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N-(3-Methylphenyl)methanesulfonamide

B. Thimme Gowda,[a]* Sabine Foro[b] and Hartmut Fuess[b]

[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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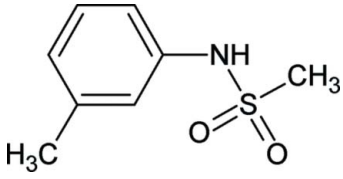
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.006 Å; R factor = 0.048; wR factor = 0.124; data-to-parameter ratio = 13.0.

The conformation of the N—H bond in the structure of the title compound (3MPMSA), $C_8H_{11}NO_2S$, is *anti* to the *meta*-methyl substituent, similar to that observed in the corresponding *meta*-nitro-substituted sulfonanilide (3NPMSA). The bond parameters in the three compounds, PMSA, 3MPMSA and 3NPMSA, are similar except in the S—N—C angle and in the S—N—C—C torsion angles. The molecules are linked into chains in the direction of the *c* axis through N—H···O hydrogen bonds.

Related literature

For related literature, see: Gowda *et al.* (2007); Gowda *et al.* (2007*a*); Gowda *et al.* (2007*b*); Gowda *et al.* (2000); Jayalakshmi & Gowda (2004); Klug (1968).



Experimental

Crystal data

$C_8H_{11}NO_2S$
M_r = 185.24
Orthorhombic, *Pccn*
a = 23.218 (2) Å
b = 8.4933 (7) Å
c = 9.2561 (8) Å
V = 1825.3 (3) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 2.84 mm^{-1}
T = 299 (2) K
0.25 × 0.10 × 0.03 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.623, T_{max} = 0.859
(expected range = 0.666–0.918)
1875 measured reflections
1618 independent reflections
975 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
3 standard reflections
frequency: 120 min
intensity decay: 2.2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.124
S = 1.02
1618 reflections
124 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5N···O3^{i}	0.856 (10)	2.144 (12)	2.990 (4)	169 (3)

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

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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: BT2331).

References

Enraf–Nonius (1996). *CAD-4-PC*. PC Version. Nonius BV, Delft, The Netherlands.
Gowda, B. T., Foro, S. & Fuess, H. (2007*a*). *Acta Cryst.* E**63**, o1975–o1976.
Gowda, B. T., Foro, S. & Fuess, H. (2007*b*). *Acta Cryst.* E**63**, o2337.
Gowda, B. T., Kozisek, J., Svoboda, I. & Fuess, H. (2007). *Z. Naturforsch. Teil A*, **62**, 91–100.
Gowda, B. T., Paulus, H. & Fuess, H. (2000). *Z. Naturforsch. Teil A*, **55**, 711–720.
Jayalakshmi, K. L. & Gowda, B. T. (2004). *Z. Naturforsch. Teil A*, **59**, 491–500.
Klug, H. P. (1968). *Acta Cryst.* B**24**, 792–802.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (1987). *REDU4*. Stoe & Cie GmbH, Darmstadt, Germany.

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supplementary materials

Acta Cryst. (2007). E**63**, o2338 [**doi:10.1107/S1600536807016443**]

N-(3-Methylphenyl)methanesulfonamide

B. T. Gowda, S. Foro and H. Fuess

Comment

The stereochemistry of biologically important alkyl sulfonanilides is of interest in explaining their biological activity. The biological activity may be due to N—H group. Therefore the structural studies of sulfonanilides are of interest. In the present work, the structure of *N*-(3-methylphenyl)-methanesulfonamde (3MPMSA) has been determined to explore the substituent effects on the structures of anilides and sulfonanilides (Gowda *et al.*, 2000, 2007, 2007a,b). The conformation of the N—H bond in the structure of 3MPMSA, is anti to the *meta*-methyl substituent (Fig.1), similar to that observed in the corresponding *meta*- nitro substituted sulfonanilide (3NPMSA)(Gowda *et al.*, 2007*b*). The bond parameters in the 3 compounds, PMSA (Klug, 1968), 3MPMSA and 3NPMSA are similar except in the S—N—C bond angle [120.0 (1)° (PMSA); 121.2 (2)° (3MPMSA); 126.3 (3)° (3NPMSA)] and in the S—N—C—C torsion angles [S2—N5—C6—C7 and S2—N5—C6—C11: 75.5 (2)° and -106.6 (2)° (PMSA); 68.1 (4)° and -114.3 (3)° (3MPMSA); 41.1 (3)°, -140.8 (2)° (3NPMSA)]. The molecules are linked in chains in the direction of *c* axis through N—H···O hydrogen bonds. (Table 1 and Fig. 2).

Experimental

The title compound was prepared according to the literature method (Jayalakshmi & Gowda, 2004). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Jayalakshmi & Gowda, 2004). Single crystals of the title compound were obtained from a slow evaporation of its ethanolic solution.

Refinement

Methyl groups were refined as riding with C—H = 0.96Å and U_{iso}(H) = 1.2 U_{eq}(C). The coordinates of the remaining H atoms were refined with U_{iso}(H) = 1.2 U_{eq}(C,*N*).

Figures

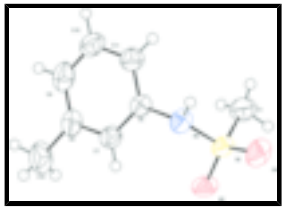
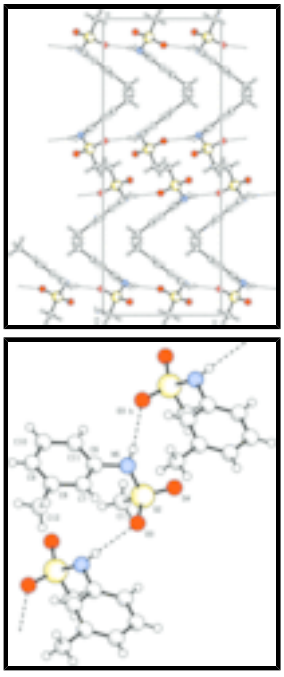


Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.
Fig. 2. The crystal packing of the title compound, viewed down the *b* axis.



_N_-(3-Methylphenyl)methanesulfonamide

Crystal data

$C_8H_{11}NO_2S$	F_{000} = 784
M_r = 185.24	D_x = 1.348 Mg m^{-3}
Orthorhombic, *Pccn*	Cu *K*α radiation λ = 1.54180 Å
Hall symbol: -P 2ab 2ac	Cell parameters from 25 reflections
a = 23.218 (2) Å	θ = 3.8–22.8º
b = 8.4933 (7) Å	μ = 2.84 mm^{-1}
c = 9.2561 (8) Å	*T* = 299 (2) K
V = 1825.3 (3) Å^3	Laminar, colourless
Z = 8	0.25 × 0.10 × 0.03 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.044
Radiation source: fine-focus sealed tube	θ_{max} = 66.8º
Monochromator: graphite	θ_{min} = 3.8º
T = 299(2) K	*h* = −27→0
ω/2θ scans	*k* = −10→2
Absorption correction: Psi-scan (North *et al.*, 1968)	*l* = −11→0
T_{min} = 0.623, T_{max} = 0.859	3 standard reflections
1875 measured reflections	every 120 min
1618 independent reflections	intensity decay: 2.2%

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

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.048$

$wR(F^2) = 0.124$

$S = 1.02$

1618 reflections

124 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: difference Fourier map

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0551P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.20$ e Å^{-3}

$\Delta\rho_{min} = -0.36$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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	0.49810 (16)	0.2700 (5)	0.0568 (4)	0.0565 (10)
H1A	0.5140	0.3265	0.1373	0.068*
H1B	0.4865	0.3432	−0.0166	0.068*
H1C	0.5267	0.1999	0.0183	0.068*
C6	0.37038 (14)	0.4150 (4)	0.1081 (4)	0.0370 (8)
C7	0.33344 (16)	0.3904 (5)	−0.0062 (4)	0.0435 (9)
H7	0.3240 (15)	0.295 (4)	−0.033 (4)	0.052*
C8	0.31135 (16)	0.5164 (5)	−0.0843 (4)	0.0492 (10)
C9	0.32608 (18)	0.6653 (6)	−0.0410 (5)	0.0575 (11)
H9	0.3117 (16)	0.744 (6)	−0.089 (5)	0.069*
C10	0.36123 (19)	0.6921 (5)	0.0767 (5)	0.0567 (12)
H10	0.3701 (16)	0.791 (5)	0.105 (5)	0.068*
C11	0.38420 (17)	0.5653 (5)	0.1511 (4)	0.0487 (10)
H11	0.4078 (16)	0.577 (5)	0.230 (4)	0.058*
C12	0.27302 (19)	0.4873 (6)	−0.2119 (5)	0.0807 (16)

H12A	0.2589	0.5860	−0.2480	0.097*
H12B	0.2411	0.4226	−0.1831	0.097*
H12C	0.2945	0.4348	−0.2863	0.097*
N5	0.39317 (13)	0.2824 (4)	0.1876 (3)	0.0431 (8)
H5N	0.4022 (15)	0.309 (4)	0.2740 (17)	0.052*
O3	0.41179 (11)	0.0963 (3)	−0.0128 (2)	0.0502 (7)
O4	0.45564 (12)	0.0557 (3)	0.2256 (3)	0.0597 (8)
S2	0.43830 (4)	0.16131 (9)	0.11400 (8)	0.0400 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.060 (2)	0.046 (2)	0.063 (2)	−0.005 (2)	−0.002 (2)	−0.004 (2)
C6	0.0430 (19)	0.0377 (17)	0.0302 (16)	0.0040 (16)	0.0050 (16)	0.0004 (18)
C7	0.048 (2)	0.043 (2)	0.0400 (19)	0.0059 (18)	−0.0015 (18)	−0.0052 (19)
C8	0.047 (2)	0.053 (2)	0.048 (2)	0.0124 (19)	−0.0021 (19)	0.005 (2)
C9	0.053 (3)	0.055 (3)	0.064 (3)	0.012 (2)	0.002 (2)	0.018 (3)
C10	0.052 (2)	0.037 (2)	0.081 (3)	−0.0026 (19)	0.007 (2)	0.000 (2)
C11	0.053 (2)	0.046 (2)	0.046 (2)	0.000 (2)	−0.0027 (19)	−0.003 (2)
C12	0.086 (3)	0.084 (4)	0.072 (3)	0.028 (3)	−0.034 (3)	−0.005 (3)
N5	0.0595 (19)	0.0441 (18)	0.0256 (14)	0.0099 (16)	−0.0017 (15)	0.0024 (14)
O3	0.0723 (17)	0.0407 (14)	0.0375 (13)	0.0003 (14)	−0.0112 (12)	−0.0093 (12)
O4	0.088 (2)	0.0473 (15)	0.0436 (14)	0.0134 (15)	−0.0116 (14)	0.0162 (13)
S2	0.0588 (5)	0.0311 (4)	0.0302 (4)	0.0028 (4)	−0.0063 (4)	0.0011 (4)

Geometric parameters (Å, °)

C1—S2	1.749 (4)	C9—H9	0.87 (4)
C1—H1A	0.9600	C10—C11	1.385 (5)
C1—H1B	0.9600	C10—H10	0.90 (4)
C1—H1C	0.9600	C11—H11	0.92 (4)
C6—C11	1.375 (5)	C12—H12A	0.9600
C6—C7	1.378 (5)	C12—H12B	0.9600
C6—N5	1.446 (4)	C12—H12C	0.9600
C7—C8	1.389 (5)	N5—S2	1.618 (3)
C7—H7	0.87 (4)	N5—H5N	0.856 (10)
C8—C9	1.370 (6)	O3—S2	1.436 (2)
C8—C12	1.500 (5)	O4—S2	1.426 (2)
C9—C10	1.380 (6)		
S2—C1—H1A	109.5	C11—C10—H10	119 (3)
S2—C1—H1B	109.5	C6—C11—C10	119.2 (4)
H1A—C1—H1B	109.5	C6—C11—H11	118 (3)
S2—C1—H1C	109.5	C10—C11—H11	123 (3)
H1A—C1—H1C	109.5	C8—C12—H12A	109.5
H1B—C1—H1C	109.5	C8—C12—H12B	109.5
C11—C6—C7	120.6 (3)	H12A—C12—H12B	109.5
C11—C6—N5	119.4 (3)	C8—C12—H12C	109.5
C7—C6—N5	120.0 (3)	H12A—C12—H12C	109.5

C6—C7—C8	120.8 (4)	H12B—C12—H12C	109.5
C6—C7—H7	121 (3)	C6—N5—S2	121.2 (2)
C8—C7—H7	118 (3)	C6—N5—H5N	111 (2)
C9—C8—C7	117.8 (4)	S2—N5—H5N	114 (2)
C9—C8—C12	122.0 (4)	O4—S2—O3	118.09 (16)
C7—C8—C12	120.2 (4)	O4—S2—N5	106.12 (15)
C8—C9—C10	122.0 (4)	O3—S2—N5	108.12 (16)
C8—C9—H9	118 (3)	O4—S2—C1	109.09 (18)
C10—C9—H9	120 (3)	O3—S2—C1	107.21 (17)
C9—C10—C11	119.5 (4)	N5—S2—C1	107.82 (18)
C9—C10—H10	121 (3)		
C11—C6—C7—C8	2.8 (6)	N5—C6—C11—C10	−178.5 (4)
N5—C6—C7—C8	−179.7 (3)	C9—C10—C11—C6	−1.5 (6)
C6—C7—C8—C9	−2.0 (6)	C11—C6—N5—S2	−114.3 (3)
C6—C7—C8—C12	177.6 (4)	C7—C6—N5—S2	68.2 (4)
C7—C8—C9—C10	−0.6 (6)	C6—N5—S2—O4	174.6 (3)
C12—C8—C9—C10	179.8 (4)	C6—N5—S2—O3	−57.7 (3)
C8—C9—C10—C11	2.3 (7)	C6—N5—S2—C1	57.9 (3)
C7—C6—C11—C10	−1.0 (6)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5N···O3^{i}	0.856 (10)	2.144 (12)	2.990 (4)	169 (3)

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

Fig. 1

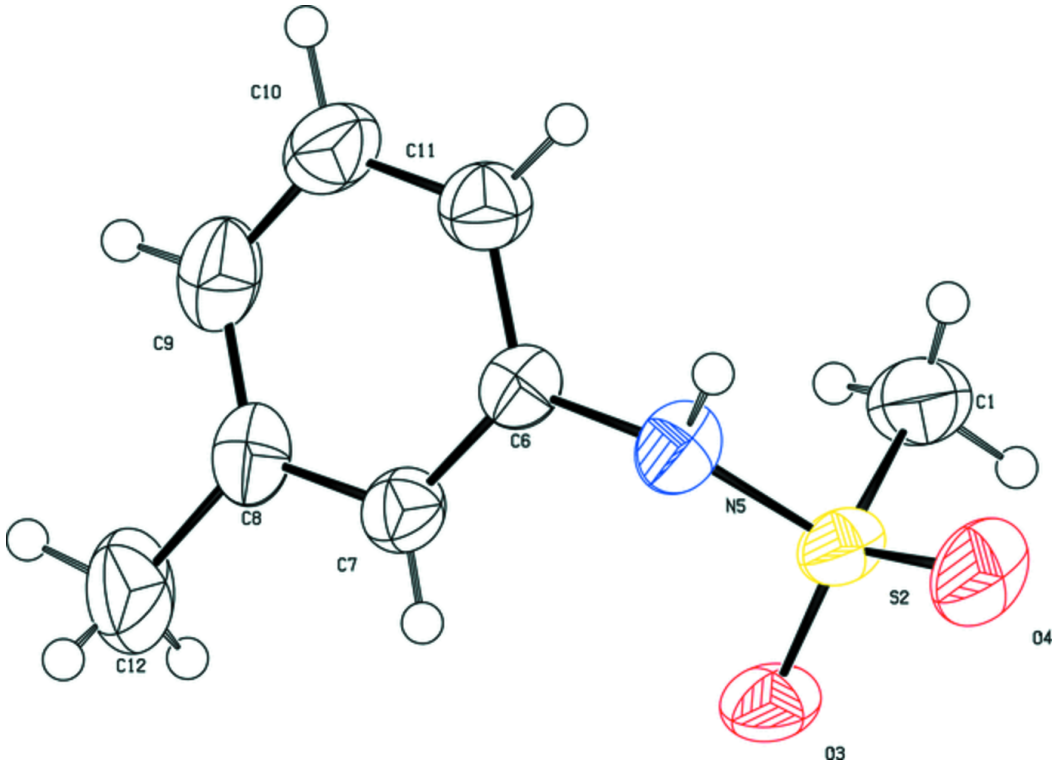


Fig. 2

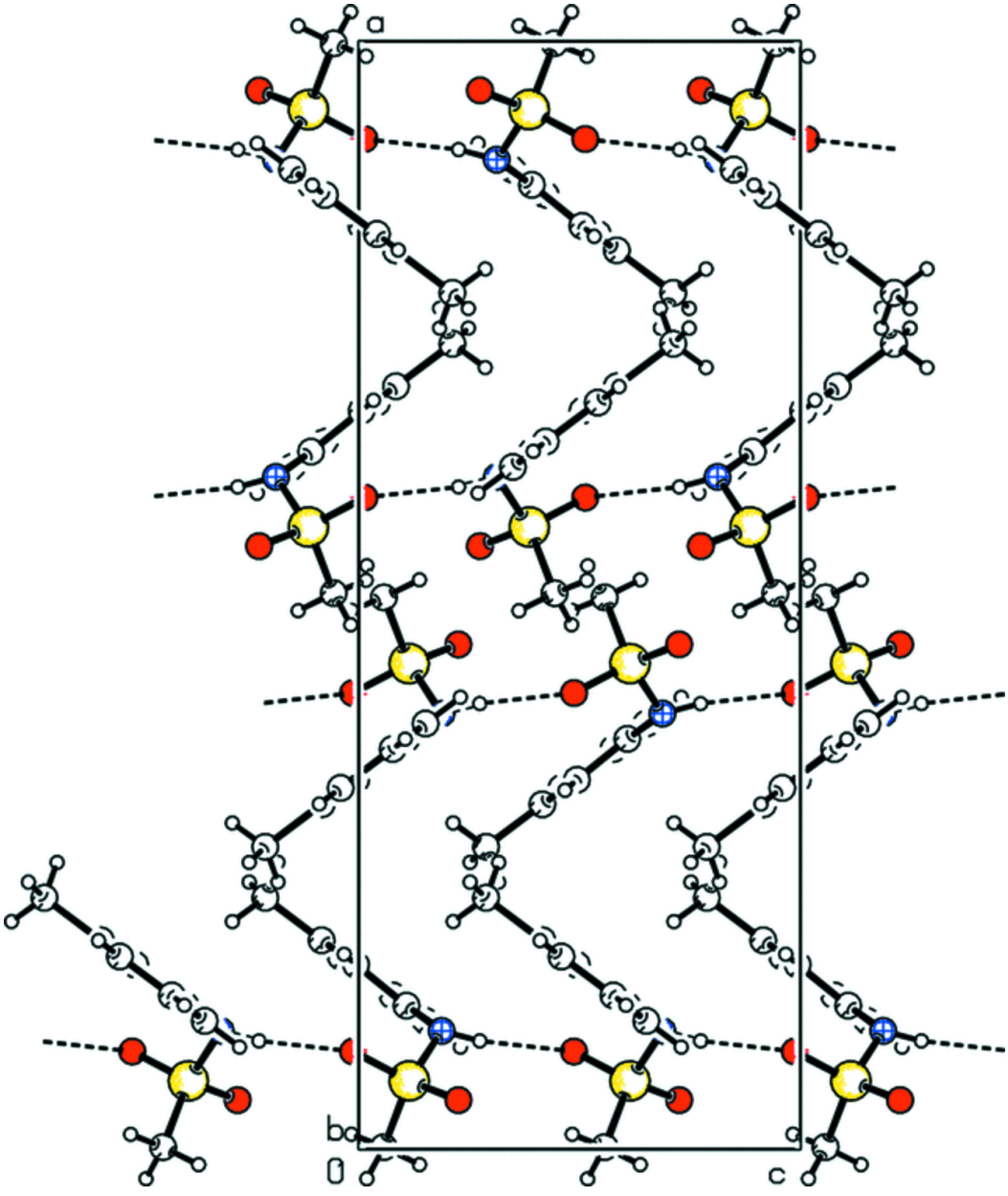


Fig. 3