Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N′-(2-Bromobenzylidene)-3,4,5-trimethoxybenzohydrazide methanol solvate

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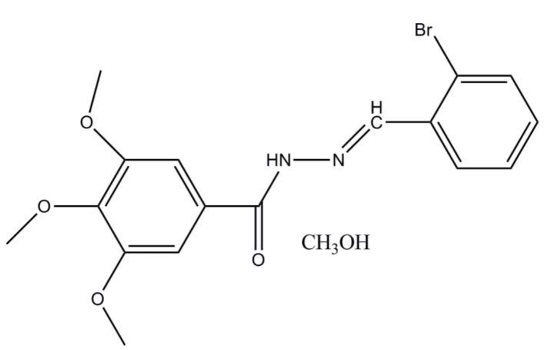
Received 8 July 2008; accepted 13 July 2008

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.005 Å; R factor = 0.030; wR factor = 0.081; data-to-parameter ratio = 15.8.

The title compound, $C_{17}H_{17}BrN_2O_4\cdot CH_4O$, was synthesized by the condensation of 3,4,5-trimethoxybenzohydrazide and 2-bromobenzaldehyde. The two aromatic rings are approximately planar, the dihedral angle being 3.08 (9)°. The molecules are linked by intermolecular N—H⋯O and O—H⋯O hydrogen bonds into chains along the *a* axis.

Related literature

For related literature, see: Constable & Holmes (1987); Ganjali *et al.* (2006); Gardner *et al.* (1991); Jing *et al.* (2006); Kuriakose *et al.* (2007); Patole *et al.* (2003); Zhou *et al.* (2005).



Experimental

Crystal data

$C_{17}H_{17}BrN_2O_4\cdot CH_4O$
M_r = 425.28
Orthorhombic, $Pna2_1$
a = 12.9234 (7) Å
b = 4.9159 (3) Å
c = 29.3975 (17) Å
V = 1867.63 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.23 mm^{-1}
T = 173 (2) K
0.36 × 0.35 × 0.33 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.455, T_{max} = 0.479
8158 measured reflections
3799 independent reflections
3206 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.080
S = 1.04
3799 reflections
240 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Absolute structure: Flack (1983), 1720 Friedel pairs
Flack parameter: −0.008 (8)

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1A⋯O5^{i}	0.88	2.01	2.871 (4)	164
O5—H5⋯O4	0.84	1.96	2.794 (3)	175

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; 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*.

The authors thank the Natural Science Youth Foundation of South China University of Technology for financial assistance (E5050570).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2271).

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supplementary materials

Acta Cryst. (2008). E**64**, o1630 [**doi:10.1107/S1600536808021764**]

N'-(2-Bromobenzylidene)-3,4,5-trimethoxybenzohydrazide methanol solvate

Y.-C. Zhu and **D.-H. He**

Comment

Hydrazones are acknowledged to possess a diverse range of bioactivities; these include antibacterial, antiviral, antineoplastic, and anti-inflammatory (Constable & Holmes, 1987; Ganjali *et al.*, 2006; Gardner *et al.*, 1991; Patole *et al.*, 2003). In addition, many hydrazones have also been used as ligands because they can readily form stable complexes with most metal ions (Kuriakose *et al.*, 2007; Zhou *et al.*, 2005). We report here the synthesis and crystal structure of the title compound, obtained by the condensation of 3,4,5-trimethoxybenzohydrazide and 2-bromobenzaldehyde.

The asymmetric unit of the title compound comprises one *N*'-(2-bromobenzylidene)-3,4,5-trimethoxybenzohydrazide and a methanol solvent molecule (Fig. 1). The two aromatic rings are approximately planar, with a dihedral angle of 3.08 (9)°. Similar geometry has been observed in related hydrazone analogues (Jing *et al.*, 2006). The methanol molecules in the crystal structure are linked to *N*'-(2-bromobenzylidene)-3,4,5-trimethoxybenzohydrazide through intermolecular N—H···O and O—H···O hydrogen bonds into chains along the *a* axis (Fig. 2).

Experimental

A mixture of 3,4,5-trimethoxybenzohydrazide (1 mmol) and 2-bromobenzaldehyde (1 mmol) in anhydrous ethanol (10 ml) was refluxed for 2 h. When the solution was cooled to room temperature, some white needles separated out. After filtration, colorless single crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol solution.

Refinement

All H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with N—H = 0.88 Å, O—H = 0.84 Å, Csp^2—H = 0.95 Å, C(methyl)—H = 0.98 Å and U_{iso}(H) = xU_{eq}(C, N, O), where x = 1.5 for the methyl and hydroxyl groups, x = 1.2 for all other H atoms.

Figures

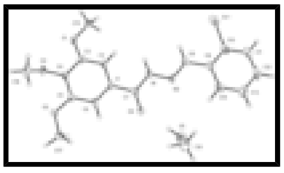

Fig. 1. The structure of the two independent molecules in the asymmetric unit of the title compound, with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are represented by spheres of arbitrary radius.

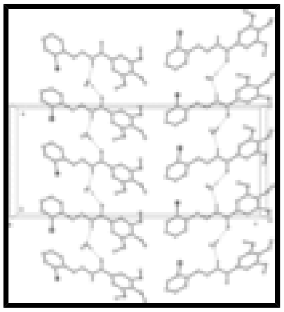

Fig. 2. The packing of the title compound, viewed down the *b* axis. The dashed lines represent the hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

N'-(2-Bromobenzylidene)-3,4,5-trimethoxybenzohydrazide methanol solvate

Crystal data

$C_{17}H_{17}BrN_2O_4 \cdot CH_4O$	F_{000} = 872
M_r = 425.28	D_x = 1.512 Mg m^{-3}
Orthorhombic, $Pna2_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2c -2n	Cell parameters from 4139 reflections
a = 12.9234 (7) Å	θ = 2.8–26.8º
b = 4.9159 (3) Å	μ = 2.23 mm^{-1}
c = 29.3975 (17) Å	*T* = 173 (2) K
V = 1867.63 (19) Å^3	Block, colorless
Z = 4	0.36 × 0.35 × 0.33 mm

Data collection

Bruker SMART 1000 CCD diffractometer	3799 independent reflections
Radiation source: fine-focus sealed tube	3206 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 173(2) K	θ_{max} = 27.0º
ω scans	θ_{min} = 1.4º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	$h = -15 \rightarrow 16$
T_{min} = 0.455, T_{max} = 0.479	$k = -2 \rightarrow 6$
8158 measured reflections	$l = -34 \rightarrow 37$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.030	$w = 1/[\sigma^2(F_o^2) + 0.8008P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.080	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.04	$\Delta\rho_{max}$ = 0.33 e Å^{-3}

3799 reflections	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
240 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 1720 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.008 (8)
Secondary atom site location: difference Fourier map	

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	0.61656 (2)	1.31840 (7)	0.659414 (16)	0.03707 (11)
C1	0.5590 (2)	0.7908 (6)	0.89278 (10)	0.0193 (6)
C2	0.6409 (2)	0.9755 (6)	0.89566 (11)	0.0195 (6)
H2	0.6593	1.0831	0.8701	0.023*
C3	0.6953 (2)	1.0008 (6)	0.93627 (11)	0.0207 (7)
C4	0.6698 (2)	0.8389 (6)	0.97327 (10)	0.0186 (6)
C5	0.5855 (2)	0.6608 (6)	0.97056 (11)	0.0215 (7)
C6	0.5308 (2)	0.6357 (6)	0.93023 (11)	0.0211 (7)
H6	0.4742	0.5129	0.9282	0.025*
C7	0.4968 (2)	0.7557 (6)	0.85047 (11)	0.0212 (7)
C8	0.5282 (3)	0.9221 (7)	0.73624 (12)	0.0276 (7)
H8	0.5962	0.9952	0.7377	0.033*
C9	0.4707 (3)	0.9235 (7)	0.69320 (11)	0.0254 (7)
C10	0.4991 (2)	1.0835 (6)	0.65573 (14)	0.0264 (7)
C11	0.4448 (3)	1.0814 (8)	0.61551 (12)	0.0337 (8)
H11	0.4657	1.1955	0.5911	0.040*
C12	0.3603 (3)	0.9139 (8)	0.61066 (13)	0.0362 (9)
H12	0.3235	0.9084	0.5827	0.043*
C13	0.3292 (3)	0.7520 (8)	0.64720 (12)	0.0344 (9)
H13	0.2709	0.6357	0.6441	0.041*
C14	0.3830 (3)	0.7604 (8)	0.68790 (14)	0.0312 (8)
H14	0.3598	0.6530	0.7127	0.037*
C15	0.8028 (3)	1.3547 (7)	0.90665 (12)	0.0254 (7)
H15A	0.8276	1.2478	0.8807	0.038*
H15B	0.8577	1.4779	0.9168	0.038*
H15C	0.7422	1.4611	0.8975	0.038*
C16	0.7819 (3)	0.6441 (7)	1.02794 (14)	0.0378 (9)

H16A	0.7402	0.4792	1.0242	0.057*
H16B	0.8003	0.6660	1.0601	0.057*
H16C	0.8451	0.6289	1.0097	0.057*
C17	0.4812 (3)	0.3298 (7)	1.00811 (13)	0.0294 (8)
H17A	0.4160	0.4211	1.0006	0.044*
H17B	0.4748	0.2407	1.0378	0.044*
H17C	0.4968	0.1932	0.9848	0.044*
C18	0.2740 (4)	0.2319 (9)	0.78016 (15)	0.0461 (11)
H18A	0.3183	0.2281	0.7531	0.069*
H18B	0.2092	0.1360	0.7737	0.069*
H18C	0.3096	0.1426	0.8055	0.069*
N2	0.4860 (2)	0.8218 (6)	0.77170 (9)	0.0247 (6)
N1	0.5432 (2)	0.8335 (6)	0.81116 (9)	0.0254 (6)
H1A	0.6079	0.8897	0.8109	0.030*
O1	0.77516 (17)	1.1759 (4)	0.94291 (7)	0.0240 (5)
O2	0.72395 (17)	0.8738 (5)	1.01327 (8)	0.0247 (5)
O3	0.56273 (16)	0.5255 (5)	1.00977 (8)	0.0279 (5)
O4	0.40936 (17)	0.6632 (5)	0.85149 (8)	0.0282 (5)
O5	0.25214 (18)	0.5045 (5)	0.79189 (9)	0.0319 (6)
H5	0.2973	0.5615	0.8101	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.03845 (18)	0.03817 (18)	0.03459 (19)	−0.00184 (16)	0.0079 (2)	0.0056 (2)
C1	0.0208 (15)	0.0234 (15)	0.0137 (16)	0.0046 (13)	−0.0037 (12)	−0.0005 (12)
C2	0.0212 (15)	0.0209 (15)	0.0165 (16)	0.0034 (13)	−0.0004 (12)	0.0008 (12)
C3	0.0181 (14)	0.0212 (16)	0.0228 (17)	0.0016 (13)	0.0009 (13)	−0.0054 (13)
C4	0.0209 (15)	0.0203 (15)	0.0144 (16)	0.0027 (13)	−0.0023 (12)	−0.0036 (12)
C5	0.0218 (15)	0.0231 (17)	0.0195 (17)	0.0003 (13)	−0.0024 (13)	0.0030 (13)
C6	0.0201 (15)	0.0238 (16)	0.0194 (17)	0.0007 (13)	−0.0051 (12)	0.0003 (13)
C7	0.0206 (15)	0.0247 (16)	0.0183 (16)	0.0010 (13)	−0.0012 (13)	−0.0004 (12)
C8	0.0235 (16)	0.0360 (18)	0.0232 (18)	−0.0025 (15)	−0.0004 (14)	0.0030 (15)
C9	0.0271 (17)	0.0318 (17)	0.0172 (17)	0.0048 (15)	−0.0029 (13)	−0.0024 (13)
C10	0.0313 (15)	0.0282 (14)	0.0196 (17)	0.0088 (12)	0.0059 (18)	−0.0007 (16)
C11	0.047 (2)	0.037 (2)	0.0170 (18)	0.0092 (18)	0.0041 (16)	0.0035 (15)
C12	0.047 (2)	0.043 (2)	0.0192 (19)	0.0102 (19)	−0.0100 (16)	−0.0003 (16)
C13	0.0344 (18)	0.042 (2)	0.027 (2)	−0.0003 (16)	−0.0079 (16)	−0.0059 (14)
C14	0.033 (2)	0.040 (2)	0.021 (2)	0.0007 (18)	−0.0008 (15)	0.0053 (14)
C15	0.0242 (16)	0.0260 (18)	0.0260 (19)	−0.0014 (15)	0.0021 (14)	−0.0016 (14)
C16	0.040 (2)	0.036 (2)	0.037 (2)	0.0072 (19)	−0.0187 (18)	−0.0032 (17)
C17	0.0250 (17)	0.0339 (19)	0.0294 (19)	−0.0035 (16)	0.0007 (14)	0.0083 (16)
C18	0.057 (3)	0.046 (2)	0.036 (2)	0.011 (2)	−0.004 (2)	−0.0082 (19)
N2	0.0217 (13)	0.0366 (16)	0.0159 (14)	−0.0002 (12)	−0.0058 (11)	0.0011 (12)
N1	0.0185 (13)	0.0413 (18)	0.0162 (14)	−0.0031 (13)	−0.0030 (10)	0.0024 (12)
O1	0.0251 (11)	0.0277 (12)	0.0193 (12)	−0.0046 (10)	−0.0042 (9)	0.0012 (9)
O2	0.0305 (12)	0.0285 (12)	0.0150 (12)	−0.0001 (10)	−0.0068 (10)	−0.0019 (9)
O3	0.0277 (12)	0.0379 (13)	0.0181 (12)	−0.0087 (11)	−0.0042 (10)	0.0067 (10)

O4	0.0232 (11)	0.0409 (14)	0.0205 (13)	−0.0073 (11)	−0.0049 (10)	0.0038 (10)
O5	0.0230 (12)	0.0402 (14)	0.0326 (14)	0.0039 (11)	−0.0045 (11)	−0.0067 (11)

Geometric parameters (Å, °)

Br1—C10	1.911 (3)	C12—H12	0.9500
C1—C6	1.388 (4)	C13—C14	1.384 (5)
C1—C2	1.397 (4)	C13—H13	0.9500
C1—C7	1.491 (4)	C14—H14	0.9500
C2—C3	1.391 (4)	C15—O1	1.427 (4)
C2—H2	0.9500	C15—H15A	0.9800
C3—O1	1.358 (4)	C15—H15B	0.9800
C3—C4	1.388 (4)	C15—H15C	0.9800
C4—O2	1.379 (4)	C16—O2	1.422 (4)
C4—C5	1.400 (5)	C16—H16A	0.9800
C5—O3	1.363 (4)	C16—H16B	0.9800
C5—C6	1.386 (4)	C16—H16C	0.9800
C6—H6	0.9500	C17—O3	1.428 (4)
C7—O4	1.218 (4)	C17—H17A	0.9800
C7—N1	1.357 (4)	C17—H17B	0.9800
C8—N2	1.276 (4)	C17—H17C	0.9800
C8—C9	1.467 (4)	C18—O5	1.412 (5)
C8—H8	0.9500	C18—H18A	0.9800
C9—C14	1.398 (5)	C18—H18B	0.9800
C9—C10	1.402 (5)	C18—H18C	0.9800
C10—C11	1.375 (5)	N2—N1	1.377 (4)
C11—C12	1.375 (6)	N1—H1A	0.8800
C11—H11	0.9500	O5—H5	0.8400
C12—C13	1.396 (5)		
C6—C1—C2	120.5 (3)	C14—C13—H13	119.9
C6—C1—C7	117.1 (3)	C12—C13—H13	119.9
C2—C1—C7	122.3 (3)	C13—C14—C9	121.4 (4)
C3—C2—C1	119.5 (3)	C13—C14—H14	119.3
C3—C2—H2	120.2	C9—C14—H14	119.3
C1—C2—H2	120.2	O1—C15—H15A	109.5
O1—C3—C4	115.6 (3)	O1—C15—H15B	109.5
O1—C3—C2	124.3 (3)	H15A—C15—H15B	109.5
C4—C3—C2	120.1 (3)	O1—C15—H15C	109.5
O2—C4—C3	118.5 (3)	H15A—C15—H15C	109.5
O2—C4—C5	121.4 (3)	H15B—C15—H15C	109.5
C3—C4—C5	119.9 (3)	O2—C16—H16A	109.5
O3—C5—C6	124.7 (3)	O2—C16—H16B	109.5
O3—C5—C4	115.2 (3)	H16A—C16—H16B	109.5
C6—C5—C4	120.1 (3)	O2—C16—H16C	109.5
C5—C6—C1	119.7 (3)	H16A—C16—H16C	109.5
C5—C6—H6	120.2	H16B—C16—H16C	109.5
C1—C6—H6	120.2	O3—C17—H17A	109.5
O4—C7—N1	122.4 (3)	O3—C17—H17B	109.5
O4—C7—C1	121.5 (3)	H17A—C17—H17B	109.5

N1—C7—C1	116.1 (3)	O3—C17—H17C	109.5
N2—C8—C9	119.3 (3)	H17A—C17—H17C	109.5
N2—C8—H8	120.3	H17B—C17—H17C	109.5
C9—C8—H8	120.3	O5—C18—H18A	109.5
C14—C9—C10	116.5 (3)	O5—C18—H18B	109.5
C14—C9—C8	120.3 (3)	H18A—C18—H18B	109.5
C10—C9—C8	123.2 (3)	O5—C18—H18C	109.5
C11—C10—C9	122.6 (3)	H18A—C18—H18C	109.5
C11—C10—Br1	117.3 (3)	H18B—C18—H18C	109.5
C9—C10—Br1	120.1 (3)	C8—N2—N1	116.2 (3)
C12—C11—C10	119.9 (3)	C7—N1—N2	117.9 (3)
C12—C11—H11	120.0	C7—N1—H1A	121.1
C10—C11—H11	120.0	N2—N1—H1A	121.1
C11—C12—C13	119.4 (3)	C3—O1—C15	118.2 (2)
C11—C12—H12	120.3	C4—O2—C16	115.3 (2)
C13—C12—H12	120.3	C5—O3—C17	117.4 (3)
C14—C13—C12	120.2 (4)	C18—O5—H5	109.5

C6—C1—C2—C3	0.9 (4)	C14—C9—C10—C11	−0.5 (5)
C7—C1—C2—C3	179.4 (3)	C8—C9—C10—C11	179.6 (3)
C1—C2—C3—O1	−179.2 (3)	C14—C9—C10—Br1	179.1 (2)
C1—C2—C3—C4	1.5 (4)	C8—C9—C10—Br1	−0.9 (4)
O1—C3—C4—O2	2.0 (4)	C9—C10—C11—C12	−1.2 (5)
C2—C3—C4—O2	−178.6 (3)	Br1—C10—C11—C12	179.2 (3)
O1—C3—C4—C5	177.0 (3)	C10—C11—C12—C13	1.5 (5)
C2—C3—C4—C5	−3.6 (4)	C11—C12—C13—C14	0.0 (6)
O2—C4—C5—O3	−0.7 (4)	C12—C13—C14—C9	−1.8 (6)
C3—C4—C5—O3	−175.6 (3)	C10—C9—C14—C13	1.9 (5)
O2—C4—C5—C6	178.2 (3)	C8—C9—C14—C13	−178.1 (3)
C3—C4—C5—C6	3.3 (4)	C9—C8—N2—N1	−178.4 (3)
O3—C5—C6—C1	177.8 (3)	O4—C7—N1—N2	4.1 (5)
C4—C5—C6—C1	−1.0 (5)	C1—C7—N1—N2	−175.7 (3)
C2—C1—C6—C5	−1.2 (5)	C8—N2—N1—C7	173.1 (3)
C7—C1—C6—C5	−179.7 (3)	C4—C3—O1—C15	−177.9 (3)
C6—C1—C7—O4	21.3 (4)	C2—C3—O1—C15	2.7 (4)
C2—C1—C7—O4	−157.2 (3)	C3—C4—O2—C16	−117.3 (3)
C6—C1—C7—N1	−159.0 (3)	C5—C4—O2—C16	67.8 (4)
C2—C1—C7—N1	22.5 (4)	C6—C5—O3—C17	4.7 (5)
N2—C8—C9—C14	−15.7 (5)	C4—C5—O3—C17	−176.5 (3)
N2—C8—C9—C10	164.3 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O5^{i}	0.88	2.01	2.871 (4)	164
O5—H5···O4	0.84	1.96	2.794 (3)	175

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

Fig. 1

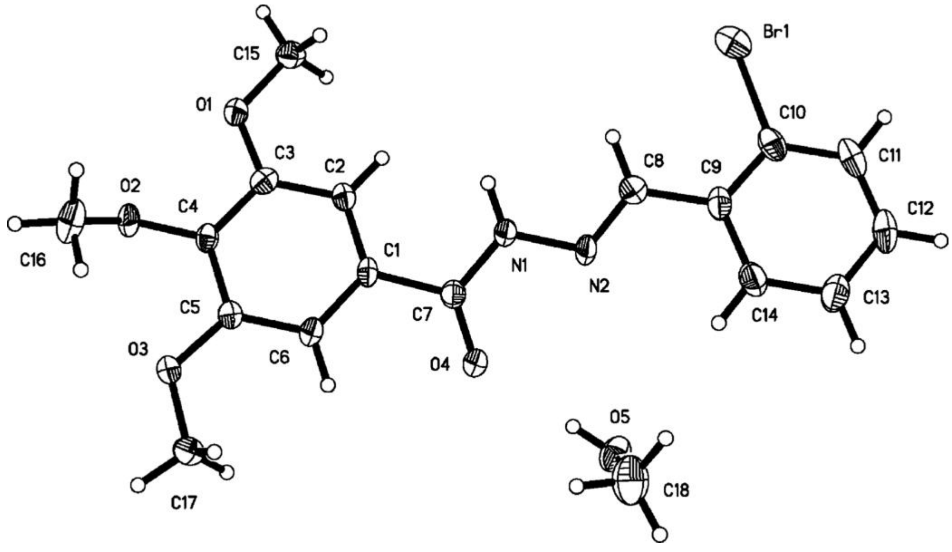
Br1
C15
O1
C10
C3
C2
C8
C9
C11
O2
C4
C12
C16
C1
N1
N2
C5
C7
C14
C13
O3
C6
O4
O5
C18
C17

Fig. 2