Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(3-Chlorophenyl)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

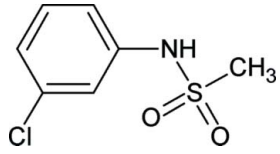
Received 6 April 2007; accepted 13 April 2007

Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.005 Å; R factor = 0.064; wR factor = 0.177; data-to-parameter ratio = 14.2.

The conformation of the N—H bond in the structure of the title compound (3CPMSA), $C_7H_8ClNO_2S$, is neither *syn* nor *anti* to the *meta*-chloro substituent, in contrast to the *anti* conformations observed for the stronger electron-withdrawing *meta*-nitro substituted (3NPMSA) and electron-donating *meta*-methyl substituted compounds (3MPMSA). The substitution of the Cl atom at the *meta* position of *N*-(phenyl)-methanesulfonamde (PMSA) changes its space group from $P2_1/c$ to $C2/c$ compared to the change over from monoclinic $P2_1/c$ to orthorhombic *Pccn* on *meta*-substitution of the electron-donating methyl group in PMSA and from monoclinic $P2_1/c$ to triclinic $P\overline{1}$, on *meta*-substitution of the stronger electron-withdrawing nitro group. The bond parameters in PMSA, 3CPMSA, 3MPMSA and 3NPMSA are similar except for some differences in the S—N—C—C torsion angles. As in other alkyl sulfonanilides, the amide hydrogen is available to a receptor molecule during its biological activity, as it sits alone on one side of the plane of the benzene ring, while the whole methanesulfonyl group is on the opposite side of the plane. The molecules in the title compound are packed into chains in the *b*-axis direction *via* N—H···O hydrogen bonds [H···O = 2.06, N···O = 2.979 (3) Å and N—H···O 169°].

Related literature

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



Experimental

Crystal data

$C_7H_8ClNO_2S$
M_r = 205.65
Monoclinic, $C2/c$
a = 23.488 (7) Å
b = 8.523 (2) Å
c = 9.216 (2) Å
β = 107.05 (2)°
V = 1763.8 (8) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 5.73 mm^{-1}
T = 299 (2) K
0.75 × 0.47 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.065, T_{max} = 0.191
(expected range = 0.061–0.179)
1675 measured reflections
1563 independent reflections
1486 reflections with $I > 2\sigma(I)$
R_{int} = 0.097
3 standard reflections
frequency: 120 min
intensity decay: 1.2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.177
S = 1.09
1563 reflections
110 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.87 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5*N*···O3^{i}	0.93	2.06	2.979 (3)	169

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

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*.

BTG thanks the Alexander von Humboldt Foundation, Bonn, Germany for an extension of his research fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2009).

References

Enraf–Nonius (1996). *CAD-4-PC*. Enraf–Nonius, Delft, The Netherlands.
Gowda, B. T., Foro, S. & Fuess, H. (2007*a*). *Acta Cryst.* E**63**, o2337.
Gowda, B. T., Foro, S. & Fuess, H. (2007*b*). *Acta Cryst.* E**63**, o2338.
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.

 doi:10.1107/S1600536807018466

supplementary materials

Acta Cryst. (2007). E**63**, o2569 [**doi:10.1107/S1600536807018466**]

N-(3-Chlorophenyl)methanesulfonamide

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

Comment

The stereochemistry of the biologically significant alkyl sulfonanilides, particularly in the vicinity of the phenyl-N—H portion is of interest in explaining their biological activity. The latter is thought to be due to the hydrogen atom of the phenyl N—H portion of the sulfonanilides as it can align itself, in relation to a receptor site. Therefore the structural studies of sulfonanilides are of interest. In the present work, the structure of *N*-(3-chlorophenyl)-methanesulfonamde (3CPMSA) has been determined to explore the substituent effects on the structures of sulfonanilides (Gowda *et al.*, 2007*a, b*). The conformation of the N—H bond in 3CPMSA is neither *syn* nor *anti* to the *meta*-chloro substituent (Fig. 1), in contrast to the *anti* conformations observed for the sulfonanilide with the stronger electron withdrawing *meta*-nitro substituent (3NPMSA)(Gowda *et al.*, 2007*a*) and for the compound with the electron donating *meta* - methyl substituent (3MPMSA)(Gowda *et al.*, 2007*b*). The substitution of Cl atom at the *meta* position of *N*-(phenyl)-methanesulfonamde (PMSA) changes its space group from P21/c (Klug, 1968) to C 2/c compared to the change over from monoclinic P21/c to orthorhombic Pccn on *meta* substitution of electron donating methyl group in PMSA and from monoclinic P21/c to triclinic P-1, on *meta* substitution of stronger electron withdrawing nitro group. The bond parameters in the 4 compounds, PMSA, 3CPMSA, 3MPMSA and 3NPMSA are similar except some difference in the torsional angles, S2N5C6C7, S2N5C6C11: 75.5 (2)°,-106.6 (2)° (PMSA); 61.7 (3)°, -120.0 (3)° (3CPMSA);68.1 (4)°, -114.3 (3)° (3MPMSA); 41.1 (3)°, -140.8 (2)° (3NPMSA), respectively. The data included for PMSA are the values determined under the present conditions as the literature values were determined by Klug, 1968. The N—H hydrogen sits alone on one side of the plane of the phenyl group, while the whole methanesulfonyl group is on the opposite side of the plane, similar to that observed in PMSA, 3NPMSA and 3MPMSA. The amide hydrogen is thus available to a receptor molecule during biological activity. The molecules in the title compound are packed into chain structure in the direction of *b* axis through N—H···O hydrogen bond (Table 1 & Fig. 2).

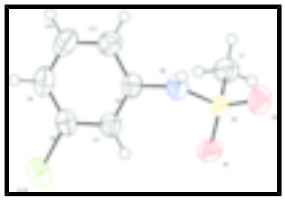
Experimental

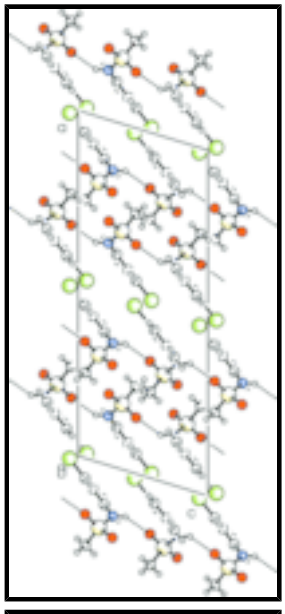
The title compound was prepared according to the literature method (Jayalakshmi & Gowda, 2004). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Jayalakshmi & Gowda, 2004). Single crystals of the title compound were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

Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.93 Å (CH aromatic) or 0.96 Å (CH_3) with U_{iso}(H) = 1.2 U_{eq}. The H atom of the NH group was located in a diffrerence map and its position refined.

Figures





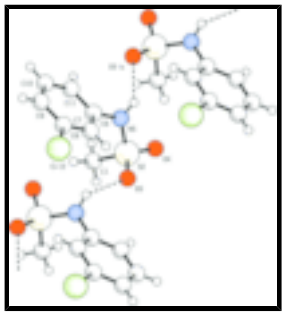


Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.
Fig. 2. Hydrogen bonding in the title compound. Hydrogen bonds are shown as dashed lines.

_N_-(3-Chlorophenyl)methanesulfonamide

Crystal data

$C_7H_8ClNO_2S$	F_{000} = 848
M_r = 205.65	D_x = 1.549 Mg m^{-3}
Monoclinic, *C*2/*c*	Cu *K*α radiation λ = 1.54180 Å
Hall symbol: -C 2yc	Cell parameters from 25 reflections
a = 23.488 (7) Å	θ = 7.9–25.4º
b = 8.523 (2) Å	μ = 5.73 mm^{-1}
c = 9.216 (2) Å	*T* = 299 (2) K
β = 107.05 (2)º	Long prism, colourless

V = 1763.8 (8) Å^3	0.75 × 0.47 × 0.30 mm
Z = 8	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.097
Radiation source: fine-focus sealed tube	θ_{max} = 67.0º
Monochromator: graphite	θ_{min} = 3.9º
T = 299(2) K	h = −26→28
ω/2θ scans	k = 0→10
Absorption correction: ψ scan (North *et al.*, 1968)	l = −10→1
T_{min} = 0.065, T_{max} = 0.191	3 standard reflections
1675 measured reflections	every 120 min
1563 independent reflections	intensity decay: 1.2%
1486 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.1311P)^2 + 1.4214P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.064	$(\Delta/\sigma)_{max}$ = 0.006
$wR(F^2)$ = 0.177	$\Delta\rho_{max}$ = 0.40 e Å^{-3}
S = 1.09	$\Delta\rho_{min}$ = −0.87 e Å^{-3}
1563 reflections	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
110 parameters	Extinction coefficient: 0.0224 (18)
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Cl12	0.01500 (4)	0.28125 (12)	0.56573 (12)	0.0759 (5)
S2	0.18925 (3)	0.58669 (7)	0.33977 (7)	0.0419 (4)
O3	0.16237 (10)	0.6527 (2)	0.4463 (2)	0.0517 (6)
O4	0.20627 (12)	0.6889 (3)	0.2374 (3)	0.0647 (7)
N5	0.14299 (11)	0.4624 (3)	0.2333 (2)	0.0480 (7)
H5N	0.1531	0.4357	0.1457	0.058*
C1	0.25175 (15)	0.4810 (4)	0.4443 (4)	0.0577 (8)
H1A	0.2799	0.5516	0.5088	0.069*
H1B	0.2698	0.4298	0.3761	0.069*
H1C	0.2398	0.4038	0.5055	0.069*
C6	0.11753 (12)	0.3372 (3)	0.2964 (3)	0.0420 (7)
C7	0.08190 (12)	0.3679 (4)	0.3865 (3)	0.0451 (7)
H7	0.0736	0.4707	0.4074	0.054*
C8	0.05832 (13)	0.2427 (4)	0.4464 (3)	0.0493 (7)
C9	0.06830 (15)	0.0902 (4)	0.4126 (4)	0.0576 (9)
H9	0.0522	0.0075	0.4534	0.069*
C10	0.10249 (15)	0.0622 (4)	0.3175 (4)	0.0618 (9)
H10	0.1085	−0.0405	0.2912	0.074*
C11	0.12804 (14)	0.1837 (4)	0.2603 (4)	0.0527 (7)
H11	0.1521	0.1633	0.1983	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl12	0.0730 (7)	0.0799 (7)	0.0904 (8)	−0.0152 (4)	0.0484 (5)	0.0030 (5)
S2	0.0540 (6)	0.0361 (5)	0.0403 (5)	−0.0044 (2)	0.0215 (3)	−0.0007 (2)
O3	0.0674 (13)	0.0441 (11)	0.0497 (11)	0.0002 (9)	0.0268 (9)	−0.0063 (8)
O4	0.0914 (18)	0.0536 (13)	0.0583 (14)	−0.0144 (12)	0.0362 (12)	0.0058 (10)
N5	0.0604 (15)	0.0514 (14)	0.0350 (11)	−0.0112 (11)	0.0181 (10)	−0.0024 (10)
C1	0.0527 (16)	0.0536 (18)	0.0658 (18)	0.0022 (14)	0.0157 (14)	−0.0049 (14)
C6	0.0422 (13)	0.0455 (15)	0.0347 (12)	−0.0080 (11)	0.0056 (10)	0.0002 (10)
C7	0.0443 (14)	0.0451 (14)	0.0450 (14)	−0.0048 (12)	0.0118 (11)	−0.0020 (11)
C8	0.0412 (15)	0.0550 (17)	0.0509 (15)	−0.0105 (12)	0.0126 (11)	0.0017 (12)
C9	0.0519 (17)	0.0496 (18)	0.067 (2)	−0.0133 (13)	0.0103 (14)	0.0069 (13)
C10	0.0582 (18)	0.0421 (15)	0.078 (2)	−0.0052 (13)	0.0083 (16)	−0.0063 (15)
C11	0.0554 (17)	0.0473 (15)	0.0548 (16)	−0.0018 (13)	0.0150 (13)	−0.0067 (13)

Geometric parameters (Å, °)

Cl12—C8	1.735 (3)	C6—C7	1.366 (4)
S2—O4	1.425 (2)	C6—C11	1.390 (4)
S2—O3	1.429 (2)	C7—C8	1.389 (4)
S2—N5	1.625 (2)	C7—H7	0.9300
S2—C1	1.751 (3)	C8—C9	1.372 (5)
N5—C6	1.428 (4)	C9—C10	1.372 (5)

N5—H5N	0.9344	C9—H9	0.9300
C1—H1A	0.9600	C10—C11	1.377 (5)
C1—H1B	0.9600	C10—H10	0.9300
C1—H1C	0.9600	C11—H11	0.9300
O4—S2—O3	118.70 (14)	C11—C6—N5	118.8 (3)
O4—S2—N5	105.47 (13)	C6—C7—C8	118.8 (3)
O3—S2—N5	108.64 (13)	C6—C7—H7	120.6
O4—S2—C1	109.04 (17)	C8—C7—H7	120.6
O3—S2—C1	107.00 (15)	C9—C8—C7	121.5 (3)
N5—S2—C1	107.54 (15)	C9—C8—Cl12	119.6 (2)
C6—N5—S2	121.81 (17)	C7—C8—Cl12	118.8 (2)
C6—N5—H5N	114.4	C8—C9—C10	118.7 (3)
S2—N5—H5N	112.7	C8—C9—H9	120.6
S2—C1—H1A	109.5	C10—C9—H9	120.6
S2—C1—H1B	109.5	C9—C10—C11	121.0 (3)
H1A—C1—H1B	109.5	C9—C10—H10	119.5
S2—C1—H1C	109.5	C11—C10—H10	119.5
H1A—C1—H1C	109.5	C10—C11—C6	119.3 (3)
H1B—C1—H1C	109.5	C10—C11—H11	120.4
C7—C6—C11	120.6 (3)	C6—C11—H11	120.4
C7—C6—N5	120.6 (3)		
O4—S2—N5—C6	178.0 (2)	C6—C7—C8—Cl12	178.0 (2)
O3—S2—N5—C6	−53.7 (3)	C7—C8—C9—C10	0.1 (5)
C1—S2—N5—C6	61.7 (3)	Cl12—C8—C9—C10	179.7 (2)
S2—N5—C6—C7	62.3 (3)	C8—C9—C10—C11	2.0 (5)
S2—N5—C6—C11	−119.8 (3)	C9—C10—C11—C6	−1.8 (5)
C11—C6—C7—C8	2.6 (4)	C7—C6—C11—C10	−0.5 (4)
N5—C6—C7—C8	−179.6 (2)	N5—C6—C11—C10	−178.4 (3)
C6—C7—C8—C9	−2.4 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5N···O3^{i}	0.93	2.06	2.979 (3)	169

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

Fig. 1

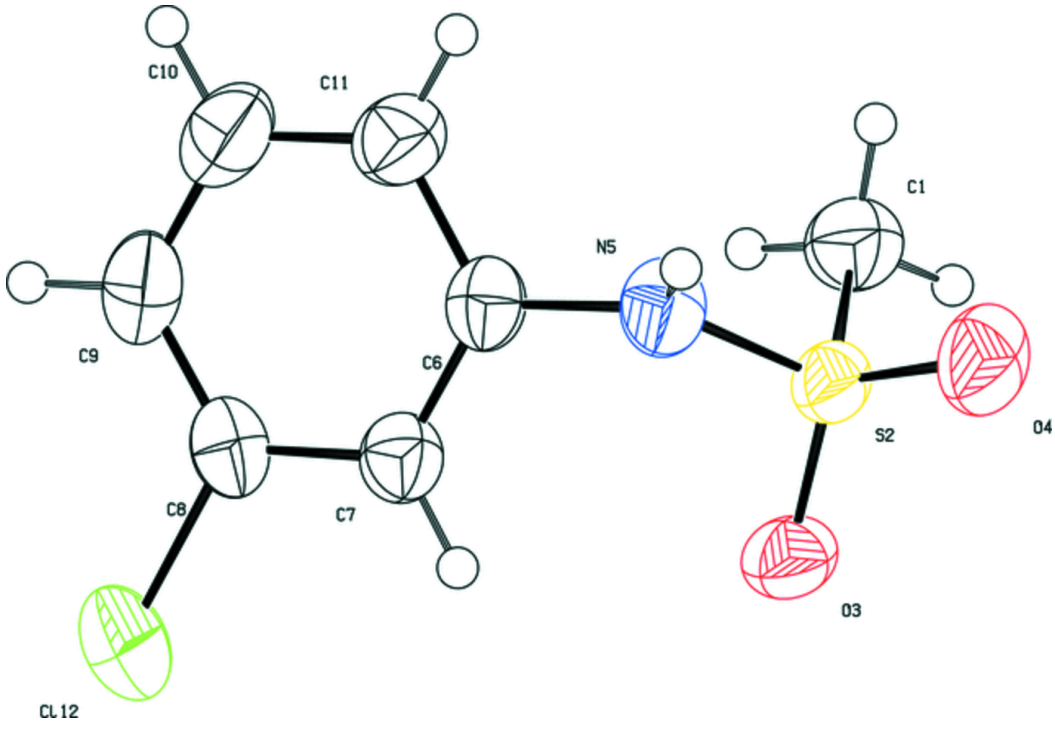


Fig. 2

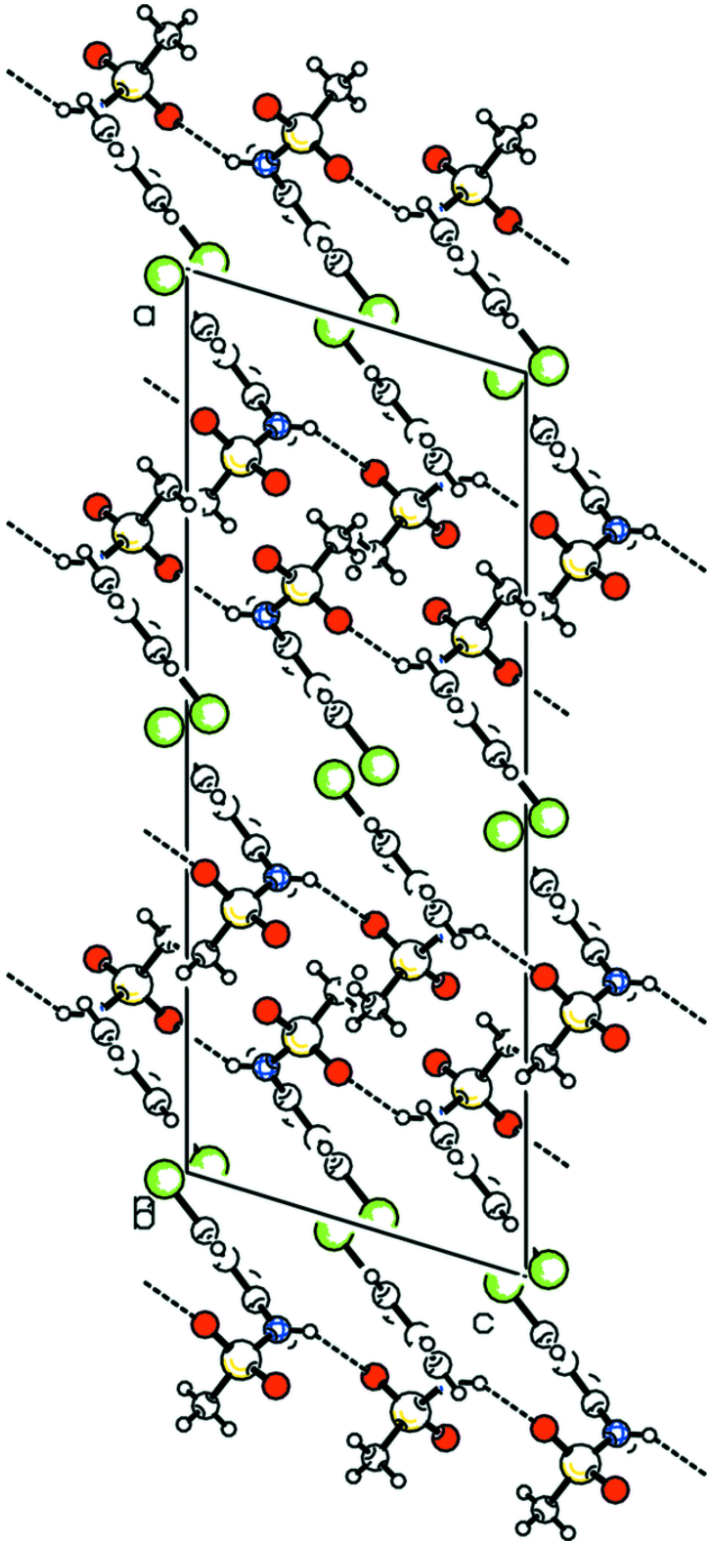


Fig. 3