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1,1′-Sulfonyldiimidazole

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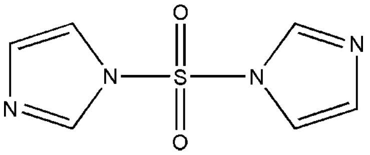
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.035; wR factor = 0.080; data-to-parameter ratio = 12.3.

The molecule of the title compound, $C_6H_6N_4O_2S$, possesses a pseudo-twofold rotation axis of symmetry which passes through the S atom. The molecules are linked through intermolecular C—H···O hydrogen bonds into a zigzag chain of C(5) graph-set motif along the b axis. Along the a axis, the chains are cross-linked through π–π stacking interactions between two symmetry-related imidazole rings [centroid-to-centroid distance = 3.667 (2) Å] and by C—H···π interactions involving the π system of the other imidazole ring. These interactions lead to the formation of a layer parallel to the ab plane.

Related literature

For general background, see: Elmer & Collier (1993); Lehn *et al.* (1989). For pseudo-symmetry analysis, see: Hepperle (2001). For related structures, see: Bettinetti & Sardone (1997); Blaton *et al.* (1979*a*,*b*); Jones *et al.* (1996); Malone *et al.* (1997); Patel *et al.* (2001, 2007); Secondo *et al.* (1996); Tiwari & Singh (1982); Ülkü *et al.* (1997). For hydrogen bonding, see: Hunter & Sanders (1990); Desiraju & Gavezzotti (1989); Bernstein *et al.* (1995).



Experimental

Crystal data

$C_6H_6N_4O_2S$
M_r = 198.21
Orthorhombic, *Pbca*
a = 7.285 (2) Å
b = 11.012 (4) Å
c = 20.646 (3) Å
V = 1656.3 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 293 K
0.12 × 0.10 × 0.05 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
1459 measured reflections
1459 independent reflections
1064 reflections with $I > 2\sigma(I)$
3 standard reflections
frequency: 60 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.081
S = 1.01
1459 reflections
119 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

Cg1 is the centroid of the C1/C2/N2/C3/N1 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O1^{i}	0.93	2.51	3.261 (3)	138
C5—H5···Cg1^{ii}	0.93	2.93	3.684 (3)	139 (3)

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); 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: CI2410).

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supplementary materials

Acta Cryst. (2007). E**63**, o3598-o3599 [**doi:10.1107/S160053680703543X**]

1,1'-Sulfonyldiimidazole

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Comment

1,1'-Sulfonyldiimidazole is a potent drug belonging to the 'sulfa' family. Also, units containing diimidazole moiety have been incorporated in the synthesis of organic polymers and macrocylic complexes (Elmer *et al.*, 1993; Lehn *et al.*, 1989). As part of a systematic study of the stereochemistry of 'sulfa' drugs (Patel *et al.*, 2001) in different chemicals as well as crystallographic environments, we have investigated the crystal and molecular structure of 1,1'-sulfonyldiimidazole.

The title molecule (Fig. 1) possesses an internal twofold symmetry. The two halves across sulfur is related by a pseudo-twofold axis with direction cosines 0.883, −0.467 and −0.046 (Hepperle, 2001). The rotation axis passes through the sulfur atom. The r.m.s. deviation on superposition about the axis is as low as 0.033 Å. The lengths of the symmetry (pseudo) related bonds such as C4—N3 and C1—N1, C5—N4 and C2—N2, S—N1 and S—N3, and C3—N2 and C6—N4 are similar (Table 1). The C3—N2 and C6—N4 bond lengths are shorter than the usual double bond observed in similar structures (Secondo *et al.*, 1996; Ülkü *et al.*, 1997). Bond angles about symmetry (pseudo) related atoms C2 and C5, and N2 and N4 are similar. The stereochemistry around sulfur, as usual in sulfonamides (Patel *et al.*, 2001; Bettinetti & Sardone, 1997) is a distorted tetrahedron: the angles vary from 104.54 (11)° [N3—S—N1] to 124.00 (12)° [O1—S—O2]. Non-bonded contact distances and the molecular geometry around sulfur are very well comparable to those of 4,4'-diaminodiphenylsulfone, a very similar structure where the sulfide bridges two phenyl rings (Tiwari & Singh, 1982). The best planes of the two planar five-membered imidazole rings are inclined at 75.05 (17)° to each other.

Unlike in other imidazole derivatives (Blaton *et al.*, 1979*a*, 1979*b*; Jones *et al.*, 1996) none of the imidazolidine N-atoms are involved in any conventional hydrogen bonding interactions. However, the intermolecular interactions responding to the structure stability are relatively weak C—H···O hydrogen bonds, C—H···π and π···π interactions as usual for an aromatic molecule (Desiraju *et al.*, 1989; Hunter & Sanders, 1990; Patel *et al.*, 2007). The molecules are linked through intermolecular C6—H6···O1^{i} hydrogen bonds into a zigzag chain of C5 graph set motif along the *b* axis (Fig. 2) (Bernstein *et al.*, 1995). Along the *a* axis, the chains are cross-linked through π-π stacking interactions between two symmetry related imidazole rings, with a $Cg2\cdots Cg2^{iii}$ distance of 3.667 (2) Å [*Cg*2 is the N3/C4/C5/N4/C6 ring centroid and symmetry code: (iii) 1/2 + *x*, *y*, 3/2 − *z*], and C—H···π interactions involving the C5—H5 group and π-system of the C1/C2/N2/C3/N1 imidazole ring (centroid *Cg*1), The C—H···π interaction (Table 2) forms the type-III geometry according to the classification of Malone *et al.* (1997). These interactions lead to the formation of a layer parallel to the *ab* plane. The layers are arranged in such a way that the molecules are arranged sinusoidally along the *c* axis (Fig. 2).

Experimental

The title compound was obtained from Sigma–Aldrich in pure powder form. Thin platy crystals of the compound were obtained from ethanol at room temperature. The crystal density was measured by flotation using mixture of benzene and carbon tetrachloride.

Refinement

The H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

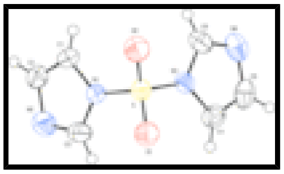

Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids.

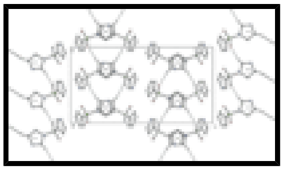

Fig. 2. The molecular packing diagram as seen along the *a* axis. π-π interactions are shown as solid lines, C—H···π interaction as double dashed lines and C—H···O interaction as dashed lines. H atoms not involved in interactions have been omitted.

1,1' sulfonyldiimidazole

Crystal data

$C_6H_6N_4O_2S$

$M_r = 198.21$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 7.285$ (2) Å

$b = 11.012$ (4) Å

$c = 20.646$ (3) Å

$V = 1656.3$ (8) Å^3

$Z = 8$

$F_{000} = 816$

$D_x = 1.590$ Mg m^{-3}

$D_m = 1.557$ Mg m^{-3}

D_m measured by flotation method

Mo *K*α radiation

$\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 25$–$35°$

$\mu = 0.36$ mm^{-1}

$T = 293$ K

Plate, colourless

0.12 × 0.10 × 0.05 mm

Data collection

Enraf–Nonius CAD-4 diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ K

ω/2θ scans

Absorption correction: none

1459 measured reflections

1459 independent reflections

1064 reflections with $I > 2\sigma(I)$

$R_{int} = 0.0000$

$\theta_{max} = 25.0°$

$\theta_{min} = 3.4°$

$h = 0 \rightarrow 8$

$k = -12 \rightarrow 0$

$l = 0 \rightarrow 24$

3 standard reflections

every 60 min

intensity decay: 1%

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.035$	$w = 1/[\sigma^2(F_o^2) + (0.028P)^2 + 0.9166P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.081$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.19$ e Å^{-3}
1459 reflections	$\Delta\rho_{min} = -0.26$ e Å^{-3}
119 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001Fc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0087 (7)
Secondary atom site location: difference Fourier map	

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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*	$U_{iso}*/U_{eq}$
S	0.66304 (8)	0.88695 (5)	0.61462 (3)	0.0380 (2)
O1	0.7673 (3)	0.99405 (16)	0.62217 (9)	0.0528 (6)
O2	0.7212 (3)	0.78547 (15)	0.57839 (8)	0.0538 (7)
N1	0.4613 (3)	0.92839 (16)	0.58525 (9)	0.0373 (7)
N2	0.2174 (3)	1.0421 (2)	0.56562 (13)	0.0606 (9)
N3	0.6173 (3)	0.83646 (17)	0.68836 (9)	0.0352 (6)
N4	0.5471 (3)	0.7087 (2)	0.76714 (11)	0.0556 (9)
C1	0.3395 (4)	0.8570 (2)	0.55011 (12)	0.0447 (9)
C2	0.1954 (4)	0.9279 (2)	0.53849 (13)	0.0509 (10)
C3	0.3767 (4)	1.0391 (2)	0.59317 (15)	0.0566 (10)
C4	0.6300 (3)	0.9021 (2)	0.74563 (12)	0.0459 (9)
C5	0.5877 (4)	0.8224 (3)	0.79227 (13)	0.0533 (10)
C6	0.5660 (4)	0.7203 (2)	0.70536 (13)	0.0476 (9)
H1	0.35530	0.77670	0.53740	0.0540*
H2	0.09260	0.90380	0.51510	0.0610*
H3	0.42790	1.10400	0.61560	0.0680*
H4	0.66100	0.98350	0.75050	0.0550*

H5	0.58590	0.84100	0.83620	0.0640*
H6	0.54740	0.65770	0.67580	0.0570*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S	0.0395 (3)	0.0406 (3)	0.0338 (3)	0.0000 (3)	0.0020 (3)	0.0011 (3)
O1	0.0503 (11)	0.0515 (10)	0.0567 (11)	−0.0169 (9)	−0.0052 (10)	0.0087 (9)
O2	0.0622 (13)	0.0561 (11)	0.0431 (10)	0.0158 (10)	0.0105 (9)	−0.0083 (9)
N1	0.0463 (13)	0.0318 (10)	0.0338 (11)	0.0018 (9)	−0.0060 (10)	−0.0020 (8)
N2	0.0603 (16)	0.0463 (14)	0.0753 (17)	0.0095 (12)	−0.0191 (14)	−0.0001 (12)
N3	0.0395 (12)	0.0344 (11)	0.0317 (10)	0.0035 (9)	0.0011 (9)	0.0006 (8)
N4	0.0567 (16)	0.0605 (15)	0.0496 (15)	0.0051 (12)	0.0048 (12)	0.0164 (12)
C1	0.0572 (17)	0.0372 (13)	0.0397 (14)	−0.0036 (13)	−0.0084 (13)	−0.0079 (11)
C2	0.0546 (18)	0.0499 (16)	0.0483 (16)	−0.0083 (14)	−0.0146 (13)	0.0024 (13)
C3	0.066 (2)	0.0326 (14)	0.0711 (19)	0.0046 (13)	−0.0187 (16)	−0.0082 (13)
C4	0.0503 (16)	0.0466 (15)	0.0407 (14)	0.0047 (12)	0.0002 (12)	−0.0088 (12)
C5	0.0494 (17)	0.078 (2)	0.0325 (14)	0.0094 (16)	0.0016 (12)	0.0002 (14)
C6	0.0539 (17)	0.0374 (15)	0.0516 (17)	0.0045 (12)	0.0029 (14)	0.0052 (12)

Geometric parameters (Å, °)

S—O1	1.411 (2)	N4—C5	1.387 (4)
S—O2	1.4099 (19)	N4—C6	1.289 (4)
S—N1	1.654 (2)	C1—C2	1.330 (4)
S—N3	1.655 (2)	C4—C5	1.339 (4)
N1—C1	1.390 (3)	C1—H1	0.93
N1—C3	1.376 (3)	C2—H2	0.93
N2—C2	1.386 (3)	C3—H3	0.93
N2—C3	1.293 (4)	C4—H4	0.93
N3—C4	1.389 (3)	C5—H5	0.93
N3—C6	1.378 (3)	C6—H6	0.93
O1···C6^{i}	3.261 (3)	C6···O1^{ix}	3.261 (3)
O2···C2^{ii}	3.373 (3)	C1···H5^{viii}	2.9900
O2···C1^{ii}	3.200 (3)	C2···H2^{iv}	3.0100
O1···H4	2.7600	C2···H5^{viii}	2.8700
O1···H3	2.7600	C5···H3^{v}	3.0700
O1···H6^{i}	2.5100	H1···O2	2.8000
O2···H6	2.7600	H1···O2^{vi}	2.6700
O2···H1	2.8000	H1···N2^{x}	2.7000
O2···H1^{ii}	2.6700	H2···N2^{iv}	2.8700
N1···N2	2.211 (3)	H2···C2^{iv}	3.0100
N2···N1	2.211 (3)	H2···H2^{iv}	2.5900
N3···N4	2.211 (3)	H3···O1	2.7600
N4···N3	2.211 (3)	H3···N4^{xi}	2.6900
N2···H1^{iii}	2.7000	H3···C5^{xi}	3.0700

N2···H2^{iv}	2.8700	H4···O1	2.7600
N4···H3^{v}	2.6900	H4···N4^{xi}	2.9300
N4···H4^{v}	2.9300	H5···C1^{vii}	2.9900
C1···O2^{vi}	3.200 (3)	H5···C2^{vii}	2.8700
C2···O2^{vi}	3.373 (3)	H6···O2	2.7600
C4···C5^{vii}	3.536 (4)	H6···O1^{ix}	2.5100
C5···C4^{viii}	3.536 (4)		
O1—S—O2	124.00 (12)	N1—C3—N2	111.9 (2)
O1—S—N1	106.74 (11)	N3—C4—C5	104.8 (2)
O1—S—N3	106.71 (11)	N4—C5—C4	111.8 (2)
O2—S—N1	106.93 (11)	N3—C6—N4	111.9 (2)
O2—S—N3	106.40 (10)	N1—C1—H1	127.00
N1—S—N3	104.54 (11)	C2—C1—H1	127.00
S—N1—C1	127.05 (16)	N2—C2—H2	124.00
S—N1—C3	126.79 (18)	C1—C2—H2	124.00
C1—N1—C3	106.1 (2)	N1—C3—H3	124.00
C2—N2—C3	105.0 (2)	N2—C3—H3	124.00
S—N3—C4	126.51 (16)	N3—C4—H4	128.00
S—N3—C6	126.93 (17)	C5—C4—H4	128.00
C4—N3—C6	106.52 (19)	N4—C5—H5	124.00
C5—N4—C6	104.9 (2)	C4—C5—H5	124.00
N1—C1—C2	105.4 (2)	N3—C6—H6	124.00
N2—C2—C1	111.6 (2)	N4—C6—H6	124.00
O1—S—N1—C1	156.4 (2)	C3—N1—C1—C2	1.1 (3)
O1—S—N1—C3	−26.7 (2)	S—N1—C3—N2	−178.30 (19)
O2—S—N1—C1	21.8 (2)	C1—N1—C3—N2	−0.9 (3)
O2—S—N1—C3	−161.3 (2)	C3—N2—C2—C1	0.5 (3)
N3—S—N1—C1	−90.8 (2)	C2—N2—C3—N1	0.3 (3)
N3—S—N1—C3	86.1 (2)	S—N3—C4—C5	−177.4 (2)
O1—S—N3—C4	17.1 (2)	C6—N3—C4—C5	0.4 (3)
O1—S—N3—C6	−160.3 (2)	S—N3—C6—N4	177.50 (19)
O2—S—N3—C4	151.3 (2)	C4—N3—C6—N4	−0.3 (3)
O2—S—N3—C6	−26.1 (3)	C6—N4—C5—C4	0.3 (3)
N1—S—N3—C4	−95.8 (2)	C5—N4—C6—N3	0.0 (3)
N1—S—N3—C6	86.9 (2)	N1—C1—C2—N2	−1.0 (3)
S—N1—C1—C2	178.51 (18)	N3—C4—C5—N4	−0.5 (3)

Symmetry codes: (i) $-x+3/2, y+1/2, z$; (ii) $x+1/2, -y+3/2, -z+1$; (iii) $-x+1/2, y+1/2, z$; (iv) $-x, -y+2, -z+1$; (v) $-x+1, y-1/2, -z+3/2$; (vi) $x-1/2, -y+3/2, -z+1$; (vii) $x+1/2, y, -z+3/2$; (viii) $x-1/2, y, -z+3/2$; (ix) $-x+3/2, y-1/2, z$; (x) $-x+1/2, y-1/2, z$; (xi) $-x+1, y+1/2, -z+3/2$.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O1^{ix}	0.93	2.51	3.261 (3)	138
C5—H5···Cg1^{vii}	0.93	2.93	3.684 (3)	139 (3)

Symmetry codes: (ix) $-x+3/2, y-1/2, z$; (vii) $x+1/2, y, -z+3/2$.

Fig. 1

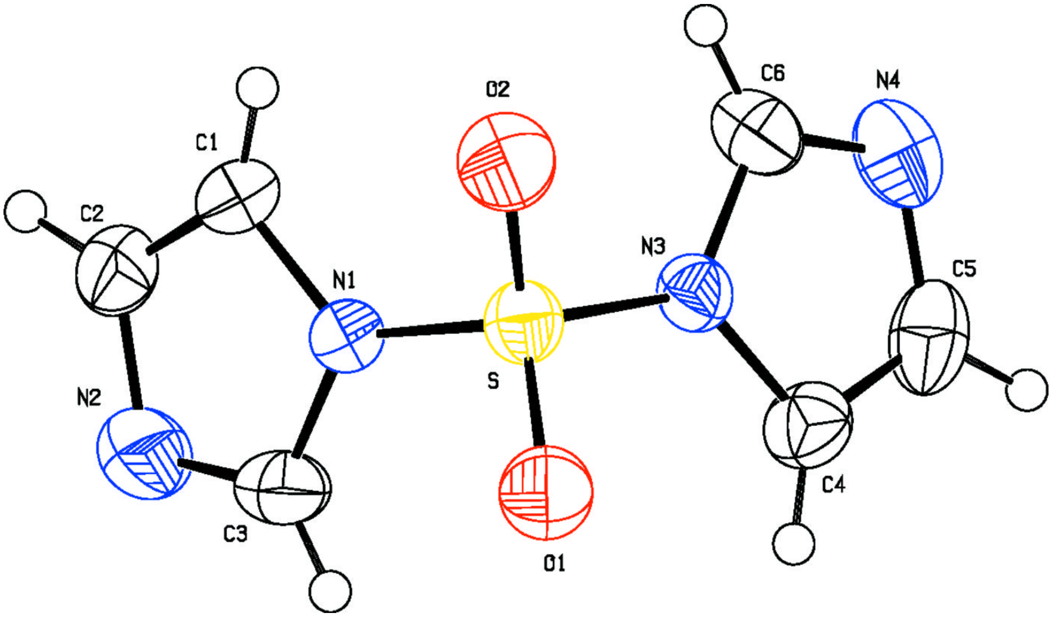

Fig. 2