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Crystal structure of *p*-toluenesulfonylmethyl isocyanide

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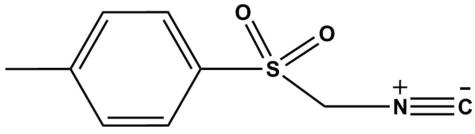
The molecule of the commercially available title compound, $C_9H_9NO_2S$, has crystallographically imposed mirror symmetry, the mirror plane passing through the isocyanide group and the *para*-C atoms, the methyl C atom and the S atom of the methyl 4-tolyl sulfone moiety. In the crystal, C—H···O hydrogen-bond interactions link the molecules into chains running parallel to the *b* axis.

Keywords: crystal structure; isocyanide derivative; hydrogen bonding.

CCDC reference: 1063415

1. Related literature

The title compound is an isocyanide derivative of methyl 4-tolyl sulfone (Ye, 2007), an important reaction intermediate obtained during the synthesis of mesotrione, a well known herbicide (Smith *et al.*, 2008).



2. Experimental

2.1. Crystal data

$C_9H_9NO_2S$
M_r = 195.23
Orthorhombic, *Pnma*
a = 22.342 (5) Å
b = 8.881 (2) Å
c = 4.8462 (12) Å
V = 961.6 (4) Å^3
Z = 4
Mo *Kα* radiation
μ = 0.30 mm^{-1}
T = 273 K
0.49 × 0.32 × 0.15 mm

2.2. Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.864, T_{max} = 0.961
5160 measured reflections
955 independent reflections
733 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.119
S = 1.11
955 reflections
77 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6*A*···O1^{i}	0.97	2.47	3.2519 (18)	138
C6—H6*A*···O1^{ii}	0.97	2.54	3.296 (4)	135
C6—H6*B*···O1^{iii}	0.97	2.54	3.296 (4)	135
C6—H6*B*···O1^{iv}	0.97	2.47	3.2519 (18)	138

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: RZ5158).

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supporting information

Acta Cryst. (2015). E**71**, o412 [doi:10.1107/S2056989015008816]

Crystal structure of *p*-toluenesulfonylmethyl isocyanide

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S1. Comment

The title compound is an isocyanide derivative of the previously reported compound methyl 4-tolyl sulfone (Ye, 2007), an important reaction intermediate obtained during the synthesis of mesotrione, a well known herbicide (Smith *et al.*, 2008). The compound was crystallized as part of our ongoing research project involving the study of the crystal structures and enzyme inhibition abilities of commercially available molecular libraries. The molecule has crystallographically imposed mirror symmetry, atoms C1, C4–C7, N1, S1 lying on the mirror plane (Fig. 1). The least-square mean line through C6, N1 and C7 forms an angle of 79.4 (3)° with the normal to the plane of the benzene ring. The crystal structure is stabilized by C6—H6A···O1, and C6—H6B···O1 intermolecular hydrogen interactions that link the molecules to form chains running parallel to the *b* axis (Fig. 2).

S2. Experimental

The title compound is a commercially available Sigma-Aldrich product. Colourless single crystals suitable for X-ray analysis were obtained from slow evaporation of a methanol solution at room temperature.

S3. Refinement

Aromatic and methylene H atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H = 0.93-0.97 Å, and with U_{iso}(H)= 1.2U_{eq}(C). The methyl H5A atom lying on a mirror plane was located in a difference Fourier map and refined isotropically, with the C5–H5A bond length constrained to be 1.1 (1) Å.

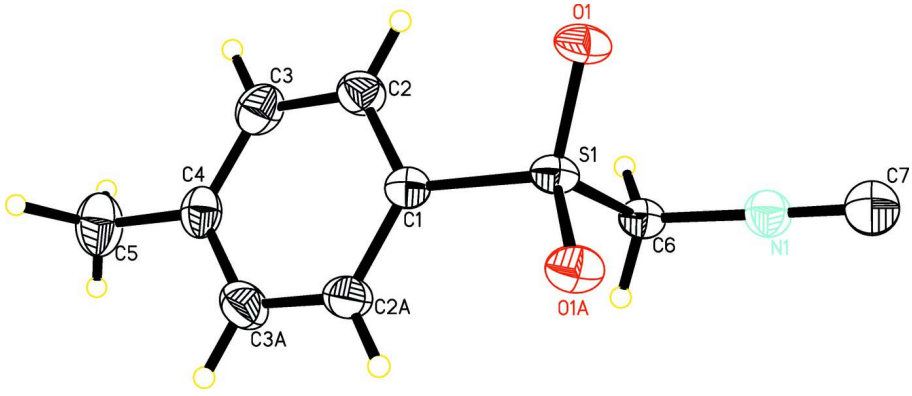

Figure 1

The molecular structure of title compound with displacement ellipsoids drawn at the 30% probability level.

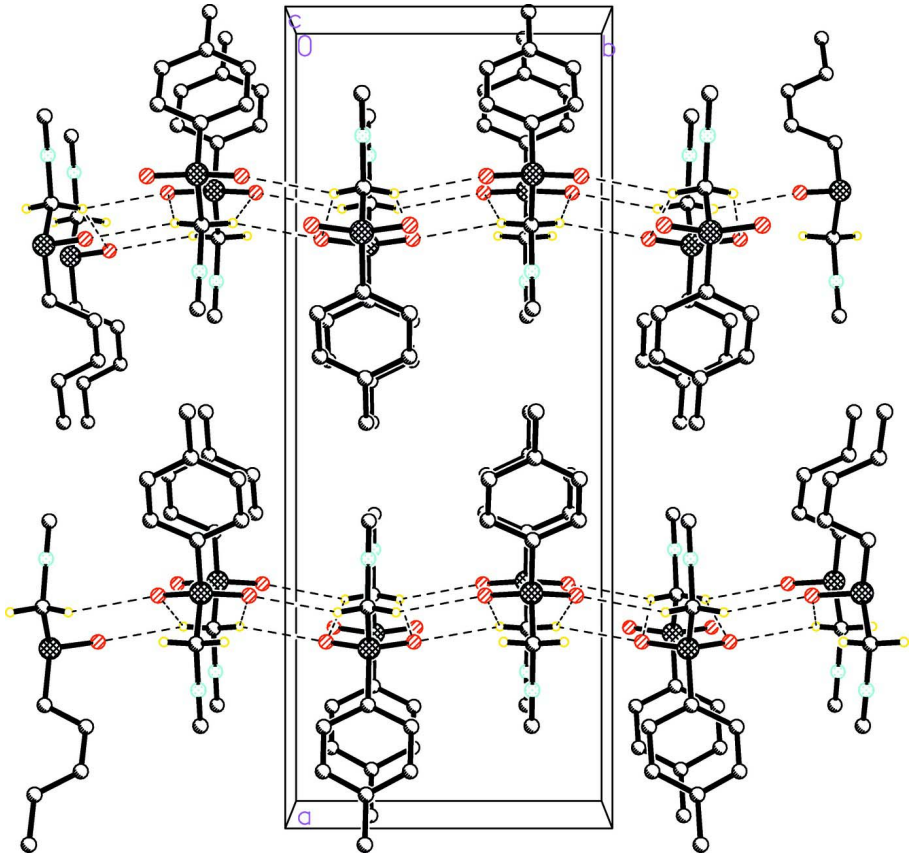

Figure 2

Crystal packing of the title compound, showing the formation of chains parallel to the *b* axis *via* C—H···O hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonding are omitted.

p-Toluenesulfonylmethyl isocyanide

Crystal data

$C_9H_9NO_2S$
M_r = 195.23
Orthorhombic, *Pnma*
Hall symbol: -P 2ac 2n
a = 22.342 (5) Å
b = 8.881 (2) Å
c = 4.8462 (12) Å
V = 961.6 (4) Å^3
Z = 4
$F(000)$ = 408
D_x = 1.349 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 830 reflections
θ = 2.9–22.3°
μ = 0.30 mm^{-1}
T = 273 K
Plate, colourless
0.49 × 0.32 × 0.15 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.864, T_{max} = 0.961
5160 measured reflections
955 independent reflections
733 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 25.5°, θ_{min} = 1.8°
h = −27→25
k = −10→10
l = −5→5

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.119$
$S = 1.11$
955 reflections
77 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0557P)^2 + 0.1844P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.28836 (4)	0.2500	0.85946 (16)	0.0354 (3)	
O1	0.28301 (8)	0.11111 (18)	1.0084 (3)	0.0462 (5)	
N1	0.17475 (16)	0.2500	0.7198 (6)	0.0483 (8)	
C1	0.35416 (16)	0.2500	0.6642 (7)	0.0379 (9)	
C2	0.37872 (13)	0.1154 (3)	0.5815 (6)	0.0488 (7)	
H2A	0.3624	0.0246	0.6398	0.059*	
C3	0.42793 (13)	0.1177 (3)	0.4109 (6)	0.0557 (8)	
H3A	0.4446	0.0268	0.3543	0.067*	
C4	0.45334 (18)	0.2500	0.3212 (7)	0.0477 (10)	
C5	0.5064 (2)	0.2500	0.1335 (11)	0.0714 (16)	
H5B	0.505 (2)	0.320 (5)	0.013 (11)	0.14 (2)*	
C6	0.23235 (16)	0.2500	0.5941 (7)	0.0383 (9)	
H6A	0.2369	0.3385	0.4788	0.046*	0.50
H6B	0.2369	0.1615	0.4788	0.046*	0.50
C7	0.1292 (2)	0.2500	0.8320 (11)	0.0707 (14)	
H5A	0.549 (2)	0.2500	0.242 (17)	0.21 (4)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0508 (6)	0.0300 (5)	0.0255 (4)	0.000	0.0031 (4)	0.000
O1	0.0676 (13)	0.0360 (10)	0.0349 (10)	0.0001 (9)	0.0045 (9)	0.0096 (7)
N1	0.051 (2)	0.0469 (19)	0.0467 (18)	0.000	0.0048 (17)	0.000
C1	0.044 (2)	0.0368 (19)	0.0330 (18)	0.000	−0.0023 (16)	0.000

C2	0.0551 (18)	0.0383 (15)	0.0531 (15)	−0.0007 (13)	0.0084 (14)	−0.0045 (12)
C3	0.0549 (19)	0.0551 (18)	0.0572 (18)	0.0105 (15)	0.0053 (15)	−0.0108 (15)
C4	0.040 (2)	0.065 (3)	0.039 (2)	0.000	−0.0021 (17)	0.000
C5	0.055 (3)	0.104 (5)	0.056 (3)	0.000	0.012 (3)	0.000
C6	0.051 (2)	0.0355 (18)	0.0288 (17)	0.000	0.0018 (16)	0.000
C7	0.066 (3)	0.059 (3)	0.087 (4)	0.000	0.008 (3)	0.000

Geometric parameters (Å, º)

S1—O1^{i}	1.4340 (16)	C2—H2A	0.9300
S1—O1	1.4341 (16)	C3—C4	1.375 (4)
S1—C1	1.748 (4)	C3—H3A	0.9300
S1—C6	1.794 (4)	C4—C3^{i}	1.375 (4)
N1—C7	1.154 (5)	C4—C5	1.494 (6)
N1—C6	1.424 (5)	C5—H5B	0.85 (5)
C1—C2^{i}	1.375 (3)	C5—H5A	1.095 (10)
C1—C2	1.375 (3)	C6—H6A	0.9700
C2—C3	1.376 (4)	C6—H6B	0.9700
O1^{i}—S1—O1	118.66 (14)	C4—C3—H3A	118.9
O1^{i}—S1—C1	110.03 (9)	C2—C3—H3A	118.9
O1—S1—C1	110.03 (9)	C3—C4—C3^{i}	117.3 (4)
O1^{i}—S1—C6	107.61 (10)	C3—C4—C5	121.33 (18)
O1—S1—C6	107.61 (10)	C3^{i}—C4—C5	121.33 (18)
C1—S1—C6	101.45 (16)	C4—C5—H5B	113 (3)
C7—N1—C6	177.2 (4)	C4—C5—H5A	114 (5)
C2^{i}—C1—C2	120.8 (3)	H5B—C5—H5A	111 (4)
C2^{i}—C1—S1	119.56 (18)	N1—C6—S1	108.9 (2)
C2—C1—S1	119.56 (18)	N1—C6—H6A	109.9
C1—C2—C3	118.8 (3)	S1—C6—H6A	109.9
C1—C2—H2A	120.6	N1—C6—H6B	109.9
C3—C2—H2A	120.6	S1—C6—H6B	109.9
C4—C3—C2	122.2 (3)	H6A—C6—H6B	108.3
O1^{i}—S1—C1—C2^{i}	−25.6 (3)	S1—C1—C2—C3	175.2 (2)
O1—S1—C1—C2^{i}	−158.2 (2)	C1—C2—C3—C4	0.2 (5)
C6—S1—C1—C2^{i}	88.1 (3)	C2—C3—C4—C3^{i}	0.6 (6)
O1^{i}—S1—C1—C2	158.2 (2)	C2—C3—C4—C5	−179.3 (4)
O1—S1—C1—C2	25.6 (3)	O1^{i}—S1—C6—N1	−64.47 (9)
C6—S1—C1—C2	−88.1 (3)	O1—S1—C6—N1	64.47 (9)
C2^{i}—C1—C2—C3	−0.9 (6)	C1—S1—C6—N1	180.0

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6*A*···O1^{ii}	0.97	2.47	3.2519 (18)	138
C6—H6*A*···O1^{iii}	0.97	2.54	3.296 (4)	135

C6—H6*B*···O1^{iv}	0.97	2.54	3.296 (4)	135
C6—H6*B*···O1^{v}	0.97	2.47	3.2519 (18)	138

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