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2-[(2-Aminophenylimino)phenylmethyl]-4-bromophenol

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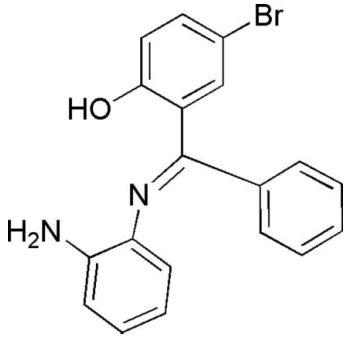
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.038; wR factor = 0.099; data-to-parameter ratio = 13.4.

In the title compound, $C_{19}H_{15}BrN_2O$, the dihedral angles formed by the imide group and the three benzene rings are 56.5 (2), 6.2 (4) and 55.7 (1)°. The molecular structure and packing are stabilized by O—H···N, N—H···O and N—H···N intermolecular hydrogen-bond interactions and C—H···π interactions.

Related literature

For related literature, see: Allen *et al.* (1987); Geraghty *et al.* (1999); Ranford & Sadler (1993); Saha *et al.* (2004); Zierkiewicz *et al.* (2000); Yang (2006); Zoroddu *et al.* (1996).



Experimental

Crystal data

$C_{19}H_{15}BrN_2O$
M_r = 367.23
Triclinic, $P\overline{1}$
a = 8.4504 (17) Å
b = 9.4206 (19) Å
c = 11.141 (2) Å
α = 68.94 (3)°
β = 85.40 (3)°
γ = 78.31 (3)°
V = 810.5 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.54 mm^{-1}
T = 295 (2) K
0.20 × 0.20 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
3365 measured reflections
2785 independent reflections
2094 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.099
S = 1.03
2785 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of rings C1–C6, C8–C13 and C14–C19, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*B*···O1^{i}	0.86	2.28	3.011 (3)	142
O1—H1···N2	0.85	1.79	2.505 (3)	141
N1—H1*A*···N2	0.86	2.41	2.734 (4)	103
N1—H1*B*···*Cg*1^{ii}	0.86	3.20	3.799 (2)	129
C19—H19*A*···*Cg*2^{iii}	0.93	2.98	3.800 (3)	148
C1—H1*C*···*Cg*3^{iv}	0.93	2.76	3.557 (3)	145

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2255).

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supplementary materials

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2-[(2-Aminophenylimino)phenylmethyl]-4-bromophenol

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Comment

Monocondensed Schiff bases are attractive because of their use as intermediates in the synthesis of unsymmetrical multidentate Schiff base ligands. Schiff bases also serve as potential chelating agents and possess biological activities (Yang, 2006). Transition metal complexes derived from Schiff bases are are of great interest since they exhibit numerous biological activities such as antitumor (Ranford *et al.*, 1993), anti-candida (Majella *et al.*, 1999), antimicrobacterial (Saha *et al.*, 2004) and antimicrobial (Zoroddu *et al.*, 1996) activities. In this paper, we have synthesized a new Schiff base compound by the condensation of 5-Bromo 2-hyoxybenzophenone with diaminobenzene and characterized it with X-ray crystallographic techniques.

All the bond lengths in the compounds are within normal ranges (Allen *et al.*, 1987). The C7—N2 bond length of 1.281 (3)Å confirms it as a double bond. The C—Br bond length [1.887 (3) Å] is agreement with other reported bonds [1.884 (2)Å (Wiktor *et al.*, 2000)].

Four atoms C4,C7,C8,N2 are in a plane (p1). The benzene ring, C8—C13, (p3), is approximately planar with its immediate substituent atoms Br1, O1, and C7, with a maximum deviation of 0.028 (1)Å for O1. The benzene ring, C14—C19, is planar with its immediate substituent atoms N1 forming the plane p4. The dihedral angles formed by p1 with the benzene ring, C1—C6, (p2), p3 and p4 are 56.5 (2), 6.2 (4) and 55.7 (1)°, respectively. The dihedral angles formed by p2 with p3 and p4 are 59.4 (2) and 61.8 (3)°. The dihedral angle between p3 and p4 is 61.8 (2)°.

The molecular structure is stabilized by intramolecular C—H···π interactions and O—H···N, N—H···O and N—H···N inter- and intra-molecular hydrogen-bond interactions [N1···C_g1 = 3.799 (2), H1B···C_g1 = 3.200 (1) Å, N1—H1B···C_g1 = 128.8 (3)° (Symmetry code: 1 − *x*,2 − *y*,-*z*); C1···C_g3 = 3.557 (3), H1C···C_g3 = 2.758 (2) Å, C1—H1C···*Cg*3 = 144.6 (2)° (Symmetry code: 1 + *x*,*y*,*z*); C19···Cg_2 = 3.800 (3), H19A···C_g2 = 2.977 (2) Å, C19—H19A···C_g2 = 148.3 (2)° (Symmetry code: 1 − *x*,1 − *y*,-*z*). C_g1, C_g2 and C_g3 are the centroids of phenyl rings C1—C6, C8—C13 and C14—C19, respectively]. Hydrogen-bond interactions are list in Table 2.

Experimental

5-Bromo-2-hyoxybenzophenone (47 g, 0.17 mol), diaminobenzene (18.4 g, 0.17 mol), piperidine (15 g, 0.18 mol) and triethylorthoformate (20 ml) were refluxed in absolute methanol (150 ml) until crystals started to appear. The solution was cooled to room temperature and the desired compound was collected by filtration. Single crystals suitable for X-ray measurements were obtained by slow evaporation of chloroform/ ethanol (1:1 *v*/*v*) at room temperature.

Refinement

H atoms except H1 were fixed geometrically and allowed to ride on their attached atoms, with C—H distances = 0.93Å and N—H = 0.86 Å, and with U_{iso}(H)=1.2U_{eq}(C). H1 wass located from a delta(F) map.

Figures

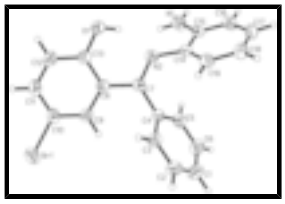


Fig. 1. The structure of the title compound showing 30% probability displacement ellipsoids and the atom-numbering scheme.

2-[(2-Aminophenylimino)phenylmethyl]-4-bromophenol

Crystal data

$C_{19}H_{15}BrN_2O$	$Z = 2$
$M_r = 367.23$	$F_{000} = 372$
Triclinic, $P\overline{1}$	$D_x = 1.505$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.4504$ (17) Å	Cell parameters from 25 reflections
$b = 9.4206$ (19) Å	$\theta = 4$–14º
$c = 11.141$ (2) Å	$\mu = 2.54$ mm^{-1}
$\alpha = 68.94$ (3)º	$T = 295$ (2) K
$\beta = 85.40$ (3)º	Block, colorless
$\gamma = 78.31$ (3)º	0.20 × 0.20 × 0.18 mm
$V = 810.5$ (3) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.018$
Radiation source: fine-focus sealed tube	$\theta_{max} = 25.0$º
Monochromator: graphite	$\theta_{min} = 2.0$º
$T = 295$(2) K	$h = -9 \rightarrow 10$
ω scans	$k = -11 \rightarrow 6$
Absorption correction: none	$l = -13 \rightarrow 12$
3365 measured reflections	3 standard reflections
2785 independent reflections	every 100 reflections
2094 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.038$	H-atom parameters constrained
$wR(F^2) = 0.099$	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
2785 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
208 parameters	$\Delta\rho_{min} = -0.27$ 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}
Br1	0.82601 (5)	0.79635 (4)	−0.41528 (3)	0.07530 (19)
O1	0.1888 (2)	0.8105 (2)	−0.1436 (2)	0.0624 (6)
H1	0.2000	0.7754	−0.0624	0.075*
N1	0.1382 (3)	0.9926 (3)	0.1374 (3)	0.0688 (8)
H1A	0.1667	1.0127	0.0581	0.083*
H1B	0.0732	1.0614	0.1604	0.083*
N2	0.3303 (3)	0.7716 (3)	0.0581 (2)	0.0517 (6)
C1	0.9008 (5)	0.6305 (5)	0.2237 (4)	0.0752 (10)
H1C	0.9945	0.6028	0.2716	0.090*
C2	0.8721 (4)	0.5433 (4)	0.1568 (3)	0.0674 (9)
H2B	0.9468	0.4547	0.1601	0.081*
C3	0.7361 (4)	0.5825 (4)	0.0847 (3)	0.0554 (8)
H3A	0.7197	0.5218	0.0386	0.066*
C4	0.6232 (4)	0.7126 (3)	0.0804 (3)	0.0454 (7)
C5	0.6508 (4)	0.8013 (4)	0.1486 (3)	0.0559 (8)
H5A	0.5755	0.8891	0.1468	0.067*
C6	0.7894 (5)	0.7604 (5)	0.2197 (3)	0.0708 (10)
H6A	0.8078	0.8211	0.2652	0.085*
C7	0.4709 (3)	0.7531 (3)	0.0073 (3)	0.0441 (7)
C8	0.4763 (3)	0.7798 (3)	−0.1316 (3)	0.0449 (7)
C9	0.6214 (4)	0.7812 (3)	−0.1996 (3)	0.0518 (7)
H9A	0.7169	0.7688	−0.1577	0.062*
C10	0.6255 (4)	0.8009 (3)	−0.3276 (3)	0.0552 (8)
C11	0.4869 (4)	0.8210 (4)	−0.3928 (3)	0.0601 (9)
H11A	0.4913	0.8332	−0.4796	0.072*
C12	0.3429 (4)	0.8230 (4)	−0.3288 (3)	0.0591 (8)
H12A	0.2485	0.8371	−0.3727	0.071*

C13	0.3342 (4)	0.8041 (3)	−0.1989 (3)	0.0500 (7)
C14	0.3017 (3)	0.7385 (3)	0.1922 (3)	0.0478 (7)
C15	0.1967 (3)	0.8507 (4)	0.2275 (3)	0.0505 (7)
C16	0.1562 (4)	0.8156 (4)	0.3567 (3)	0.0607 (9)
H16A	0.0891	0.8903	0.3833	0.073*
C17	0.2127 (4)	0.6739 (4)	0.4455 (3)	0.0657 (9)
H17A	0.1807	0.6521	0.5310	0.079*
C18	0.3161 (4)	0.5631 (4)	0.4103 (3)	0.0646 (9)
H18A	0.3555	0.4669	0.4713	0.078*
C19	0.3607 (4)	0.5967 (4)	0.2831 (3)	0.0585 (8)
H19A	0.4316	0.5227	0.2581	0.070*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0749 (3)	0.0860 (3)	0.0579 (2)	−0.0128 (2)	0.01688 (19)	−0.0216 (2)
O1	0.0479 (13)	0.0774 (16)	0.0585 (13)	0.0055 (11)	−0.0083 (11)	−0.0275 (12)
N1	0.0678 (19)	0.0588 (17)	0.0656 (18)	0.0057 (14)	0.0118 (15)	−0.0169 (15)
N2	0.0490 (16)	0.0552 (16)	0.0471 (15)	−0.0011 (12)	0.0011 (12)	−0.0184 (12)
C1	0.057 (2)	0.090 (3)	0.071 (2)	−0.021 (2)	−0.0160 (19)	−0.014 (2)
C2	0.050 (2)	0.071 (2)	0.068 (2)	−0.0008 (17)	−0.0046 (18)	−0.014 (2)
C3	0.055 (2)	0.0535 (19)	0.0539 (19)	−0.0049 (15)	−0.0050 (16)	−0.0165 (15)
C4	0.0471 (17)	0.0469 (17)	0.0386 (15)	−0.0092 (14)	0.0009 (13)	−0.0108 (14)
C5	0.063 (2)	0.0550 (19)	0.0518 (18)	−0.0184 (16)	0.0030 (16)	−0.0187 (16)
C6	0.075 (3)	0.089 (3)	0.060 (2)	−0.038 (2)	−0.0054 (19)	−0.027 (2)
C7	0.0477 (18)	0.0388 (16)	0.0444 (16)	−0.0034 (13)	−0.0003 (14)	−0.0154 (13)
C8	0.0451 (18)	0.0404 (16)	0.0454 (16)	−0.0001 (13)	−0.0034 (14)	−0.0143 (13)
C9	0.0512 (19)	0.0508 (18)	0.0504 (18)	−0.0053 (14)	−0.0057 (15)	−0.0154 (15)
C10	0.068 (2)	0.0489 (18)	0.0446 (17)	−0.0046 (15)	0.0011 (16)	−0.0152 (14)
C11	0.078 (3)	0.055 (2)	0.0434 (18)	−0.0033 (17)	−0.0032 (18)	−0.0175 (15)
C12	0.060 (2)	0.062 (2)	0.0532 (19)	0.0037 (16)	−0.0163 (17)	−0.0227 (17)
C13	0.0491 (19)	0.0452 (17)	0.0521 (18)	0.0017 (13)	−0.0047 (15)	−0.0176 (14)
C14	0.0408 (17)	0.0561 (19)	0.0463 (17)	−0.0079 (14)	0.0011 (14)	−0.0186 (16)
C15	0.0414 (17)	0.057 (2)	0.0550 (19)	−0.0139 (14)	0.0023 (14)	−0.0196 (17)
C16	0.059 (2)	0.071 (2)	0.063 (2)	−0.0192 (17)	0.0155 (17)	−0.036 (2)
C17	0.075 (2)	0.083 (3)	0.0431 (18)	−0.031 (2)	0.0044 (17)	−0.0192 (19)
C18	0.065 (2)	0.068 (2)	0.051 (2)	−0.0121 (18)	−0.0023 (17)	−0.0094 (17)
C19	0.057 (2)	0.057 (2)	0.057 (2)	−0.0036 (15)	−0.0007 (16)	−0.0186 (17)

Geometric parameters (Å, °)

Br1—C10	1.887 (3)	C7—C8	1.475 (4)
O1—C13	1.330 (4)	C8—C9	1.389 (4)
O1—H1	0.8499	C8—C13	1.401 (4)
N1—C15	1.373 (4)	C9—C10	1.369 (4)
N1—H1A	0.8600	C9—H9A	0.9300
N1—H1B	0.8600	C10—C11	1.372 (5)
N2—C7	1.281 (3)	C11—C12	1.361 (4)
N2—C14	1.423 (3)	C11—H11A	0.9300

C1—C2	1.356 (5)	C12—C13	1.391 (4)
C1—C6	1.373 (6)	C12—H12A	0.9300
C1—H1C	0.9300	C14—C19	1.378 (4)
C2—C3	1.366 (5)	C14—C15	1.387 (4)
C2—H2B	0.9300	C15—C16	1.387 (4)
C3—C4	1.380 (4)	C16—C17	1.363 (5)
C3—H3A	0.9300	C16—H16A	0.9300
C4—C5	1.377 (4)	C17—C18	1.370 (5)
C4—C7	1.487 (4)	C17—H17A	0.9300
C5—C6	1.376 (5)	C18—C19	1.375 (4)
C5—H5A	0.9300	C18—H18A	0.9300
C6—H6A	0.9300	C19—H19A	0.9300
C13—O1—H1	108.9	C8—C9—H9A	119.6
C15—N1—H1A	120.0	C9—C10—C11	121.2 (3)
C15—N1—H1B	120.0	C9—C10—Br1	119.4 (3)
H1A—N1—H1B	120.0	C11—C10—Br1	119.4 (2)
C7—N2—C14	124.1 (3)	C12—C11—C10	119.1 (3)
C2—C1—C6	119.1 (4)	C12—C11—H11A	120.5
C2—C1—H1C	120.5	C10—C11—H11A	120.5
C6—C1—H1C	120.5	C11—C12—C13	121.2 (3)
C1—C2—C3	121.6 (3)	C11—C12—H12A	119.4
C1—C2—H2B	119.2	C13—C12—H12A	119.4
C3—C2—H2B	119.2	O1—C13—C12	117.7 (3)
C2—C3—C4	119.8 (3)	O1—C13—C8	122.6 (3)
C2—C3—H3A	120.1	C12—C13—C8	119.7 (3)
C4—C3—H3A	120.1	C19—C14—C15	120.5 (3)
C5—C4—C3	119.1 (3)	C19—C14—N2	122.5 (3)
C5—C4—C7	120.3 (3)	C15—C14—N2	116.7 (3)
C3—C4—C7	120.6 (3)	N1—C15—C14	120.8 (3)
C6—C5—C4	120.1 (3)	N1—C15—C16	121.5 (3)
C6—C5—H5A	119.9	C14—C15—C16	117.7 (3)
C4—C5—H5A	119.9	C17—C16—C15	121.3 (3)
C1—C6—C5	120.4 (3)	C17—C16—H16A	119.4
C1—C6—H6A	119.8	C15—C16—H16A	119.4
C5—C6—H6A	119.8	C16—C17—C18	120.9 (3)
N2—C7—C8	116.4 (3)	C16—C17—H17A	119.6
N2—C7—C4	123.2 (2)	C18—C17—H17A	119.6
C8—C7—C4	120.3 (2)	C17—C18—C19	118.8 (3)
C9—C8—C13	118.0 (3)	C17—C18—H18A	120.6
C9—C8—C7	121.2 (3)	C19—C18—H18A	120.6
C13—C8—C7	120.7 (3)	C18—C19—C14	120.8 (3)
C10—C9—C8	120.7 (3)	C18—C19—H19A	119.6
C10—C9—H9A	119.6	C14—C19—H19A	119.6

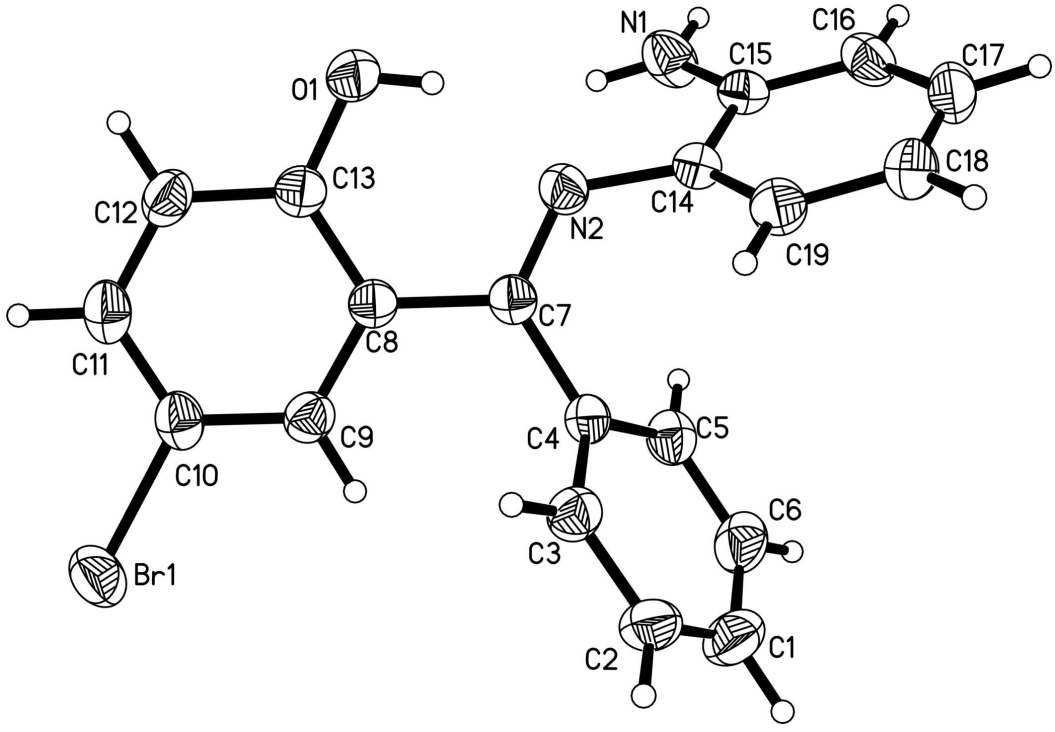
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1B···O1^{i}	0.86	2.28	3.011 (3)	142
O1—H1···N2	0.85	1.79	2.505 (3)	141

N1—H1A···N2	0.86	2.41	2.734 (4)	103
N1—H1B···Cg1^{ii}	0.86	3.20	3.799 (2)	129
C19—H19A···Cg2^{iii}	0.93	2.98	3.800 (3)	148
C1—H1C···Cg3^{iv}	0.93	2.76	3.557 (3)	145

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

Fig. 1


N1
C16
C15
C17
O1
C18
C13
C14
C12
N2
C19
C7
C8
C11
C4
C5
C9
C10
C6
C3
Br1
C2
C1