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N-(2-Chlorobenzoyl)-3-nitrobenzene-sulfonamide

P. A. Suchetan,[a] Sabine Foro[b] and B. Thimme Gowda[a]*

[a]Department of Chemistry, Mangalore University, Mangalagangotri 574 199, Mangalore, India, and [b]Institute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287 Darmstadt, Germany
Correspondence e-mail: gowdabt@yahoo.com

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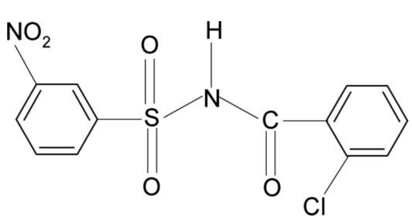
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.058; wR factor = 0.104; data-to-parameter ratio = 14.1.

In the molecule of the title compound, $C_{13}H_9ClN_2O_5S$, the dihedral angle between the two aromatic rings is 84.3 (1)°. In the crystal, molecules are linked into chains *via* N—H···O(S) hydrogen bonds.

Related literature

For studies, including ours, of the effects of substituents on the structures and other aspects of *N*-(aryl)-amides, see: Bowes *et al.* (2003); Gowda *et al.* (1999, 2003); of *N*-(aryl)-methanesulfonamides, see: Gowda *et al.* (2007); of *N*-(aryl)-arylsulfonamides, see: Shetty & Gowda (2005); of *N*-(substituted benzoyl)-arylsulfonamides, see: Suchetan *et al.* (2012); of *N*-chloroarylamides, see: Jyothi & Gowda (2004); and of *N*-bromoarylsulfonamides, see: Usha & Gowda (2006).



Experimental

Crystal data

$C_{13}H_9ClN_2O_5S$
M_r = 340.73
Monoclinic, $P2_1/n$
a = 14.606 (2) Å
b = 5.1159 (4) Å
c = 18.742 (2) Å
β = 93.336 (9)°
V = 1398.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 293 K
0.36 × 0.10 × 0.06 mm

Data collection

Oxford Xcalibur diffractometer with Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
T_{min} = 0.855, T_{max} = 0.974
5313 measured reflections
2844 independent reflections
2005 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.104
S = 1.19
2844 reflections
202 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O2^i	0.83 (2)	2.09 (2)	2.919 (3)	173 (3)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *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: BT5798).

References

Bowes, K. F., Glidewell, C., Low, J. N., Skakle, J. M. S. & Wardell, J. L. (2003). *Acta Cryst.* C**59**, o1–o3.
Gowda, B. T., Bhat, D. K., Fuess, H. & Weiss, A. (1999). *Z. Naturforsch. Teil A*, **54**, 261–267.
Gowda, B. T., Foro, S. & Fuess, H. (2007). *Acta Cryst.* E**63**, o2337.
Gowda, B. T., Usha, K. M. & Jayalakshmi, K. L. (2003). *Z. Naturforsch. Teil A*, **61**, 801–806.
Jyothi, K. & Gowda, B. T. (2004). *Z. Naturforsch. Teil A*, **59**, 64–68.
Oxford Diffraction (2009). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Yarnton, Oxfordshire, England.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shetty, M. & Gowda, B. T. (2005). *Z. Naturforsch. Teil A*, **60**, 113–120.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Suchetan, P. A., Foro, S. & Gowda, B. T. (2012). *Acta Cryst.* E**68**, o244.
Usha, K. M. & Gowda, B. T. (2006). *J. Chem. Sci.* **118**, 351–359.

supplementary materials

Acta Cryst. (2012). E**68**, o543 [**doi:10.1107/S1600536812003236**]

N-(2-Chlorobenzoyl)-3-nitrobenzenesulfonamide

P. A. Suchetan, S. Foro and B. T. Gowda

Comment

Diaryl acylsulfonamides are known as potent antitumor agents against a broad spectrum of human tumor xenografts in nude mice. As part of our studies on the substituent effects on the structures and other aspects of *N*-(aryl)-amides (Bowes *et al.*, 2003; Gowda *et al.*, 1999, 2003), *N*-(aryl)-methanesulfonamides (Gowda *et al.*, 2007), *N*-(aryl)-arylsulfonamides (Shetty & Gowda, 2005); *N*-(substitutedbenzoyl)-arylsulfonamides (Suchetan *et al.*, 2012); *N*-chloroarylsulfonamides (Jyothi & Gowda, 2004) and *N*-bromoarylsulfonamides (Usha & Gowda, 2006), in the present work, the crystal structure of *N*-(2-chlorobenzoyl)-3-nitrobenzenesulfonamide (I) has been determined (Fig.1).

The conformation between the N—H and C═O bonds in the C—SO_2—NH—C(O) segment is *anti* and the N—C bond in the segment has *gauche* torsion with respect to the S═O bonds (Fig. 1), similar to that observed in *N*-(3-chlorobenzoyl)-3-nitrobenzene-sulfonamide (II) (Suchetan *et al.*, 2012). Further, in (I), the conformation between the N—H bond and the *meta*-nitro group in the sulfonyl benzene ring is *syn*, similar to that observed in (II). The conformation of the C═O is also *syn* to the *ortho*-Cl atom in the benzoyl ring, in contrast to the *anti* conformation observed between the C═O and the *meta*-Cl atom in (II)

The molecule is twisted at the S—N bond with the torsional angle of -61.82 (29)°, compared to the value of -60.40 (29)° in (II).

The dihedral angle between the sulfonyl benzene ring and the —SO_2—NH—C—O segment is 80.4 (1)°, compared to the value of 77.0 (1)° in (II). Furthermore, the dihedral angle between the sulfonyl and the benzoyl benzene rings is 84.3 (1)°, compared to the value of 83.5 (1)° in (II).

The packing of molecules linked by of N—H···O(S) hydrogen bonds (Table 1) is shown in Fig. 2.

Experimental

The title compound was prepared by refluxing a mixture of 2-chlorobenzoic acid (0.02 mole), 3-nitrobenzenesulfonamide (0.02 mole) and excess phosphorous oxychloride for 3 h on a water bath. The resultant mixture was cooled and poured into crushed ice. The solid, *N*-(2-chlorobenzoyl)-3-nitrobenzenesulfonamide, obtained was filtered, washed thoroughly with water and then dissolved in sodium bicarbonate solution. The compound was later reprecipitated by acidifying the filtered solution with dilute HCl. It was filtered, dried and recrystallized.

Rod like colourless single crystals of the title compound used in X-ray diffraction studies were obtained by slow evaporation of its toluene solution at room temperature.

Refinement

The H atom of the NH group was located in a difference map and later restrained to N—H = 0.86 (2) %A. The other H atoms were positioned with idealized geometry using a riding model with C—H = 0.93 Å. All H atoms were refined with isotropic displacement parameters (set to 1.2 times of the U_{eq} of the parent atom).

Figures

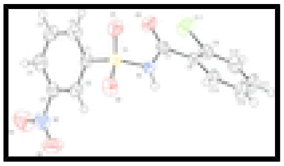

Fig. 1. Molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

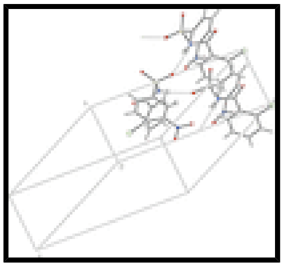

Fig. 2. Molecular packing in the title compound. Hydrogen bonds are shown as dashed lines.

N-(2-Chlorobenzoyl)-3-nitrobenzenesulfonamide

Crystal data

$C_{13}H_9ClN_2O_5S$	$F(000) = 696$
$M_r = 340.73$	$D_x = 1.619$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 1612 reflections
$a = 14.606$ (2) Å	$\theta = 2.6–27.7°$
$b = 5.1159$ (4) Å	$\mu = 0.45$ mm^{-1}
$c = 18.742$ (2) Å	$T = 293$ K
$\beta = 93.336$ (9)°	Rod, colourless
$V = 1398.1$ (3) Å^3	0.36 × 0.10 × 0.06 mm
$Z = 4$	

Data collection

Oxford Xcalibur diffractometer with Sapphire CCD detector	2844 independent reflections
Radiation source: fine-focus sealed tube	2005 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.028$
Rotation method data acquisition using ω scans	$\theta_{max} = 26.4°$, $\theta_{min} = 3.4°$
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)	$h = -17\rightarrow18$

T_{min} = 0.855, T_{max} = 0.974	k = −6→6
5313 measured reflections	l = −23→14

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.058	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.104	H atoms treated by a mixture of independent and constrained refinement
S = 1.19	$w = 1/[\sigma^2(F_o^2) + (0.0156P)^2 + 1.9016P]$ where $P = (F_o^2 + 2F_c^2)/3$
2844 reflections	$(\Delta/\sigma)_{max}$ = 0.001
202 parameters	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
1 restraint	$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Special details

Experimental. CrysAlis RED (Oxford Diffraction, 2009) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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}
C1	0.1617 (2)	0.3605 (6)	0.91163 (16)	0.0303 (7)
C2	0.2244 (2)	0.5563 (6)	0.92952 (17)	0.0327 (8)
H2	0.2658	0.6146	0.8971	0.039*
C3	0.2233 (2)	0.6616 (7)	0.99714 (17)	0.0340 (8)
C4	0.1637 (2)	0.5785 (7)	1.04683 (18)	0.0405 (9)
H4	0.1647	0.6535	1.0921	0.049*
C5	0.1028 (3)	0.3823 (8)	1.02791 (18)	0.0454 (10)
H5	0.0627	0.3218	1.0610	0.055*
C6	0.1003 (2)	0.2736 (7)	0.96009 (18)	0.0395 (9)
H6	0.0580	0.1437	0.9472	0.047*
C7	0.0183 (2)	0.4942 (6)	0.77389 (16)	0.0301 (7)
C8	−0.0148 (2)	0.6786 (6)	0.71599 (16)	0.0292 (7)
C9	−0.0867 (2)	0.8548 (7)	0.72383 (17)	0.0343 (8)

C10	−0.1108 (3)	1.0338 (7)	0.67100 (19)	0.0443 (9)
H10	−0.1579	1.1521	0.6774	0.053*
C11	−0.0651 (3)	1.0377 (8)	0.60867 (19)	0.0498 (10)
H11	−0.0807	1.1605	0.5735	0.060*
C12	0.0037 (3)	0.8594 (8)	0.59861 (18)	0.0491 (10)
H12	0.0333	0.8586	0.5560	0.059*
C13	0.0285 (2)	0.6831 (7)	0.65139 (16)	0.0381 (8)
H13	0.0751	0.5639	0.6440	0.046*
N1	0.10998 (18)	0.4193 (5)	0.76979 (13)	0.0299 (6)
H1N	0.1464 (19)	0.515 (6)	0.7492 (16)	0.036*
N2	0.2880 (2)	0.8740 (6)	1.01653 (16)	0.0460 (8)
O1	0.11150 (18)	−0.0212 (4)	0.82834 (12)	0.0460 (7)
O2	0.25475 (16)	0.2152 (5)	0.80566 (12)	0.0443 (6)
O3	−0.02699 (16)	0.4097 (5)	0.82055 (12)	0.0427 (6)
O4	0.2823 (2)	0.9787 (6)	1.07436 (15)	0.0686 (9)
O5	0.3436 (2)	0.9354 (6)	0.97376 (15)	0.0724 (10)
Cl1	−0.14856 (7)	0.8669 (2)	0.80000 (5)	0.0528 (3)
S1	0.16187 (6)	0.21592 (16)	0.82617 (4)	0.0321 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0364 (18)	0.0269 (18)	0.0272 (16)	0.0043 (16)	−0.0002 (14)	0.0024 (14)
C2	0.0375 (19)	0.0297 (19)	0.0310 (17)	0.0041 (16)	0.0042 (14)	0.0028 (15)
C3	0.0378 (19)	0.0322 (19)	0.0314 (17)	0.0017 (17)	−0.0026 (14)	−0.0030 (15)
C4	0.045 (2)	0.046 (2)	0.0303 (18)	0.0063 (19)	0.0006 (16)	−0.0068 (17)
C5	0.046 (2)	0.058 (3)	0.0327 (18)	−0.002 (2)	0.0094 (16)	0.0058 (19)
C6	0.039 (2)	0.042 (2)	0.0374 (19)	−0.0046 (18)	0.0026 (15)	0.0026 (17)
C7	0.0307 (18)	0.0299 (18)	0.0295 (17)	−0.0044 (15)	0.0009 (14)	−0.0040 (15)
C8	0.0277 (17)	0.0306 (18)	0.0289 (16)	−0.0040 (15)	−0.0030 (13)	−0.0012 (14)
C9	0.0305 (18)	0.041 (2)	0.0316 (17)	−0.0018 (17)	0.0004 (14)	−0.0038 (16)
C10	0.042 (2)	0.043 (2)	0.047 (2)	0.0105 (19)	−0.0038 (17)	0.0013 (19)
C11	0.060 (3)	0.051 (3)	0.037 (2)	0.012 (2)	−0.0019 (19)	0.0154 (19)
C12	0.054 (2)	0.063 (3)	0.0307 (19)	0.008 (2)	0.0058 (17)	0.0055 (19)
C13	0.0383 (19)	0.049 (2)	0.0272 (17)	0.0081 (18)	0.0031 (14)	0.0026 (17)
N1	0.0308 (16)	0.0316 (16)	0.0275 (14)	−0.0010 (13)	0.0019 (11)	0.0052 (12)
N2	0.052 (2)	0.0432 (19)	0.0419 (18)	−0.0030 (17)	−0.0049 (16)	−0.0041 (16)
O1	0.0690 (18)	0.0245 (13)	0.0436 (14)	−0.0033 (13)	−0.0048 (13)	0.0003 (11)
O2	0.0416 (14)	0.0530 (16)	0.0385 (13)	0.0174 (13)	0.0040 (11)	−0.0081 (12)
O3	0.0404 (14)	0.0489 (16)	0.0397 (13)	0.0002 (13)	0.0118 (11)	0.0108 (12)
O4	0.076 (2)	0.070 (2)	0.0592 (18)	−0.0126 (17)	0.0022 (16)	−0.0354 (16)
O5	0.084 (2)	0.079 (2)	0.0552 (18)	−0.0441 (19)	0.0119 (17)	−0.0091 (17)
Cl1	0.0486 (6)	0.0624 (7)	0.0493 (5)	0.0118 (5)	0.0195 (4)	0.0037 (5)
S1	0.0401 (5)	0.0272 (4)	0.0288 (4)	0.0064 (4)	0.0003 (3)	−0.0023 (4)

Geometric parameters (Å, °)

C1—C6	1.386 (4)	C8—C9	1.398 (5)
C1—C2	1.386 (4)	C9—C10	1.379 (5)

C1—S1	1.764 (3)	C9—Cl1	1.735 (3)
C2—C3	1.378 (4)	C10—C11	1.379 (5)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.379 (5)	C11—C12	1.377 (5)
C3—N2	1.471 (4)	C11—H11	0.9300
C4—C5	1.374 (5)	C12—C13	1.372 (5)
C4—H4	0.9300	C12—H12	0.9300
C5—C6	1.386 (5)	C13—H13	0.9300
C5—H5	0.9300	N1—S1	1.637 (3)
C6—H6	0.9300	N1—H1N	0.834 (18)
C7—O3	1.207 (4)	N2—O5	1.216 (4)
C7—N1	1.399 (4)	N2—O4	1.216 (4)
C7—C8	1.497 (4)	O1—S1	1.421 (2)
C8—C13	1.398 (4)	O2—S1	1.431 (2)

C6—C1—C2	121.1 (3)	C8—C9—Cl1	122.7 (3)
C6—C1—S1	119.7 (3)	C11—C10—C9	120.1 (3)
C2—C1—S1	119.1 (2)	C11—C10—H10	119.9
C3—C2—C1	117.5 (3)	C9—C10—H10	119.9
C3—C2—H2	121.2	C12—C11—C10	119.9 (3)
C1—C2—H2	121.2	C12—C11—H11	120.0
C2—C3—C4	122.9 (3)	C10—C11—H11	120.0
C2—C3—N2	118.3 (3)	C13—C12—C11	120.1 (3)
C4—C3—N2	118.8 (3)	C13—C12—H12	120.0
C5—C4—C3	118.4 (3)	C11—C12—H12	120.0
C5—C4—H4	120.8	C12—C13—C8	121.4 (3)
C3—C4—H4	120.8	C12—C13—H13	119.3
C4—C5—C6	120.8 (3)	C8—C13—H13	119.3
C4—C5—H5	119.6	C7—N1—S1	123.2 (2)
C6—C5—H5	119.6	C7—N1—H1N	120 (2)
C1—C6—C5	119.3 (3)	S1—N1—H1N	113 (2)
C1—C6—H6	120.3	O5—N2—O4	123.8 (3)
C5—C6—H6	120.3	O5—N2—C3	118.2 (3)
O3—C7—N1	120.6 (3)	O4—N2—C3	118.0 (3)
O3—C7—C8	125.7 (3)	O1—S1—O2	120.39 (16)
N1—C7—C8	113.8 (3)	O1—S1—N1	109.88 (15)
C13—C8—C9	117.4 (3)	O2—S1—N1	103.81 (14)
C13—C8—C7	119.7 (3)	O1—S1—C1	107.69 (15)
C9—C8—C7	122.9 (3)	O2—S1—C1	107.25 (15)
C10—C9—C8	121.0 (3)	N1—S1—C1	107.12 (15)
C10—C9—Cl1	116.3 (3)		

C6—C1—C2—C3	−0.2 (5)	C9—C10—C11—C12	1.2 (6)
S1—C1—C2—C3	−178.9 (2)	C10—C11—C12—C13	−1.9 (6)
C1—C2—C3—C4	0.6 (5)	C11—C12—C13—C8	0.2 (6)
C1—C2—C3—N2	−178.6 (3)	C9—C8—C13—C12	2.2 (5)
C2—C3—C4—C5	0.0 (5)	C7—C8—C13—C12	−176.2 (3)
N2—C3—C4—C5	179.2 (3)	O3—C7—N1—S1	0.2 (4)
C3—C4—C5—C6	−1.0 (6)	C8—C7—N1—S1	−179.1 (2)
C2—C1—C6—C5	−0.9 (5)	C2—C3—N2—O5	−4.8 (5)

S1—C1—C6—C5	177.9 (3)	C4—C3—N2—O5	175.9 (3)
C4—C5—C6—C1	1.5 (5)	C2—C3—N2—O4	174.9 (3)
O3—C7—C8—C13	−154.9 (3)	C4—C3—N2—O4	−4.4 (5)
N1—C7—C8—C13	24.4 (4)	C7—N1—S1—O1	54.9 (3)
O3—C7—C8—C9	26.8 (5)	C7—N1—S1—O2	−175.1 (3)
N1—C7—C8—C9	−153.9 (3)	C7—N1—S1—C1	−61.8 (3)
C13—C8—C9—C10	−2.9 (5)	C6—C1—S1—O1	−15.0 (3)
C7—C8—C9—C10	175.4 (3)	C2—C1—S1—O1	163.7 (2)
C13—C8—C9—Cl1	178.4 (3)	C6—C1—S1—O2	−146.0 (3)
C7—C8—C9—Cl1	−3.2 (5)	C2—C1—S1—O2	32.8 (3)
C8—C9—C10—C11	1.3 (6)	C6—C1—S1—N1	103.1 (3)
Cl1—C9—C10—C11	−180.0 (3)	C2—C1—S1—N1	−78.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O2^{i}	0.83 (2)	2.09 (2)	2.919 (3)	173 (3)

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

Fig. 1

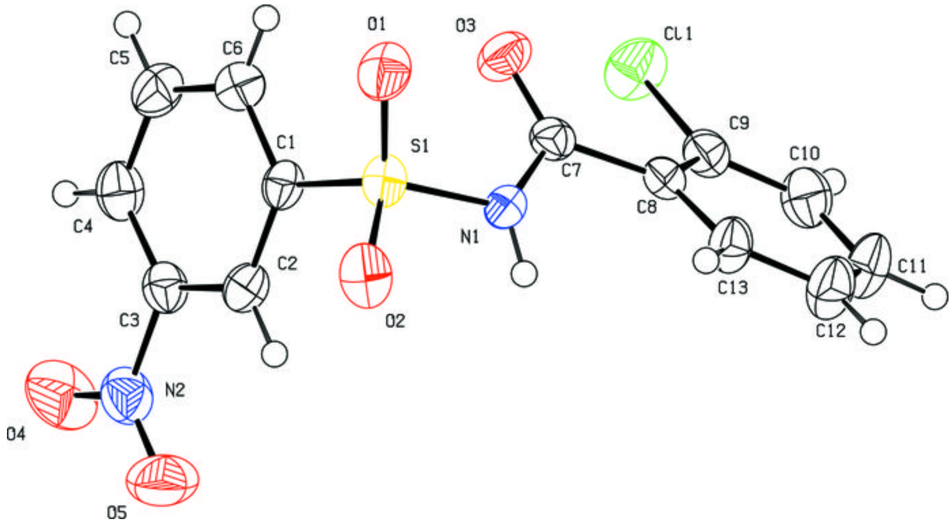

Fig. 2