organic compounds

4-[(2-Hydroxy-5-nitrobenzylidene)-amino]benzenesulfonamide

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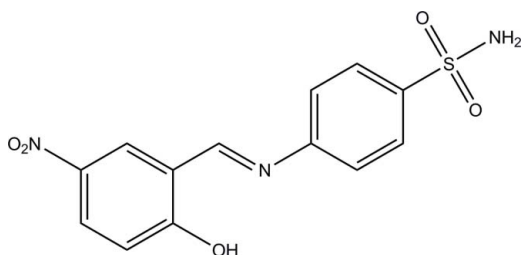
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The title Schiff base compound, $C_{13}H_{11}N_3O_5S$, exists in an *E* configuration with respect to the C=N double bond. The benzene rings are almost coplanar, making a dihedral angle of 2.82 (6). The sulfonamide group is twisted away from the attached phenyl ring with an N—S—C—C torsion angle of 64.84 (11)°. An intramolecular O—H⋯N hydrogen bond stabilizes the molecule, generating an $S(6)$ ring motif. In the crystal, intermolecular N—H⋯O and C—H⋯O hydrogen bonds link the molecules into a three-dimensional network.

Related literature

For background and the biological activity of sulfonamide and its derivatives, see: Kremer *et al.* (2006); Chumakov *et al.* (2006); Mohamed & Sharaby (2007); Wang *et al.* (2010); Sharaby (2007); Aziz-ur-Rehman *et al.* (2010); Subashini *et al.* (2009); Loughrey *et al.* (2009). For a related structure, see: Fun *et al.* (2010). For bond-length data, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).

Experimental

Crystal data

$C_{13}H_{11}N_3O_5S$	$V = 1337.21$ (3) Å^3
$M_r = 321.31$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 6.7698$ (1) Å	$\mu = 0.27$ mm^{-1}
$b = 26.4754$ (3) Å	$T = 100$ K
$c = 9.9683$ (1) Å	$0.41 \times 0.27 \times 0.06$ mm
$\beta = 131.544$ (1)°	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	29377 measured reflections
	4825 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)	4104 reflections with $I > 2\sigma(I)$
$T_{min} = 0.896$, $T_{max} = 0.985$	$R_{int} = 0.031$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.110$	
$S = 1.06$	
4825 reflections	$\Delta\rho_{max} = 0.60$ e Å^{-3}
211 parameters	$\Delta\rho_{min} = -0.43$ e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N2—H2N2⋯O5[i]	0.82 (3)	2.07 (3)	2.891 (2)	172 (3)
N2—H1N2⋯O2[ii]	0.84 (3)	2.58 (2)	3.1378 (15)	125 (2)
N2—H1N2⋯O4[iii]	0.84 (3)	2.11 (3)	2.883 (2)	153 (2)
O1—H1O1⋯N1	0.96 (3)	1.67 (3)	2.5626 (15)	154 (4)
C5—H5A⋯O3[iv]	0.93	2.55	3.3350 (17)	143
C7—H7A⋯O3[iv]	0.93	2.36	3.187 (2)	148
C10—H10A⋯O1[v]	0.93	2.58	3.1861 (19)	123

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; 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* and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5036).

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supplementary materials

4-[(2-Hydroxy-5-nitrobenzylidene)amino]benzenesulfonamide

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Comment

Sulfanilamide which is also known as sulfonamide and its derivatives are extensively used in medicine as they possess a wide range of medicinal, pharmacological and antimicrobial properties (Kremer *et al.*, 2006, Chumakov *et al.*, 2006). Sulfanilamide was the first drug that had been found to be used as a preventive and therapeutic agent towards a variety of diseases or bacterial infections in human biological systems. Schiff bases derived from sulfanilamide exhibit various pharmacological activities including antibacterial, antifungal, antiviral, antimicrobial, anticonvulsant, antitumor, antiulcer, anti-neoplastic, and anti-inflammatory properties as well as acting as enzymatic inhibitors (Wang *et al.*, 2010, Sharaby, 2007, Kremer *et al.*, 2006, Chumakov *et al.*, 2006, Aziz-ur-Rehman *et al.*, 2010, Subashini *et al.*, 2009, Loughrey *et al.*, 2009). The biological activity could be increased by the complexation with metal ions (Mohamed & Sharaby, 2007; Kremer *et al.*, 2006).

The title Schiff base compound (Fig. 1) exists in an *E* configuration with respect to the C7═N1 double bond. The phenyl rings (C1–C6 & C8–C13) are almost coplanar with each other with a dihedral angle of 2.82 (6)°. The sulfonamide group (S1/O3/O4/N2) is twisted away from the attached phenyl ring with the torsion angle between N2–S1–C11–C12 being 64.84 (11)°. An intramolecular O1—H1O1···N1 hydrogen bond stabilized the molecule, generating an *S*(6) ring motif (Bernstein *et al.*, 1995). Bond lengths (Allen *et al.*, 1987) and angles are within the normal ranges and are comparable to the related structure (Fun *et al.*, 2010).

In the crystal packing (Fig. 2), intermolecular N2—H2N2···O5, N2—H1N2···O2, N2—H1N2···O4, C5—H5A···O3, C7—H7A···O3 and C10—H10A···O1 hydrogen bonds (Table 1) link the molecules into three-dimensional network.

Experimental

The title compound was synthesized by the general method of condensation of sulfanilamide with 2-hydroxy-5-nitrobenzaldehyde. To a methanolic solution (10 ml) of sulfanilamide (0.3444 g, 2 mmol), sodium acetate (0.1641 g, 2 mmol) was added. The resulting solution was heated to reflux on a water bath. A methanolic solution (10 ml) of 2-hydroxy-5-nitrobenzaldehyde (0.3342 g, 2 mmol) was then added dropwise to the solution. The solution was left under reflux (65–70°C) for 1 h. After half an hour, yellowish orange precipitate started to form during refluxing. The resulting mixture was filtered and the filtrate was left to evaporate slowly at room temperature. Orange crystals of the title compound suitable for X-ray diffraction were obtained after 1 week.

Refinement

N– and O– bound H atoms were located from difference Fourier map and refined freely with the N–H bond lengths being 0.83 (2) to 0.84 (2) Å and the O–H distance 0.96 (3) Å. The remaining H atoms were positioned geometrically and refined using a riding model, with $U_{iso}(H) = 1.2\ U_{eq}(C)$ [C–H = 0.93 Å].
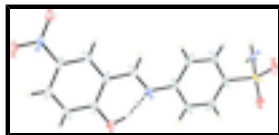
supplementary materials

Figures

Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme. The dashed line indicates the intramolecular hydrogen bond.

Fig. 2. The crystal packing of the title compound, viewed along the *a* axis, showing the three-dimensional network. Intermolecular interactions are shown as dashed lines. H atoms not involved in the intermolecular interactions (dashed lines) have been omitted for clarity.

4-[(2-Hydroxy-5-nitrobenzylidene)amino]benzenesulfonamide

Crystal data

$C_{13}H_{11}N_3O_5S$	$F(000) = 664$
$M_r = 321.31$	$D_x = 1.596$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 9950 reflections
$a = 6.7698$ (1) Å	$\theta = 2.8–35.5°$
$b = 26.4754$ (3) Å	$\mu = 0.27$ mm^{-1}
$c = 9.9683$ (1) Å	$T = 100$ K
$\beta = 131.544$ (1)°	Plate, orange
$V = 1337.21$ (3) Å^3	$0.41 \times 0.27 \times 0.06$ mm
$Z = 4$	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	4825 independent reflections
Radiation source: fine-focus sealed tube	4104 reflections with $I > 2\sigma(I)$

graphite	$R_{int} = 0.031$
φ and ω scans	$\theta_{max} = 32.5°$, $\theta_{min} = 2.8°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)	$h = -10 \rightarrow 10$
$T_{min} = 0.896$, $T_{max} = 0.985$	$k = -40 \rightarrow 36$
29377 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.039$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.110$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2 + 0.7191P]$ where $P = (F_o^2 + 2F_c^2)/3$
4825 reflections	$(\Delta/\sigma)_{max} = 0.002$
211 parameters	$\Delta\rho_{max} = 0.60$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.43$ e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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	$U_{iso}*/U_{eq}$
S1	0.25811 (6)	0.770137 (11)	0.29838 (4)	0.01433 (8)
O1	0.69814 (19)	1.06412 (4)	0.38905 (13)	0.01833 (18)
O2	1.2322 (2)	1.14670 (4)	0.11034 (15)	0.0251 (2)
O3	1.1687 (2)	1.06896 (4)	0.02207 (13)	0.0217 (2)
O4	0.46897 (19)	0.73446 (4)	0.38253 (15)	0.0264 (2)
O5	0.1385 (2)	0.77870 (4)	0.37367 (14)	0.0243 (2)
N1	0.6474 (2)	0.97162 (4)	0.29501 (13)	0.01443 (19)
N2	0.0283 (2)	0.75128 (4)	0.09717 (14)	0.01538 (19)
N3	1.1534 (2)	1.10368 (4)	0.09747 (14)	0.0166 (2)

C1	0.8033 (2)	1.07306 (5)	0.31518 (15)	0.0146 (2)
C2	0.8745 (2)	1.12251 (5)	0.31389 (16)	0.0169 (2)
H2A	0.8429	1.1487	0.3599	0.020*
C3	0.9919 (2)	1.13262 (5)	0.24433 (16)	0.0167 (2)
H3A	1.0412	1.1654	0.2442	0.020*
C4	1.0352 (2)	1.09290 (5)	0.17442 (15)	0.0142 (2)
C5	0.9623 (2)	1.04378 (5)	0.17048 (15)	0.0146 (2)
H5A	0.9913	1.0181	0.1215	0.018*
C6	0.8442 (2)	1.03309 (5)	0.24119 (15)	0.0139 (2)
C7	0.7632 (2)	0.98178 (5)	0.23515 (16)	0.0158 (2)
H7A	0.7949	0.9561	0.1879	0.019*
C8	0.5618 (2)	0.92230 (5)	0.29004 (15)	0.0135 (2)
C9	0.4354 (2)	0.91795 (5)	0.35687 (16)	0.0152 (2)
H9A	0.4130	0.9465	0.4000	0.018*
C10	0.3425 (2)	0.87159 (5)	0.35986 (16)	0.0158 (2)
H10A	0.2583	0.8689	0.4045	0.019*
C11	0.3773 (2)	0.82917 (5)	0.29516 (15)	0.0139 (2)
C12	0.5046 (2)	0.83273 (5)	0.22825 (16)	0.0163 (2)
H12A	0.5280	0.8040	0.1862	0.020*
C13	0.5958 (2)	0.87914 (5)	0.22483 (16)	0.0164 (2)
H13A	0.6792	0.8818	0.1796	0.020*
H2N2	0.074 (4)	0.7439 (7)	0.041 (3)	0.028 (5)*
H1N2	−0.119 (4)	0.7655 (8)	0.038 (3)	0.030 (5)*
H1O1	0.655 (5)	1.0290 (11)	0.368 (4)	0.068 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01492 (14)	0.01229 (14)	0.01464 (13)	−0.00158 (10)	0.00933 (11)	0.00082 (9)
O1	0.0243 (5)	0.0160 (5)	0.0229 (4)	0.0000 (4)	0.0191 (4)	−0.0007 (3)
O2	0.0303 (5)	0.0155 (5)	0.0373 (5)	−0.0009 (4)	0.0257 (5)	0.0052 (4)
O3	0.0270 (5)	0.0219 (5)	0.0227 (4)	−0.0038 (4)	0.0192 (4)	−0.0036 (4)
O4	0.0152 (4)	0.0161 (5)	0.0320 (5)	0.0019 (4)	0.0090 (4)	0.0079 (4)
O5	0.0372 (6)	0.0225 (5)	0.0267 (5)	−0.0090 (4)	0.0268 (5)	−0.0048 (4)
N1	0.0162 (4)	0.0123 (5)	0.0157 (4)	−0.0014 (4)	0.0110 (4)	−0.0003 (3)
N2	0.0137 (4)	0.0156 (5)	0.0161 (4)	−0.0005 (4)	0.0096 (4)	−0.0019 (4)
N3	0.0167 (5)	0.0155 (5)	0.0175 (4)	0.0006 (4)	0.0112 (4)	0.0032 (4)
C1	0.0147 (5)	0.0149 (5)	0.0142 (4)	0.0010 (4)	0.0096 (4)	0.0005 (4)
C2	0.0200 (5)	0.0117 (5)	0.0197 (5)	0.0014 (4)	0.0134 (5)	−0.0002 (4)
C3	0.0170 (5)	0.0134 (5)	0.0181 (5)	0.0001 (4)	0.0110 (5)	0.0010 (4)
C4	0.0148 (5)	0.0132 (5)	0.0146 (5)	−0.0003 (4)	0.0098 (4)	0.0011 (4)
C5	0.0179 (5)	0.0118 (5)	0.0154 (5)	−0.0005 (4)	0.0116 (4)	−0.0002 (4)
C6	0.0165 (5)	0.0118 (5)	0.0143 (4)	−0.0007 (4)	0.0105 (4)	−0.0006 (4)
C7	0.0195 (5)	0.0134 (5)	0.0171 (5)	−0.0009 (4)	0.0132 (5)	−0.0005 (4)
C8	0.0136 (5)	0.0122 (5)	0.0137 (4)	−0.0007 (4)	0.0087 (4)	−0.0002 (4)
C9	0.0183 (5)	0.0127 (5)	0.0185 (5)	−0.0005 (4)	0.0138 (5)	−0.0016 (4)
C10	0.0173 (5)	0.0158 (6)	0.0178 (5)	−0.0015 (4)	0.0132 (5)	−0.0012 (4)
C11	0.0143 (5)	0.0129 (5)	0.0139 (4)	−0.0017 (4)	0.0091 (4)	−0.0005 (4)

C12	0.0196 (5)	0.0138 (5)	0.0187 (5)	−0.0021 (4)	0.0140 (5)	−0.0030 (4)
C13	0.0202 (5)	0.0146 (6)	0.0199 (5)	−0.0020 (4)	0.0157 (5)	−0.0022 (4)

Geometric parameters (Å, °)

S1—O4	1.4301 (10)	C3—C4	1.3958 (17)
S1—O5	1.4408 (10)	C3—H3A	0.9300
S1—N2	1.5980 (11)	C4—C5	1.3822 (17)
S1—C11	1.7689 (12)	C5—C6	1.4014 (15)
O1—C1	1.3417 (14)	C5—H5A	0.9300
O1—H1O1	0.96 (3)	C6—C7	1.4513 (17)
O2—N3	1.2278 (14)	C7—H7A	0.9300
O3—N3	1.2345 (14)	C8—C9	1.3951 (15)
N1—C7	1.2892 (15)	C8—C13	1.4068 (16)
N1—C8	1.4160 (16)	C9—C10	1.3881 (17)
N2—H2N2	0.83 (2)	C9—H9A	0.9300
N2—H1N2	0.84 (2)	C10—C11	1.3908 (17)
N3—C4	1.4576 (15)	C10—H10A	0.9300
C1—C2	1.3982 (17)	C11—C12	1.3999 (16)
C1—C6	1.4181 (16)	C12—C13	1.3855 (17)
C2—C3	1.3837 (17)	C12—H12A	0.9300
C2—H2A	0.9300	C13—H13A	0.9300
O4—S1—O5	119.05 (7)	C4—C5—H5A	120.4
O4—S1—N2	106.97 (6)	C6—C5—H5A	120.4
O5—S1—N2	106.71 (6)	C5—C6—C1	118.97 (11)
O4—S1—C11	107.71 (6)	C5—C6—C7	119.61 (10)
O5—S1—C11	106.92 (6)	C1—C6—C7	121.42 (10)
N2—S1—C11	109.23 (6)	N1—C7—C6	120.34 (11)
C1—O1—H1O1	104.2 (17)	N1—C7—H7A	119.8
C7—N1—C8	122.45 (11)	C6—C7—H7A	119.8
S1—N2—H2N2	115.9 (13)	C9—C8—C13	119.57 (11)
S1—N2—H1N2	117.2 (14)	C9—C8—N1	115.21 (10)
H2N2—N2—H1N2	115.7 (19)	C13—C8—N1	125.21 (10)
O2—N3—O3	123.25 (11)	C10—C9—C8	120.88 (11)
O2—N3—C4	118.61 (11)	C10—C9—H9A	119.6
O3—N3—C4	118.14 (10)	C8—C9—H9A	119.6
O1—C1—C2	118.81 (11)	C9—C10—C11	119.06 (10)
O1—C1—C6	120.75 (11)	C9—C10—H10A	120.5
C2—C1—C6	120.44 (11)	C11—C10—H10A	120.5
C3—C2—C1	120.11 (11)	C10—C11—C12	120.90 (11)
C3—C2—H2A	119.9	C10—C11—S1	119.05 (9)
C1—C2—H2A	119.9	C12—C11—S1	120.04 (9)
C2—C3—C4	119.01 (11)	C13—C12—C11	119.77 (11)
C2—C3—H3A	120.5	C13—C12—H12A	120.1
C4—C3—H3A	120.5	C11—C12—H12A	120.1
C5—C4—C3	122.27 (11)	C12—C13—C8	119.81 (10)
C5—C4—N3	118.65 (11)	C12—C13—H13A	120.1
C3—C4—N3	119.05 (11)	C8—C13—H13A	120.1
C4—C5—C6	119.17 (11)		

O1—C1—C2—C3	177.73 (11)	C1—C6—C7—N1	1.12 (18)
C6—C1—C2—C3	−1.66 (18)	C7—N1—C8—C9	−178.76 (11)
C1—C2—C3—C4	0.62 (18)	C7—N1—C8—C13	1.41 (19)
C2—C3—C4—C5	0.68 (19)	C13—C8—C9—C10	−0.02 (18)
C2—C3—C4—N3	178.64 (11)	N1—C8—C9—C10	−179.86 (11)
O2—N3—C4—C5	−175.78 (11)	C8—C9—C10—C11	0.06 (19)
O3—N3—C4—C5	4.36 (16)	C9—C10—C11—C12	0.21 (18)
O2—N3—C4—C3	6.19 (17)	C9—C10—C11—S1	−179.82 (9)
O3—N3—C4—C3	−173.67 (11)	O4—S1—C11—C10	−128.97 (10)
C3—C4—C5—C6	−0.92 (18)	O5—S1—C11—C10	0.07 (12)
N3—C4—C5—C6	−178.88 (10)	N2—S1—C11—C10	115.18 (10)
C4—C5—C6—C1	−0.13 (17)	O4—S1—C11—C12	51.00 (12)
C4—C5—C6—C7	179.03 (11)	O5—S1—C11—C12	−179.95 (10)
O1—C1—C6—C5	−177.97 (11)	N2—S1—C11—C12	−64.84 (11)
C2—C1—C6—C5	1.41 (18)	C10—C11—C12—C13	−0.51 (18)
O1—C1—C6—C7	2.88 (18)	S1—C11—C12—C13	179.51 (10)
C2—C1—C6—C7	−177.74 (11)	C11—C12—C13—C8	0.55 (19)
C8—N1—C7—C6	179.21 (11)	C9—C8—C13—C12	−0.29 (18)
C5—C6—C7—N1	−178.02 (11)	N1—C8—C13—C12	179.54 (11)

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2N2···O5[i]	0.82 (3)	2.07 (3)	2.891 (2)	172 (3)
N2—H1N2···O2[ii]	0.84 (3)	2.58 (2)	3.1378 (15)	125 (2)
N2—H1N2···O4[iii]	0.84 (3)	2.11 (3)	2.883 (2)	153 (2)
O1—H1O1···N1	0.96 (3)	1.67 (3)	2.5626 (15)	154 (4)
C5—H5A···O3[iv]	0.93	2.55	3.3350 (17)	143
C7—H7A···O3[iv]	0.93	2.36	3.187 (2)	148
C10—H10A···O1[v]	0.93	2.58	3.1861 (19)	123

Symmetry codes: (i) x, $-y+3/2$, $z-1/2$; (ii) $-x+1$, $-y+2$, $-z$; (iii) $x-1$, $-y+3/2$, $z-1/2$; (iv) $-x+2$, $-y+2$, $-z$; (v) $-x+1$, $-y+2$, $-z+1$.
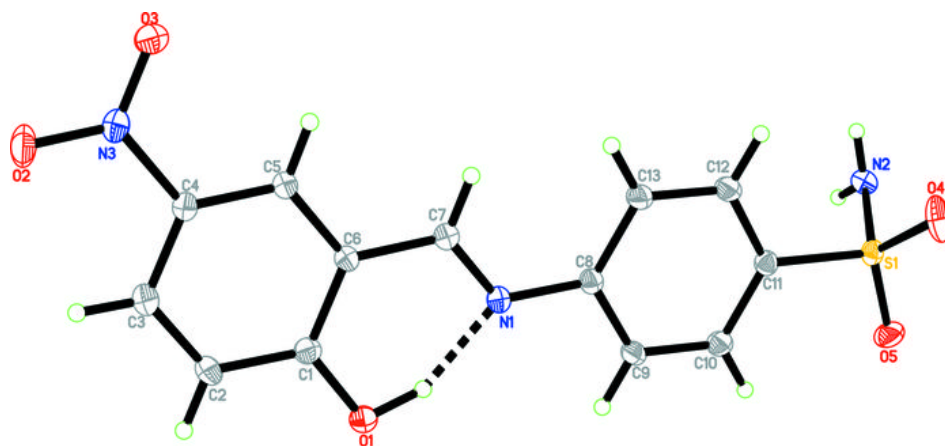
Fig. 1

Fig. 2