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## Structure Reports

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## 4-Methyl-N-(3-oxo-2,3-dihydro-1,2-benzisothiazol-2-yl)benzenesulfonamide

Corrado Rizzoli,<sup>a\*</sup> Paola Vicini<sup>b</sup> and Matteo Incerti<sup>b</sup><sup>a</sup>Dipartimento di Chimica Generale ed Inorganica, Chimica Analitica, Chimica Fisica, Viale G. P. Usberti 17/A, Università di Parma, I-43100 Parma, Italy, and<sup>b</sup>Dipartimento Farmaceutico, Viale G. P. Usberti 27/A, Università di Parma, I-43100 Parma, Italy

Correspondence e-mail: corrado.rizzoli@unipr.it

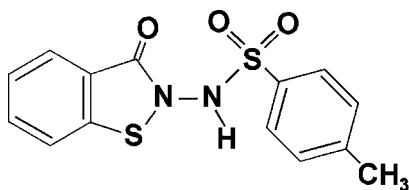
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.040;  $wR$  factor = 0.089; data-to-parameter ratio = 18.1.

In the title molecule,  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_3\text{S}_2$ , the benzisothiazolone ring system is essentially planar and forms a dihedral angle of  $67.37(6)^\circ$  with the plane of the benzene ring. In the crystal structure, molecules are linked *via* intermolecular  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds to form chains parallel to the  $b$  axis.

## Related literature

For the chemical and biological properties of 1,2-benzisothiazol-3(2H)-one derivatives, see: Clerici *et al.* (2007); Siegemund *et al.* (2002). For 2-amino-1,2-benzisothiazol-3(2H)-one derivatives with antiplatelet/spasmolytic effects, see: Vicini *et al.* (1997,2000). For derivatives with antimicrobial properties, see: Vicini *et al.* (2002); Zani *et al.* (2004). For the synthesis of the title compound, see: Vicini *et al.* (2009). For the crystal structures of related compounds, see: Cavalca *et al.* (1970); Ranganathan *et al.* (2002); Steinfeld & Kersting (2006); Kim *et al.* (1996); Xu *et al.* (2006); Sarma & Mughesh (2007); Kolberg *et al.* (1999).



## Experimental

## Crystal data

 $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}_3\text{S}_2$  $M_r = 320.38$ Monoclinic,  $P2_1/n$  $a = 8.051(3)$  Å $b = 7.655(3)$  Å $c = 23.910(10)$  Å $\beta = 98.490(8)^\circ$  $V = 1457.4(10)$  Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 0.38$  mm<sup>-1</sup> $T = 296(2)$  K $0.28 \times 0.26 \times 0.12$  mm

## Data collection

Bruker SMART 1000 CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Bruker, 1997)

 $T_{\min} = 0.892$ ,  $T_{\max} = 0.957$ 

17685 measured reflections

3521 independent reflections

1888 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.041$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.040$  $wR(F^2) = 0.089$  $S = 1.01$ 

3521 reflections

194 parameters

1 restraint

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.23$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.28$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N2}-\text{H2}\cdots\text{O1}^{\text{i}}$	0.848 (17)	1.948 (17)	2.784 (3)	168.3 (15)
$\text{C6}-\text{H6}\cdots\text{O2}^{\text{ii}}$	0.93	2.56	3.492 (3)	175

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

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and SCHAKAL (Keller, 1997); software used to prepare material for publication: SHELXL97 and PARST95 (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2764).

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**supplementary materials**

*Acta Cryst.* (2009). E65, o425-o426 [ doi:10.1107/S1600536809003201 ]

## 4-Methyl-*N*-(3-oxo-2,3-dihydro-1,2-benzisothiazol-2-yl)benzenesulfonamide

C. Rizzoli, P. Vicini and M. Incerti

### Comment

Over the past decades a substantial number of 1,2-benzisothiazol-3(2*H*)-one derivatives have been reported to possess a wide range of biological activities including antimicrobial, antiviral, anticancer, anti-inflammatory, cartilage antidegenerative and other pharmacological activities (Clerici *et al.*, 2007; Siegemund *et al.*, 2002). As part of our program aimed at developing novel biologically active 1,2-benzisothiazol-3(2*H*)-ones, we have synthesized in the last years 2-amino-1,2-benzisothiazol-3(2*H*)-one derivatives resulted in the discovery of new compounds active as antiplatelet/spasmolytic agents (Vicini *et al.*, 1997; Vicini *et al.*, 2000) and of compounds endowed with very interesting antimicrobial properties (Vicini *et al.*, 2002; Zani *et al.*, 2004). Recently, in our continuing efforts to find novel effective 2-amino-1,2-benzisothiazol-3(2*H*)-one derivatives, we have synthesized a series of 2-(phenylsulfonyl)amino-1,2-benzisothiazol-3(2*H*)-ones which exhibit anti-HIV-1 activity against wild type virus and against viral strains carrying clinically relevant mutations (Vicini *et al.*, 2009). Experimental evidences suggest non classical targets for this novel class of anti-HIV-1 agents. In order to study their binding sites at a molecular level we thought it appropriate to obtain X-ray crystallographic data for a prototype.

The molecule of the title compound (Fig. 1) shows no unusual geometric features, with the S1—N1 (1.7116 (19) Å) and S1—C1 (1.721 (2) Å) bond distances corresponding to those observed in similar structures (Cavalca *et al.*, 1970; Ranganathan *et al.*, 2002; Steinfeld & Kersting, 2006; Kim *et al.*, 1996; Xu *et al.*, 2006; Sarma & Mugesh, 2007). The N1—N2 bond distance (1.364 (2) Å) is just significantly shorter than that observed in 4,5-dimethyl-2-(3-nitrobenzenesulfonylamino)isothiazol-3(2*H*)-one 1,1-dioxide (1.387 (4) Å; Kolberg *et al.*, 1999). The benzoisothiazole rings system is essentially planar (maximum deviation 0.019 (4) Å for atom C4) and forms a dihedral angle of 67.37 (6)° with the plane of the C8—C13 benzene ring. In the crystal structure (Fig. 2), molecules are linked into chains running parallel to the *b* axis by intermolecular N—H···O and C—H···O hydrogen bonding interactions (Table 1).

### Experimental

The title compound was synthesized as described elsewhere (Vicini *et al.*, 2009). Freshly prepared chlorocarbonylsulfonylchloride (18 mmol) in dried CCl<sub>4</sub> (40 ml) was added dropwise to a stirred, ice-cooled solution of 2-tosylhydrazine (20 mmol) in pyridine (18 ml). After 2 h the reaction mixture was allowed to cool to room temperature and the crude product was filtered, purified by base-acid (Na<sub>2</sub>CO<sub>3</sub>—HCl) exchange and silica-gel column chromatography (eluent CH<sub>2</sub>Cl<sub>2</sub>—EtOH 95:5 *v/v*). Pale yellow single crystals of the title compound suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution at room temperature.

### Refinement

The H atoms bound to the N2 atom was located in a difference Fourier map and refined isotropically with the N—H distance constrained to 0.87 (1) Å. All other H atoms were placed at calculated positions and refined using a riding model, with C—H = 0.93–0.96 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$  or  $1.5 U_{\text{eq}}(\text{C})$  for methyl H atoms.

## Figures

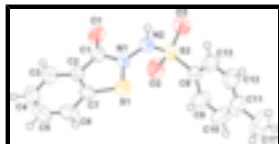


Fig. 1. The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

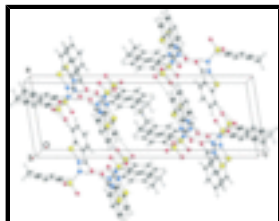


Fig. 2. Crystal packing of the title compound viewed approximately along the *b* axis. Intermolecular N—H...O and C—H...O hydrogen bonds are shown as dashed lines.

## 4-Methyl-*N*-(3-oxo-2,3-dihydro-1,2-benzisothiazol-2-yl)benzenesulfonamide

### Crystal data

$C_{14}H_{12}N_2O_3S_2$

$M_r = 320.38$

Monoclinic,  $P2_1/n$

Hall symbol:  $-P\ 2_1/n$

$a = 8.051\ (3)\ \text{\AA}$

$b = 7.655\ (3)\ \text{\AA}$

$c = 23.910\ (10)\ \text{\AA}$

$\beta = 98.490\ (8)^\circ$

$V = 1457.4\ (10)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 664$

$D_x = 1.460\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1208 reflections

$\theta = 3.1\text{--}54.7^\circ$

$\mu = 0.38\ \text{mm}^{-1}$

$T = 296\ (2)\ \text{K}$

Prism, pale yellow

$0.28 \times 0.26 \times 0.12\ \text{mm}$

### Data collection

Bruker SMART 1000 CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 296\ (2)\ \text{K}$

$\omega$  scans

Absorption correction: multi-scan (SADABS; Bruker, 1997)

$T_{\min} = 0.892$ ,  $T_{\max} = 0.957$

17685 measured reflections

3521 independent reflections

1888 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.041$

$\theta_{\text{max}} = 28.0^\circ$

$\theta_{\text{min}} = 1.7^\circ$

$h = -10 \rightarrow 10$

$k = -10 \rightarrow 10$

$l = -31 \rightarrow 31$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$$R[F^2 > 2\sigma(F^2)] = 0.040$$

$$wR(F^2) = 0.089$$

$$S = 1.01$$

3521 reflections

194 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0354P)^2]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 0.23 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.28 \text{ e } \text{\AA}^{-3}$$

Extinction correction: none

### Special details

**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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.07092 (8)	0.54275 (7)	0.15129 (2)	0.0674 (2)
S2	-0.38794 (7)	0.64261 (7)	0.12617 (2)	0.06196 (18)
O1	-0.25352 (19)	0.2912 (2)	0.21942 (6)	0.0740 (4)
O2	-0.4086 (2)	0.48129 (18)	0.09686 (6)	0.0795 (5)
O3	-0.5189 (2)	0.7130 (2)	0.15313 (7)	0.0826 (5)
N1	-0.1134 (2)	0.4976 (2)	0.17603 (7)	0.0585 (5)
N2	-0.2283 (3)	0.6277 (2)	0.17766 (8)	0.0692 (5)
H2	-0.247 (3)	0.670 (3)	0.2089 (6)	0.085 (8)*
C1	-0.1300 (3)	0.3352 (2)	0.19864 (8)	0.0524 (5)
C2	0.0211 (2)	0.2380 (2)	0.19334 (8)	0.0469 (5)
C3	0.0556 (3)	0.0671 (3)	0.21027 (8)	0.0584 (5)
H3	-0.0221	0.0028	0.2269	0.070*
C4	0.2040 (3)	-0.0051 (3)	0.20233 (10)	0.0702 (6)
H4	0.2268	-0.1211	0.2122	0.084*
C5	0.3219 (3)	0.0936 (3)	0.17950 (10)	0.0796 (7)
H5	0.4249	0.0432	0.1758	0.096*
C6	0.2925 (3)	0.2611 (3)	0.16232 (10)	0.0722 (6)
H6	0.3724	0.3250	0.1467	0.087*
C7	0.1378 (3)	0.3337 (2)	0.16900 (8)	0.0527 (5)
C8	-0.3251 (2)	0.7991 (3)	0.08016 (8)	0.0544 (5)
C9	-0.3198 (3)	0.7587 (3)	0.02474 (10)	0.0815 (7)
H9	-0.3454	0.6466	0.0111	0.098*
C10	-0.2757 (4)	0.8877 (4)	-0.01057 (10)	0.0977 (9)
H10	-0.2729	0.8606	-0.0483	0.117*
C11	-0.2362 (3)	1.0529 (4)	0.00758 (12)	0.0789 (7)
C12	-0.2448 (3)	1.0894 (3)	0.06352 (11)	0.0793 (7)

## supplementary materials

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H12	-0.2203	1.2017	0.0772	0.095*
C13	-0.2886 (3)	0.9645 (3)	0.09934 (10)	0.0708 (6)
H13	-0.2935	0.9922	0.1369	0.085*
C14	-0.1871 (4)	1.1911 (4)	-0.03204 (12)	0.1226 (12)
H14A	-0.1661	1.2993	-0.0120	0.184*
H14B	-0.2766	1.2068	-0.0629	0.184*
H14C	-0.0874	1.1549	-0.0464	0.184*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0837 (4)	0.0494 (3)	0.0742 (4)	-0.0037 (3)	0.0287 (3)	0.0081 (3)
S2	0.0711 (4)	0.0537 (3)	0.0623 (4)	0.0114 (3)	0.0140 (3)	0.0072 (3)
O1	0.0561 (9)	0.0904 (11)	0.0790 (10)	0.0106 (8)	0.0222 (8)	0.0324 (9)
O2	0.1055 (13)	0.0531 (9)	0.0784 (11)	-0.0047 (8)	0.0092 (9)	-0.0016 (8)
O3	0.0789 (11)	0.0863 (11)	0.0896 (12)	0.0260 (9)	0.0360 (9)	0.0181 (9)
N1	0.0668 (12)	0.0489 (10)	0.0626 (11)	0.0159 (9)	0.0193 (9)	0.0127 (8)
N2	0.0929 (14)	0.0660 (12)	0.0483 (11)	0.0358 (11)	0.0092 (10)	0.0007 (10)
C1	0.0538 (13)	0.0556 (13)	0.0484 (12)	0.0027 (10)	0.0099 (10)	0.0099 (10)
C2	0.0457 (12)	0.0437 (11)	0.0508 (11)	0.0001 (9)	0.0055 (9)	0.0021 (9)
C3	0.0598 (14)	0.0514 (13)	0.0610 (13)	0.0000 (10)	-0.0004 (11)	0.0053 (10)
C4	0.0759 (17)	0.0548 (13)	0.0760 (16)	0.0139 (13)	-0.0013 (13)	-0.0038 (12)
C5	0.0670 (16)	0.0808 (18)	0.0911 (18)	0.0205 (14)	0.0121 (14)	-0.0180 (14)
C6	0.0622 (15)	0.0765 (16)	0.0834 (16)	-0.0070 (13)	0.0287 (13)	-0.0146 (14)
C7	0.0552 (13)	0.0498 (12)	0.0543 (12)	-0.0030 (10)	0.0122 (10)	-0.0045 (9)
C8	0.0579 (13)	0.0556 (12)	0.0491 (12)	0.0104 (10)	0.0056 (10)	0.0034 (10)
C9	0.111 (2)	0.0751 (16)	0.0603 (16)	-0.0120 (15)	0.0195 (14)	-0.0075 (13)
C10	0.125 (2)	0.119 (2)	0.0504 (15)	-0.0115 (19)	0.0165 (15)	0.0051 (16)
C11	0.0669 (16)	0.0886 (19)	0.0774 (19)	-0.0017 (14)	-0.0021 (13)	0.0278 (16)
C12	0.0940 (19)	0.0613 (15)	0.0808 (19)	-0.0026 (13)	0.0065 (14)	0.0065 (14)
C13	0.0920 (18)	0.0637 (15)	0.0571 (14)	0.0010 (13)	0.0125 (13)	-0.0009 (12)
C14	0.108 (2)	0.143 (3)	0.114 (2)	-0.014 (2)	0.0065 (18)	0.070 (2)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

S1—N1	1.7116 (19)	C5—H5	0.9300
S1—C7	1.721 (2)	C6—C7	1.394 (3)
S2—O2	1.4175 (16)	C6—H6	0.9300
S2—O3	1.4205 (15)	C8—C13	1.364 (3)
S2—N2	1.647 (2)	C8—C9	1.368 (3)
S2—C8	1.751 (2)	C9—C10	1.380 (3)
O1—C1	1.223 (2)	C9—H9	0.9300
N1—N2	1.364 (2)	C10—C11	1.359 (3)
N1—C1	1.370 (2)	C10—H10	0.9300
N2—H2	0.844 (9)	C11—C12	1.378 (3)
C1—C2	1.448 (3)	C11—C14	1.511 (3)
C2—C3	1.385 (3)	C12—C13	1.364 (3)
C2—C7	1.386 (2)	C12—H12	0.9300
C3—C4	1.355 (3)	C13—H13	0.9300

C3—H3	0.9300	C14—H14A	0.9600
C4—C5	1.387 (3)	C14—H14B	0.9600
C4—H4	0.9300	C14—H14C	0.9600
C5—C6	1.356 (3)		
N1—S1—C7	89.03 (9)	C5—C6—H6	121.3
O2—S2—O3	120.93 (11)	C7—C6—H6	121.3
O2—S2—N2	109.30 (10)	C2—C7—C6	120.65 (19)
O3—S2—N2	103.69 (10)	C2—C7—S1	112.83 (15)
O2—S2—C8	107.99 (10)	C6—C7—S1	126.50 (17)
O3—S2—C8	109.17 (10)	C13—C8—C9	120.0 (2)
N2—S2—C8	104.56 (10)	C13—C8—S2	119.47 (17)
N2—N1—C1	123.02 (17)	C9—C8—S2	120.50 (18)
N2—N1—S1	119.29 (14)	C8—C9—C10	118.6 (2)
C1—N1—S1	117.36 (13)	C8—C9—H9	120.7
N1—N2—S2	119.16 (15)	C10—C9—H9	120.7
N1—N2—H2	120.6 (16)	C11—C10—C9	122.7 (2)
S2—N2—H2	114.6 (16)	C11—C10—H10	118.7
O1—C1—N1	122.89 (18)	C9—C10—H10	118.7
O1—C1—C2	129.65 (18)	C10—C11—C12	117.1 (2)
N1—C1—C2	107.45 (17)	C10—C11—C14	121.4 (3)
C3—C2—C7	120.20 (18)	C12—C11—C14	121.5 (3)
C3—C2—C1	126.50 (18)	C13—C12—C11	121.5 (2)
C7—C2—C1	113.30 (17)	C13—C12—H12	119.3
C4—C3—C2	119.2 (2)	C11—C12—H12	119.3
C4—C3—H3	120.4	C12—C13—C8	120.2 (2)
C2—C3—H3	120.4	C12—C13—H13	119.9
C3—C4—C5	120.1 (2)	C8—C13—H13	119.9
C3—C4—H4	119.9	C11—C14—H14A	109.5
C5—C4—H4	119.9	C11—C14—H14B	109.5
C6—C5—C4	122.3 (2)	H14A—C14—H14B	109.5
C6—C5—H5	118.8	C11—C14—H14C	109.5
C4—C5—H5	118.8	H14A—C14—H14C	109.5
C5—C6—C7	117.5 (2)	H14B—C14—H14C	109.5

Hydrogen-bond geometry (Å, °)

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N2—H2 $\cdots$ O1 <sup>i</sup>	0.848 (17)	1.948 (17)	2.784 (3)	168.3 (15)
C6—H6 $\cdots$ O2 <sup>ii</sup>	0.93	2.56	3.492 (3)	175

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



Fig. 1

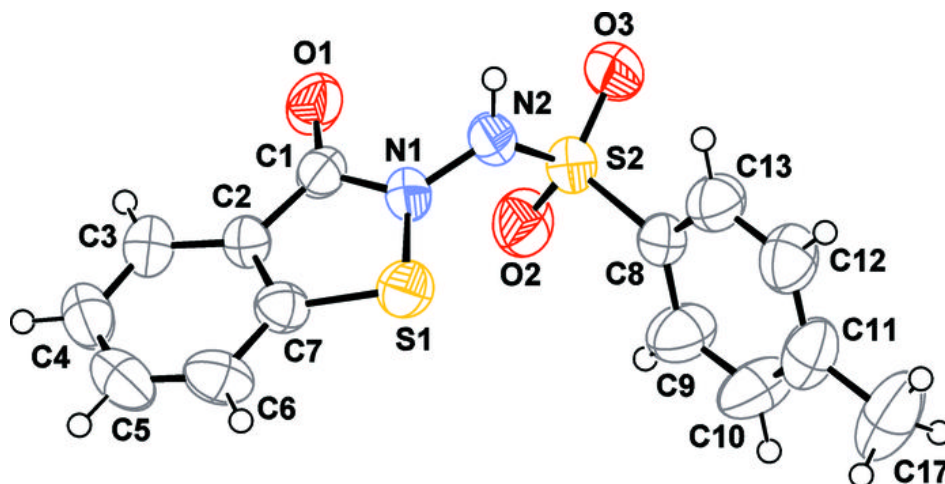


Fig. 2

