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2-Bromo-*N*′-[(*E*)-4-hydroxybenzylidene]-5-methoxybenzohydrazide

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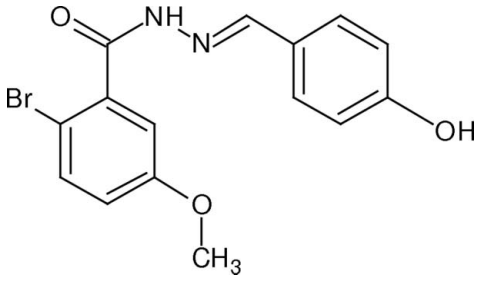
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.064; data-to-parameter ratio = 17.7.

The geometric parameters of the title compound, $C_{15}H_{13}BrN_2O_3$, are in the usual ranges. The C=N double bond is *trans* configured. The C=N—N—CO– group itself is planar, with an r.m.s. deviation of 0.044 Å, and makes a dihedral angle of 10.73 (19)° with the hydroxyphenyl ring, but forms a dihedral angle of 67.90 (8)° with the other aromatic ring. The crystal packing is stabilized by N—H···O, O—H···O and O—H···N hydrogen bonds.

Related literature

For related structures, see: Yang & Pan (2004; 2005); Butcher *et al.* (2007); Chang *et al.* (2007); Narayana *et al.* (2007); Yathirajan *et al.* (2007). For related literature, see: Hodnett & Dunn (1970); Misra *et al.* (1981); Varma *et al.* (1986); Singh & Dash (1988); Pandey *et al.* (1999); El-Masry *et al.* (2000); Aydoğan *et al.* (2001); Desai *et al.* (2001); Taggi *et al.* (2002).



Experimental

Crystal data

$C_{15}H_{13}BrN_2O_3$
M_r = 349.18
Orthorhombic, $P2_12_12_1$
a = 9.4902 (6) Å
b = 10.9347 (8) Å
c = 14.8687 (10) Å
V = 1542.96 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.68 mm^{-1}
T = 173 (2) K
0.27 × 0.25 × 0.23 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.532, T_{max} = 0.578 (expected range = 0.497–0.541)
13120 measured reflections
3536 independent reflections
3204 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.064
S = 1.06
3536 reflections
200 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}
Absolute structure: Flack (1983), with 1510 Friedel pairs
Flack parameter: −0.004 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.84 (5)	2.07 (4)	2.799 (3)	145 (4)
O2—H2···N2^{i}	0.84 (5)	2.32 (5)	2.995 (3)	137 (4)
N1—H1···O2^{ii}	0.86 (3)	2.01 (3)	2.866 (3)	170 (3)

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); 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: AT2377).

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supplementary materials

Acta Cryst. (2007). E**63**, o3862-o3863 [**doi:10.1107/S1600536807040603**]

2-Bromo-*N*'-[(*E*)-4-hydroxybenzylidene]-5-methoxybenzohydrazide

B. K. Sarojini, B. Narayana, K. Sunil, H. S. Yathirajan and M. Bolte

Comment

Schiff bases are known to have biological activities such as antimicrobial (El-Masry *et al.*, 2000; Pandey *et al.*, 1999), antifungal (Singh *et al.*, 1988; Varma *et al.*, 1986), antitumor (Hodnett *et al.*, 1970; Misra *et al.* 1981; Desai *et al.*, 2001), and as herbicides. Schiff bases have also been employed as ligands for complexation of metal ions (Aydoğan *et al.*, 2001). On the industrial scale, they have wide range of applications such as dyes and pigments (Taggi *et al.*, 2002). The crystal structures of 2-bromo-*N*-[(*E*)-4-chlorobenzylidene]-5-methoxybenzohydrazide (Butcher *et al.*, 2007), 2-bromo-5-methoxy-*N*-[(*E*)-(2-nitrophenyl)methylene]benzohydrazide (Yathirajan *et al.*, 2007), 2-bromo-*N*-[(*E*)-(4-fluorophenyl)methylene]-5-methoxybenzohydrazide monohydrate (Narayana *et al.*, 2007), *N*'-[(1E)-(5-chloro-2-hydroxyphenyl)(phenyl)methylene]-2-hydroxybenzohydrazide (Chang *et al.*, 2007), 2'-(3,4-dimethoxybenzylidene)-2-hydroxybenzohydrazide, (Yang & Pan, 2004) and 2'-(2-fluorobenzylidene)-2-hydroxybenzohydrazide (Yang & Pan, 2005) have been reported. A new Schiff base, $C_{15}H_{13}BrN_2O_3$, was synthesized and its crystal structure is here reported.

Geometric parameters of the title compound (Fig. 1) are in the usual ranges. The C═N double bond is *trans* configured. The C═N—N—CO– moiety itself is planar (r.m.s. deviation 0.044 Å). It makes a dihedral angle of 10.73 (19)°, with the hydroxyphenyl ring, but forms a dihedral angle of 67.90 (8)° with the other aromatic ring. The crystal packing is stabilized by N—H···O, O—H···O and O—H···N hydrogen bonds. The hydroxyl group forms a bifurcated H bond to the hydrazon N atom and the carbonyl group.

Experimental

A mixture of 2-bromo-5-methoxybenzohydrazide (0.735 g, 0.003 mol) and 4-hydroxybenzaldehyde (0.366 g, 0.003 mol) in 15 ml of absolute ethanol containing 2 drops of sulfuric acid was refluxed for about 3 h. On cooling, the solid separated was filtered and recrystalized from DMF (m.p.: above 523 K). Analysis found: C 51.51, H 3.71, N 7.95%; $C_{15}H_{13}BrN_2O_3$, requires: C 51.60, H 3.75, N 8.02%.

Refinement

H atoms were found in a difference map, but those bonded to C were refined using a riding model with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) for $C_{aromatic}$ and C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C) for C_{methyl}. The methyl group was allowed to rotate but not to tip. The H atoms bonded to N and O were freely refined.

Figures

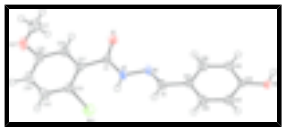

Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

Fig. 2. The formation of the title compound.

2-Bromo-*N*'-[(*E*)-4-hydroxybenzylidene]-5-methoxybenzohydrazide

Crystal data

$C_{15}H_{13}BrN_2O_3$	F_{000} = 704
M_r = 349.18	D_x = 1.503 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 13820 reflections
a = 9.4902 (6) Å	θ = 3.9–27.7º
b = 10.9347 (8) Å	μ = 2.68 mm^{-1}
c = 14.8687 (10) Å	T = 173 (2) K
V = 1542.96 (18) Å^3	Block, colourless
Z = 4	0.27 × 0.25 × 0.23 mm

Data collection

Stoe IPDSII two-circle diffractometer	3536 independent reflections
Radiation source: fine-focus sealed tube	3204 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.044
T = 173(2) K	θ_{max} = 27.6º
ω scans	θ_{min} = 4.0º
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	h = −12→10
T_{min} = 0.532, T_{max} = 0.578	k = −14→11
13120 measured reflections	l = −19→19

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0288P)^2 + 0.3101P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.032	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.064	$\Delta\rho_{max}$ = 0.37 e Å^{-3}
S = 1.06	$\Delta\rho_{min}$ = −0.58 e Å^{-3}
3536 reflections	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
200 parameters	Extinction coefficient: 0.0078 (8)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), with 1510 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.004 (8)

Hydrogen site location: inferred from neighbouring sites

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	0.82669 (3)	0.43390 (3)	0.193021 (18)	0.03868 (10)
C1	0.6507 (2)	0.6879 (2)	0.18939 (15)	0.0214 (5)
O1	0.6900 (3)	0.78219 (16)	0.22737 (11)	0.0330 (5)
O2	0.0445 (2)	0.60418 (16)	0.63181 (11)	0.0272 (4)
H2	0.068 (5)	0.664 (4)	0.665 (3)	0.076 (14)*
N1	0.5450 (2)	0.6169 (2)	0.21810 (12)	0.0241 (4)
H1	0.527 (3)	0.552 (3)	0.1878 (17)	0.022 (6)*
N2	0.4773 (2)	0.64534 (18)	0.29896 (13)	0.0232 (4)
C2	0.3686 (2)	0.5793 (2)	0.31537 (15)	0.0237 (5)
H2A	0.3412	0.5197	0.2723	0.028*
C11	0.7159 (3)	0.6461 (2)	0.10162 (15)	0.0211 (5)
C12	0.7929 (3)	0.5383 (2)	0.09271 (16)	0.0247 (5)
C13	0.8508 (3)	0.5061 (3)	0.00963 (17)	0.0319 (6)
H13	0.9046	0.4332	0.0040	0.038*
C14	0.8296 (3)	0.5809 (3)	−0.06481 (15)	0.0324 (5)
H14	0.8690	0.5590	−0.1213	0.039*
C15	0.7508 (3)	0.6875 (3)	−0.05688 (16)	0.0275 (6)
C16	0.6950 (3)	0.7216 (2)	0.02622 (15)	0.0234 (5)
H16	0.6431	0.7955	0.0318	0.028*
O17	0.7327 (2)	0.7531 (2)	−0.13480 (12)	0.0392 (5)
C17	0.6250 (4)	0.8451 (3)	−0.1348 (2)	0.0440 (8)
H17A	0.5357	0.8090	−0.1149	0.066*
H17B	0.6139	0.8779	−0.1957	0.066*
H17C	0.6517	0.9112	−0.0937	0.066*
C21	0.2849 (3)	0.5918 (2)	0.39774 (14)	0.0214 (5)
C22	0.1683 (3)	0.5158 (2)	0.40985 (14)	0.0260 (5)
H22	0.1440	0.4586	0.3643	0.031*
C23	0.0871 (3)	0.5224 (2)	0.48754 (16)	0.0258 (5)
H23	0.0065	0.4717	0.4945	0.031*
C24	0.1255 (3)	0.6041 (2)	0.55512 (14)	0.0205 (5)
C25	0.2405 (3)	0.6819 (2)	0.54426 (17)	0.0239 (5)

H25	0.2646	0.7383	0.5903	0.029*
C26	0.3199 (3)	0.6764 (2)	0.46560 (14)	0.0252 (5)
H26	0.3979	0.7299	0.4577	0.030*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.04558 (16)	0.03697 (14)	0.03348 (13)	0.01019 (15)	−0.00287 (13)	0.00721 (12)
C1	0.0258 (13)	0.0210 (10)	0.0173 (9)	−0.0010 (9)	0.0012 (10)	−0.0001 (9)
O1	0.0473 (13)	0.0280 (9)	0.0236 (7)	−0.0128 (10)	0.0101 (9)	−0.0082 (7)
O2	0.0409 (11)	0.0212 (9)	0.0195 (7)	−0.0053 (8)	0.0122 (8)	−0.0018 (7)
N1	0.0281 (11)	0.0262 (11)	0.0180 (9)	−0.0055 (9)	0.0068 (8)	−0.0077 (8)
N2	0.0271 (10)	0.0270 (10)	0.0154 (8)	0.0011 (8)	0.0064 (9)	−0.0035 (8)
C2	0.0282 (12)	0.0240 (12)	0.0189 (9)	0.0019 (10)	0.0023 (9)	−0.0016 (9)
C11	0.0220 (12)	0.0224 (12)	0.0188 (10)	−0.0060 (10)	0.0024 (9)	−0.0031 (8)
C12	0.0256 (14)	0.0246 (13)	0.0239 (11)	0.0005 (10)	−0.0013 (9)	−0.0013 (9)
C13	0.0303 (16)	0.0316 (14)	0.0338 (13)	0.0099 (12)	0.0025 (11)	−0.0088 (10)
C14	0.0340 (13)	0.0398 (15)	0.0232 (10)	0.0041 (15)	0.0083 (11)	−0.0064 (10)
C15	0.0294 (15)	0.0355 (15)	0.0177 (11)	−0.0026 (12)	0.0026 (10)	−0.0002 (10)
C16	0.0230 (15)	0.0251 (12)	0.0222 (10)	−0.0043 (11)	0.0049 (10)	−0.0022 (9)
O17	0.0472 (13)	0.0501 (13)	0.0204 (8)	0.0101 (10)	0.0085 (8)	0.0074 (9)
C17	0.052 (2)	0.0474 (19)	0.0329 (14)	0.0081 (15)	0.0011 (13)	0.0137 (13)
C21	0.0248 (12)	0.0220 (12)	0.0174 (9)	0.0016 (9)	0.0019 (8)	−0.0023 (8)
C22	0.0321 (13)	0.0262 (11)	0.0197 (9)	−0.0033 (13)	0.0023 (11)	−0.0065 (8)
C23	0.0286 (14)	0.0257 (12)	0.0230 (11)	−0.0080 (10)	0.0052 (10)	−0.0034 (9)
C24	0.0286 (12)	0.0163 (11)	0.0165 (9)	0.0026 (9)	0.0055 (9)	0.0003 (8)
C25	0.0315 (14)	0.0197 (12)	0.0205 (11)	−0.0010 (11)	0.0039 (10)	−0.0054 (9)
C26	0.0265 (13)	0.0241 (11)	0.0248 (10)	−0.0046 (13)	0.0029 (12)	−0.0023 (9)

Geometric parameters (Å, °)

Br1—C12	1.905 (2)	C15—O17	1.373 (3)
C1—O1	1.234 (3)	C15—C16	1.395 (3)
C1—N1	1.338 (3)	C16—H16	0.9500
C1—C11	1.515 (3)	O17—C17	1.434 (4)
O2—C24	1.375 (3)	C17—H17A	0.9800
O2—H2	0.84 (5)	C17—H17B	0.9800
N1—N2	1.398 (3)	C17—H17C	0.9800
N1—H1	0.86 (3)	C21—C22	1.396 (4)
N2—C2	1.282 (3)	C21—C26	1.409 (3)
C2—C21	1.466 (3)	C22—C23	1.390 (3)
C2—H2A	0.9500	C22—H22	0.9500
C11—C12	1.393 (3)	C23—C24	1.394 (3)
C11—C16	1.406 (3)	C23—H23	0.9500
C12—C13	1.397 (3)	C24—C25	1.392 (4)
C13—C14	1.391 (4)	C25—C26	1.393 (3)
C13—H13	0.9500	C25—H25	0.9500
C14—C15	1.390 (4)	C26—H26	0.9500
C14—H14	0.9500		

O1—C1—N1	124.5 (2)	C15—C16—H16	120.1
O1—C1—C11	121.5 (2)	C11—C16—H16	120.1
N1—C1—C11	114.0 (2)	C15—O17—C17	117.1 (2)
C24—O2—H2	110 (3)	O17—C17—H17A	109.5
C1—N1—N2	119.3 (2)	O17—C17—H17B	109.5
C1—N1—H1	117.8 (18)	H17A—C17—H17B	109.5
N2—N1—H1	122.7 (18)	O17—C17—H17C	109.5
C2—N2—N1	114.07 (19)	H17A—C17—H17C	109.5
N2—C2—C21	122.8 (2)	H17B—C17—H17C	109.5
N2—C2—H2A	118.6	C22—C21—C26	119.1 (2)
C21—C2—H2A	118.6	C22—C21—C2	118.8 (2)
C12—C11—C16	119.7 (2)	C26—C21—C2	122.1 (2)
C12—C11—C1	123.5 (2)	C23—C22—C21	121.0 (2)
C16—C11—C1	116.9 (2)	C23—C22—H22	119.5
C11—C12—C13	120.2 (2)	C21—C22—H22	119.5
C11—C12—Br1	121.37 (17)	C22—C23—C24	119.2 (2)
C13—C12—Br1	118.36 (19)	C22—C23—H23	120.4
C14—C13—C12	119.9 (2)	C24—C23—H23	120.4
C14—C13—H13	120.0	O2—C24—C25	122.3 (2)
C12—C13—H13	120.0	O2—C24—C23	116.9 (2)
C15—C14—C13	120.2 (2)	C25—C24—C23	120.9 (2)
C15—C14—H14	119.9	C26—C25—C24	119.7 (2)
C13—C14—H14	119.9	C26—C25—H25	120.1
O17—C15—C14	115.7 (2)	C24—C25—H25	120.1
O17—C15—C16	124.1 (3)	C25—C26—C21	120.1 (2)
C14—C15—C16	120.2 (2)	C25—C26—H26	120.0
C15—C16—C11	119.7 (2)	C21—C26—H26	120.0
O1—C1—N1—N2	−3.6 (4)	C14—C15—C16—C11	−1.5 (4)
C11—C1—N1—N2	179.3 (2)	C12—C11—C16—C15	0.4 (4)
C1—N1—N2—C2	173.1 (2)	C1—C11—C16—C15	−179.2 (2)
N1—N2—C2—C21	178.2 (2)	C14—C15—O17—C17	164.8 (3)
O1—C1—C11—C12	115.3 (3)	C16—C15—O17—C17	−14.7 (4)
N1—C1—C11—C12	−67.5 (3)	N2—C2—C21—C22	−180.0 (2)
O1—C1—C11—C16	−65.2 (3)	N2—C2—C21—C26	−1.1 (4)
N1—C1—C11—C16	112.0 (3)	C26—C21—C22—C23	−0.1 (4)
C16—C11—C12—C13	0.9 (4)	C2—C21—C22—C23	178.7 (2)
C1—C11—C12—C13	−179.6 (2)	C21—C22—C23—C24	−1.7 (4)
C16—C11—C12—Br1	179.08 (19)	C22—C23—C24—O2	−177.9 (2)
C1—C11—C12—Br1	−1.4 (3)	C22—C23—C24—C25	2.3 (4)
C11—C12—C13—C14	−1.1 (4)	O2—C24—C25—C26	179.0 (2)
Br1—C12—C13—C14	−179.3 (2)	C23—C24—C25—C26	−1.2 (4)
C12—C13—C14—C15	−0.1 (4)	C24—C25—C26—C21	−0.6 (4)
C13—C14—C15—O17	−178.2 (3)	C22—C21—C26—C25	1.3 (4)
C13—C14—C15—C16	1.4 (4)	C2—C21—C26—C25	−177.5 (2)
O17—C15—C16—C11	178.0 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

O2—H2···O1^{i}	0.84 (5)	2.07 (4)	2.799 (3)	145 (4)
O2—H2···N2^{i}	0.84 (5)	2.32 (5)	2.995 (3)	137 (4)
N1—H1···O2^{ii}	0.86 (3)	2.01 (3)	2.866 (3)	170 (3)

Symmetry codes: (i) *x*−1/2, −*y*+3/2, −*z*+1; (ii) −*x*+1/2, −*y*+1, *z*−1/2.

Fig. 1

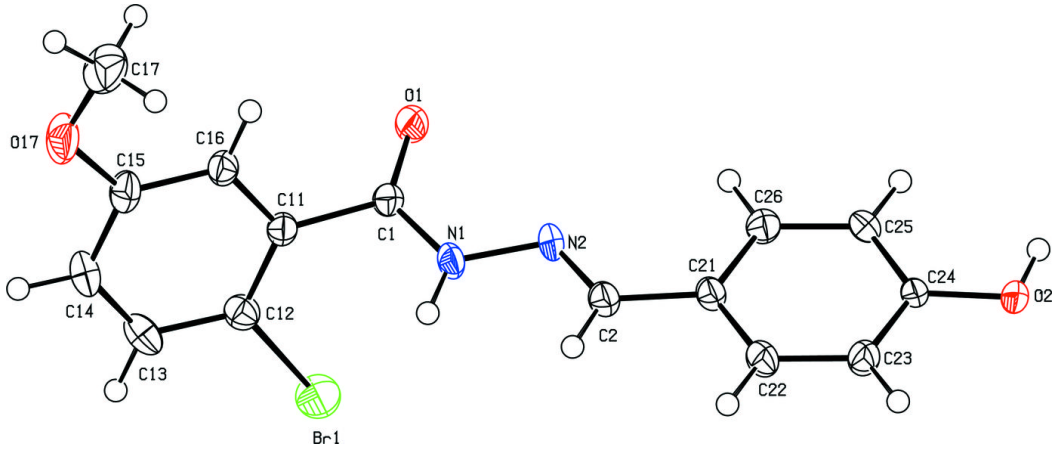
C17
O17
C15
C16
O1
C11
C1
N1
N2
C21
C26
C25
C24
O2
C14
C12
C2
C23
C13
C22
Br1

Fig. 2