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2-(Hydrazinocarbonyl)benzenesulfonamide

Shu-Yan Wang,[a] Wan-Cheng Guo[b] and Ning Ma[a]*

[a]Department of Chemistry, School of Science, Tianjin University, Tianjin 300072, People's Republic of China, and [b]Elemento-Organic Chemistry Institute, State Key Laboratory of Elemento-Organic Chemistry, Nankai University, Tianjin 300071, People's Republic of China
Correspondence e-mail: mntju@tju.edu.cn

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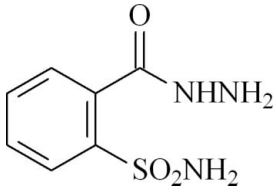
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.026; wR factor = 0.071; data-to-parameter ratio = 14.0.

In the title compound, $C_7H_9N_3O_3S$, the chiral conformation of the molecule is determined by an intramolecular N—H···O hydrogen bond between the sulfonamide and hydrazinocarbonyl groups, with the former group acting as a donor in hydrogen bonding. The crystal structure is stabilized by intermolecular N—H···O and N—H···N hydrogen bonds and π–π stacking interactions between the benzene rings [the interplanar distance is 3.755 (3) Å].

Related literature

For the crystal structure of an analogous sulfonamide compound, see: Michaux *et al.* (2006). For related literature, see: Winum *et al.* (2005).



Experimental

Crystal data

$C_7H_9N_3O_3S$
M_r = 215.23
Monoclinic, $C2/c$
a = 11.857 (2) Å
b = 11.562 (2) Å
c = 13.840 (3) Å
β = 111.72 (3)°
V = 1762.6 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 113 (2) K
0.24 × 0.20 × 0.20 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.902, T_{max} = 0.932
10255 measured reflections
2057 independent reflections
1878 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.071
S = 1.07
2057 reflections
147 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···O3^{i}	0.890 (18)	2.333 (18)	2.9424 (14)	125.7 (14)
N3—H3A···O1^{ii}	0.874 (19)	2.139 (19)	3.0098 (16)	173.9 (15)
N2—H2A···O2^{iii}	0.809 (18)	2.098 (19)	2.9070 (15)	177.0 (17)
N1—H1B···O3	0.834 (19)	2.251 (19)	2.9731 (16)	145.1 (16)
N1—H1A···N3^{iv}	0.831 (19)	2.342 (19)	3.1662 (16)	171.6 (17)

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2082).

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supplementary materials

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2-(Hydrazinocarbonyl)benzenesulfonamide

S.-Y. Wang, W.-C. Guo and N. Ma

Comment

Sulfonamide compounds attract much attention due to their diverse biological activities. Here we report the crystal structure of 2-hydrazinocarbonylbenzenesulfonamide.

The title compound has a basal plane which involves the benzene ring, the S atom and the C7 atom of the carbonyl group with a mean deviation of 0.037 (3) Å. The C, O atoms of the carbonyl group and the two N atoms of the hydrazino group lie in another plane (mean deviation 0.051 (2) Å) with a dihedral angle of 57.5 (2)° to the basal plane.

The intramolecular N1—H1B···O3 hydrogen bond forces the O atom of carbonyl group and the N atom of sulfamoyl group to lie on the same side of the basal plane (Fig. 1) and thus the molecule adopts a chiral conformation. The crystal structure is stabilized by intermolecular hydrogen bonds (Table 1) and π-π stacking interactions between the phenyl rings. (distance of 3.755 (3) Å, Fig. 2).

Experimental

20 ml of ethanol, 2.16 g of 2-methoxycarbonylbenzenesulfonamide and 1.2 g of 80% hydrazine hydrate were added to a flask and refluxed for 5 h. The mixture was cooled to room temperature and concentrated in vaccuo. The solid residue was recrystallized from ethanol and the title compound was obtained as white crystals. Its melting point and PMR data were consistent with the literature (Winum *et al.*, 2005). Colouress crystals suitable for X-ray analysis were obtained by recrystallization from ethanol at room temperature.

Refinement

The H atoms bonded to N were located in electron-density difference maps; their positional parameters were refined and U_{iso}(H) = 1.2U_{eq}(N). Remaining H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and with U_{iso}(H) = 1.2 times U_{eq}(C).

Figures

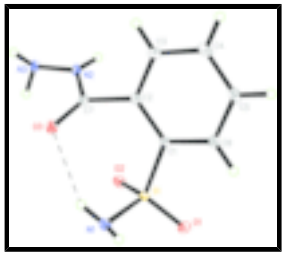

Fig. 1. Molecular structure of the title compound with the displacement ellipsoids drawn at the 35% probability level. The intramolecular hydrogen bond is indicated as dashed line.

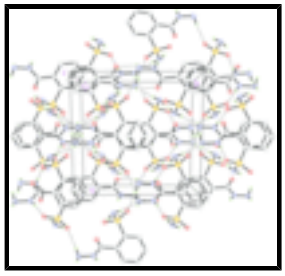

Fig. 2. Crystal packing showing intermolecular hydrogen bonds and π-π stacking interactions. The intermolecular hydrogen bonds are indicated as dashed lines.

2-(hydrazinocarbonyl)benzenesulfonamide

Crystal data

$C_7H_9N_3O_3S$	D_x = 1.622 Mg m^{-3}
M_r = 215.23	Melting point: 451 K
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
a = 11.857 (2) Å	Cell parameters from 3162 reflections
b = 11.562 (2) Å	θ = 2.6–27.9º
c = 13.840 (3) Å	μ = 0.35 mm^{-1}
β = 111.72 (3)º	*T* = 113 (2) K
V = 1762.6 (6) Å^3	Prism, colourless
Z = 8	0.24 × 0.20 × 0.20 mm
F_{000} = 896	

Data collection

Rigaku Saturn diffractometer	2057 independent reflections
Radiation source: Rotating anode	1878 reflections with $I > 2\sigma(I)$
Monochromator: confocal	R_{int} = 0.021
T = 113(2) K	θ_{max} = 27.9º
ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (Jacobson, 1998)	*h* = −15→15
T_{min} = 0.902, T_{max} = 0.932	*k* = −15→15
10255 measured reflections	*l* = −18→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.026	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.071	$w = 1/[\sigma^2(F_o^2) + (0.0332P)^2 + 1.8027P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.001

2057 reflections	$\Delta\rho_{max}$ = 0.38 e Å^{-3}
147 parameters	$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
S1	0.24521 (2)	0.16461 (2)	0.24825 (2)	0.01188 (10)
O1	0.31684 (8)	0.08049 (8)	0.32136 (7)	0.0197 (2)
O2	0.21968 (8)	0.27287 (7)	0.28704 (7)	0.01659 (19)
O3	0.09252 (8)	0.32950 (7)	0.05596 (7)	0.0175 (2)
N1	0.31502 (10)	0.19390 (10)	0.17075 (9)	0.0167 (2)
H1A	0.3400 (16)	0.1340 (16)	0.1522 (14)	0.029 (4)*
H1B	0.2715 (16)	0.2362 (16)	0.1226 (14)	0.026 (4)*
N2	−0.06435 (9)	0.36156 (9)	0.10942 (8)	0.0138 (2)
H2A	−0.1060 (16)	0.3347 (14)	0.1388 (14)	0.024 (4)*
N3	−0.07007 (10)	0.48286 (9)	0.09366 (9)	0.0155 (2)
H3A	0.0043 (17)	0.5084 (15)	0.1227 (13)	0.024 (4)*
H3B	−0.0961 (16)	0.4945 (15)	0.0253 (15)	0.026 (4)*
C1	0.10417 (10)	0.10049 (10)	0.17415 (9)	0.0113 (2)
C2	0.00556 (10)	0.16743 (9)	0.11057 (9)	0.0120 (2)
C3	−0.10350 (11)	0.11141 (11)	0.05679 (9)	0.0159 (2)
H3	−0.1706	0.1541	0.0158	0.019*
C4	−0.11318 (11)	−0.00830 (11)	0.06378 (9)	0.0175 (2)
H4	−0.1867	−0.0447	0.0275	0.021*
C5	−0.01455 (12)	−0.07293 (10)	0.12401 (10)	0.0171 (3)
H5	−0.0209	−0.1529	0.1267	0.021*
C6	0.09466 (11)	−0.01826 (10)	0.18084 (9)	0.0142 (2)
H6	0.1608	−0.0613	0.2230	0.017*
C7	0.01711 (10)	0.29415 (10)	0.09073 (9)	0.0131 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.00969 (15)	0.01151 (15)	0.01456 (15)	−0.00050 (9)	0.00463 (11)	−0.00085 (9)

O1	0.0136 (4)	0.0213 (5)	0.0207 (5)	0.0027 (3)	0.0023 (4)	0.0047 (3)
O2	0.0160 (4)	0.0147 (4)	0.0211 (4)	−0.0029 (3)	0.0093 (3)	−0.0061 (3)
O3	0.0174 (4)	0.0154 (4)	0.0237 (5)	0.0035 (3)	0.0125 (4)	0.0056 (3)
N1	0.0150 (5)	0.0162 (5)	0.0225 (5)	−0.0004 (4)	0.0112 (4)	−0.0005 (4)
N2	0.0142 (5)	0.0113 (5)	0.0181 (5)	0.0021 (4)	0.0084 (4)	0.0038 (4)
N3	0.0158 (5)	0.0110 (5)	0.0214 (5)	0.0027 (4)	0.0090 (4)	0.0038 (4)
C1	0.0112 (5)	0.0115 (5)	0.0122 (5)	−0.0008 (4)	0.0054 (4)	−0.0010 (4)
C2	0.0135 (5)	0.0115 (5)	0.0125 (5)	0.0005 (4)	0.0066 (4)	−0.0002 (4)
C3	0.0127 (5)	0.0202 (6)	0.0141 (5)	0.0005 (4)	0.0042 (4)	−0.0012 (4)
C4	0.0155 (6)	0.0202 (6)	0.0183 (6)	−0.0066 (5)	0.0080 (5)	−0.0067 (5)
C5	0.0209 (6)	0.0122 (5)	0.0223 (6)	−0.0042 (4)	0.0129 (5)	−0.0040 (4)
C6	0.0159 (6)	0.0117 (5)	0.0174 (5)	0.0013 (4)	0.0089 (4)	0.0006 (4)
C7	0.0129 (5)	0.0130 (5)	0.0119 (5)	0.0013 (4)	0.0030 (4)	0.0019 (4)

Geometric parameters (Å, °)

S1—O1	1.4335 (10)	C1—C6	1.3836 (16)
S1—O2	1.4378 (9)	C1—C2	1.4067 (16)
S1—N1	1.6148 (11)	C2—C3	1.3903 (17)
S1—C1	1.7687 (13)	C2—C7	1.5063 (15)
O3—C7	1.2314 (15)	C3—C4	1.3953 (17)
N1—H1A	0.831 (19)	C3—H3	0.9300
N1—H1B	0.834 (19)	C4—C5	1.3781 (18)
N2—C7	1.3387 (15)	C4—H4	0.9300
N2—N3	1.4171 (14)	C5—C6	1.3932 (17)
N2—H2A	0.809 (18)	C5—H5	0.9300
N3—H3A	0.874 (19)	C6—H6	0.9300
N3—H3B	0.890 (18)		
O1—S1—O2	118.60 (6)	C3—C2—C1	118.14 (11)
O1—S1—N1	107.20 (6)	C3—C2—C7	119.00 (10)
O2—S1—N1	107.21 (6)	C1—C2—C7	122.59 (10)
O1—S1—C1	108.12 (6)	C2—C3—C4	120.60 (11)
O2—S1—C1	107.27 (5)	C2—C3—H3	119.7
N1—S1—C1	108.05 (6)	C4—C3—H3	119.7
S1—N1—H1A	111.1 (12)	C5—C4—C3	120.44 (11)
S1—N1—H1B	109.6 (12)	C5—C4—H4	119.8
H1A—N1—H1B	115.4 (17)	C3—C4—H4	119.8
C7—N2—N3	122.90 (10)	C4—C5—C6	119.92 (11)
C7—N2—H2A	119.5 (12)	C4—C5—H5	120.0
N3—N2—H2A	117.0 (12)	C6—C5—H5	120.0
N2—N3—H3A	106.3 (11)	C1—C6—C5	119.62 (11)
N2—N3—H3B	107.0 (11)	C1—C6—H6	120.2
H3A—N3—H3B	109.4 (15)	C5—C6—H6	120.2
C6—C1—C2	121.22 (11)	O3—C7—N2	124.23 (11)
C6—C1—S1	117.40 (9)	O3—C7—C2	121.48 (10)
C2—C1—S1	121.38 (9)	N2—C7—C2	114.22 (10)
O1—S1—C1—C6	−13.09 (11)	C2—C3—C4—C5	−0.14 (18)
O2—S1—C1—C6	−142.08 (9)	C3—C4—C5—C6	1.91 (18)
N1—S1—C1—C6	102.63 (10)	C2—C1—C6—C5	−0.25 (17)

O1—S1—C1—C2	167.14 (9)	S1—C1—C6—C5	179.98 (9)
O2—S1—C1—C2	38.15 (11)	C4—C5—C6—C1	−1.71 (18)
N1—S1—C1—C2	−77.15 (10)	N3—N2—C7—O3	−1.86 (18)
C6—C1—C2—C3	1.97 (17)	N3—N2—C7—C2	−178.78 (10)
S1—C1—C2—C3	−178.27 (9)	C3—C2—C7—O3	−118.69 (13)
C6—C1—C2—C7	−172.00 (11)	C1—C2—C7—O3	55.23 (16)
S1—C1—C2—C7	7.77 (15)	C3—C2—C7—N2	58.33 (14)
C1—C2—C3—C4	−1.77 (17)	C1—C2—C7—N2	−127.76 (12)
C7—C2—C3—C4	172.42 (11)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3B···O3^{i}	0.890 (18)	2.333 (18)	2.9424 (14)	125.7 (14)
N3—H3A···O1^{ii}	0.874 (19)	2.139 (19)	3.0098 (16)	173.9 (15)
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N1—H1B···O3	0.834 (19)	2.251 (19)	2.9731 (16)	145.1 (16)
N1—H1A···N3^{iv}	0.831 (19)	2.342 (19)	3.1662 (16)	171.6 (17)

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

Fig. 1

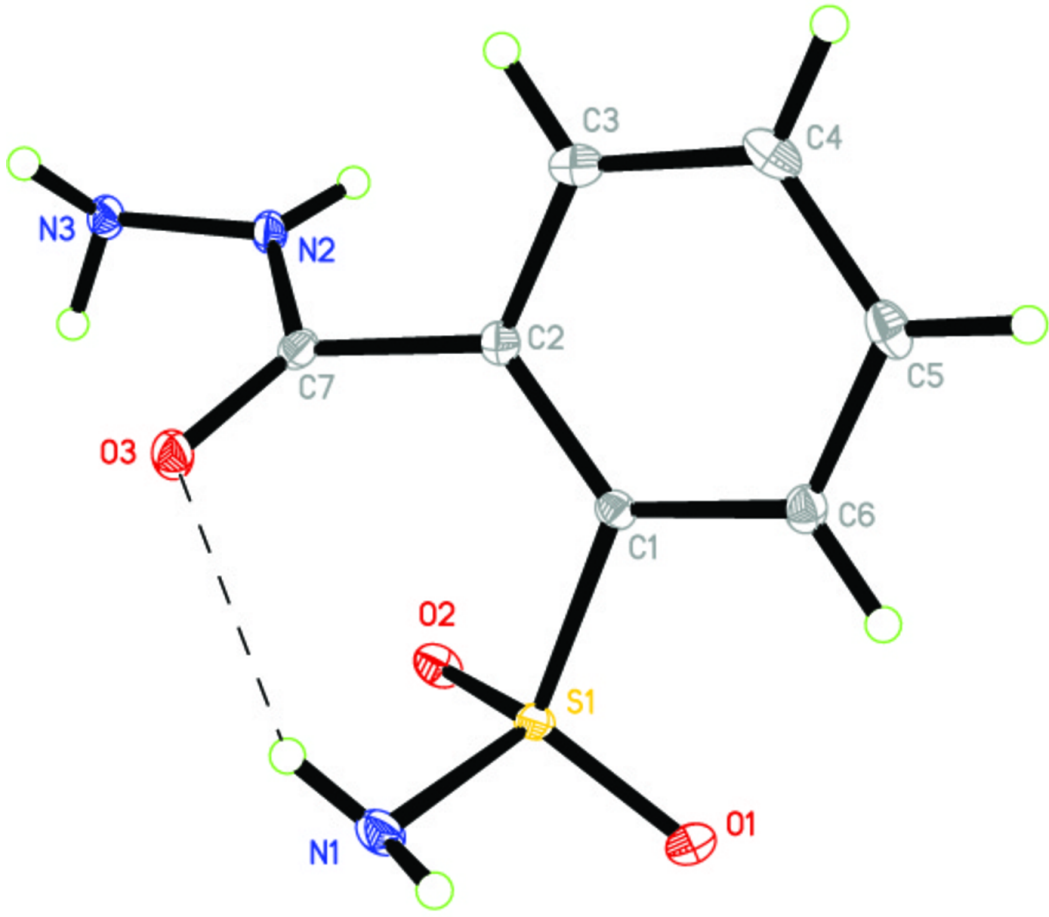
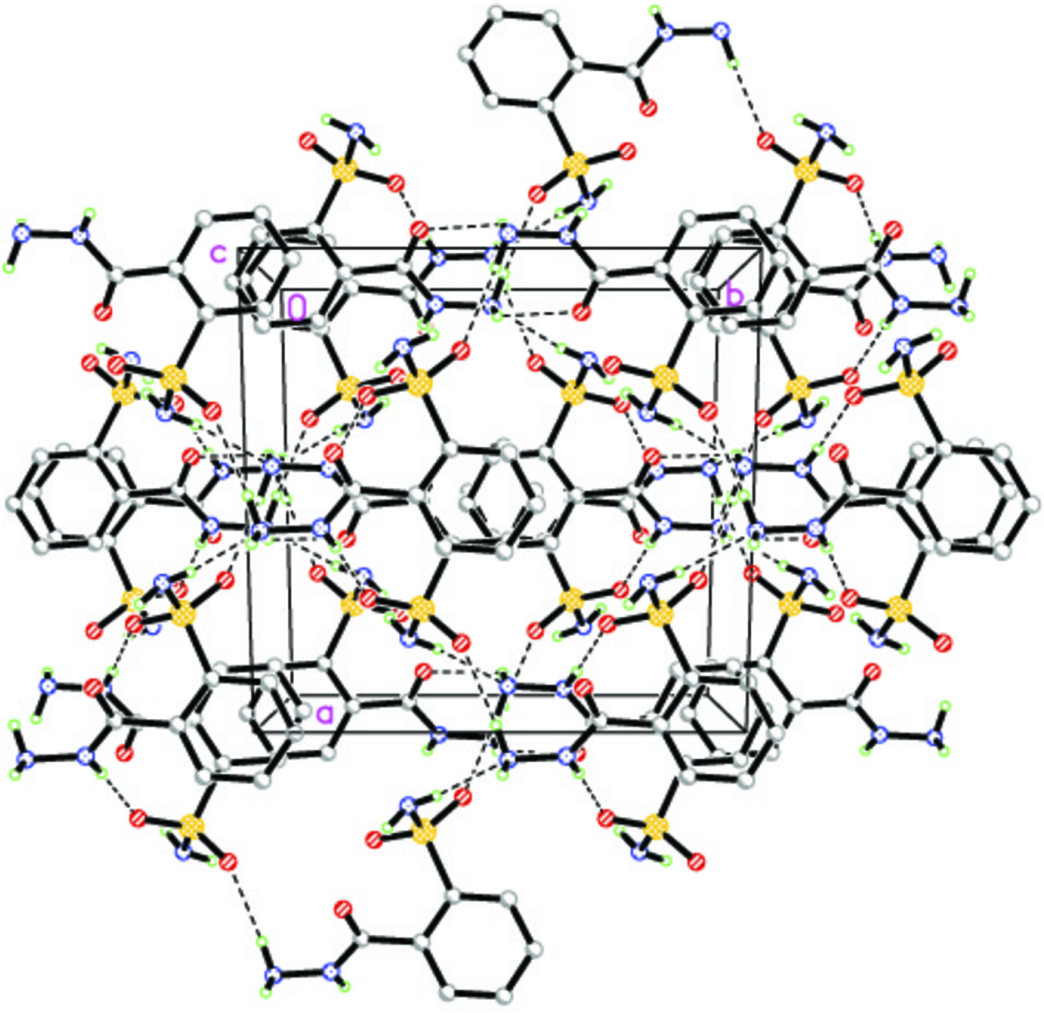
Fig. 2