109.4 | C16—C17—H17 | 119.7 |
| C4—C5—H5B | 109.4 | C19—C18—C17 | 118.5 (6) |
| H5A—C5—H5B | 108.0 | C19—C18—H18 | 120.7 |
| N2—C6—C5 | 108.9 (6) | C17—C18—H18 | 120.7 |
| N2—C6—C1 | 108.2 (7) | C18—C19—C20 | 122.7 (5) |
| C5—C6—C1 | 111.2 (7) | C18—C19—Br2 | 118.3 (4) |
| N2—C6—H6 | 109.5 | C20—C19—Br2 | 119.0 (4) |
| C5—C6—H6 | 109.5 | C19—C20—C15 | 119.5 (5) |
| C1—C6—H6 | 109.5 | C19—C20—H20 | 120.2 |
| N1—C7—C8 | 120.9 (6) | C15—C20—H20 | 120.2 |
| | | | |
| C7—N1—C1—C2 | −106.0 (7) | C9—C10—C11—C12 | −0.3 (10) |

| | | | |
|---|---|---|---|
| C7—N1—C1—C6 | 132.8 (6) | C10—C11—C12—C13 | 0.4 (9) |
| N1—C1—C2—C3 | −174.3 (7) | C10—C11—C12—Br1 | −179.6 (5) |
| C6—C1—C2—C3 | −53.9 (9) | C11—C12—C13—C8 | −1.4 (9) |
| C1—C2—C3—C4 | 56.4 (11) | Br1—C12—C13—C8 | 178.5 (4) |
| C2—C3—C4—C5 | −57.8 (10) | C9—C8—C13—C12 | 2.4 (9) |
| C3—C4—C5—C6 | 58.7 (10) | C7—C8—C13—C12 | −176.7 (5) |
| C14—N2—C6—C5 | −109.5 (7) | C6—N2—C14—C15 | 177.7 (6) |
| C14—N2—C6—C1 | 129.6 (7) | N2—C14—C15—C20 | 178.8 (6) |
| C4—C5—C6—N2 | −175.8 (7) | N2—C14—C15—C16 | 0.4 (9) |
| C4—C5—C6—C1 | −56.7 (9) | C20—C15—C16—O2 | 179.1 (5) |
| N1—C1—C6—N2 | −66.8 (7) | C14—C15—C16—O2 | −2.4 (8) |
| C2—C1—C6—N2 | 173.0 (5) | C20—C15—C16—C17 | −0.6 (9) |
| N1—C1—C6—C5 | 173.7 (5) | C14—C15—C16—C17 | 177.9 (6) |
| C2—C1—C6—C5 | 53.5 (8) | O2—C16—C17—C18 | −179.7 (6) |
| C1—N1—C7—C8 | 178.9 (6) | C15—C16—C17—C18 | 0.1 (10) |
| N1—C7—C8—C13 | −179.5 (6) | C16—C17—C18—C19 | −0.1 (10) |
| N1—C7—C8—C9 | 1.5 (9) | C17—C18—C19—C20 | 0.7 (9) |
| C13—C8—C9—O1 | 176.9 (5) | C17—C18—C19—Br2 | −179.2 (5) |
| C7—C8—C9—O1 | −4.1 (9) | C18—C19—C20—C15 | −1.3 (9) |
| C13—C8—C9—C10 | −2.3 (9) | Br2—C19—C20—C15 | 178.6 (4) |
| C7—C8—C9—C10 | 176.7 (5) | C16—C15—C20—C19 | 1.2 (8) |
| O1—C9—C10—C11 | −177.9 (6) | C14—C15—C20—C19 | −177.3 (5) |
| C8—C9—C10—C11 | 1.3 (10) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*O*···N1 | 0.84 | 1.82 | 2.581 (7) | 150 |
| O2—H2*O*···N2 | 0.84 | 1.87 | 2.626 (7) | 149 |