

N-(4-Chlorophenyl)-1,1,1-trifluoro-N-(trifluoromethylsulfonyl)methanesulfonamide

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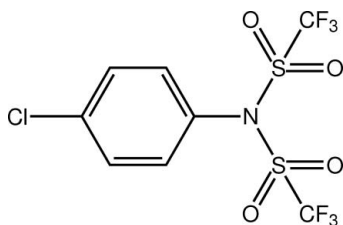
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Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.031; wR factor = 0.082; data-to-parameter ratio = 15.3.

The title molecule, also called 4-chloro-*N,N*-bis(trifluoromethanesulfonyl)aniline, $\text{C}_8\text{H}_4\text{ClF}_6\text{NO}_4\text{S}_2$, has non-crystallographic twofold symmetry with the pseudo-axis aligned along the Cl—C···C—N backbone of the molecule: the SO_2CF_3 residues lie to either side of the benzene ring. In the crystal, the presence of C—H···O contacts lead to the formation of a sequence of 12-membered $\{\cdots\text{HC}_2\text{NSO}\}_2$ synthons within a supramolecular chain aligned along [101].

Related literature

For uses of *N,N*-bis(trifluoromethanesulfonyl)aniline derivatives, see: Zeller (2001); Wulff *et al.* (1986). For general background to the synthesis, see: Deprez *et al.* (1995); Greenfield & Crosanu (2008). For a previous synthesis of the title compound, see: Laali *et al.* (2007).



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Experimental

Crystal data

$\text{C}_8\text{H}_4\text{ClF}_6\text{NO}_4\text{S}_2$
 $M_r = 391.70$
 Monoclinic, $P2_1/c$
 $a = 11.5998$ (3) Å
 $b = 13.4423$ (4) Å
 $c = 9.0548$ (2) Å
 $\beta = 108.014$ (2)°

$V = 1342.69$ (6) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.68$ mm⁻¹
 $T = 120$ K
 $0.40 \times 0.25 \times 0.25$ mm

Data collection

Nonius KappaCCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2007)
 $T_{\min} = 0.821$, $T_{\max} = 1.000$

17100 measured reflections
 3047 independent reflections
 2806 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.082$
 $S = 1.04$
 3047 reflections

199 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.62$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.41$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O3 ⁱ	0.95	2.57	3.496 (2)	164
C5—H5···O1 ⁱⁱ	0.95	2.59	3.385 (2)	141

Symmetry codes: (i) $-x + 1, -y + 2, -z + 1$; (ii) $-x + 2, -y + 2, -z + 2$.

Data collection: COLLECT (Hooft, 1998); cell refinement: DENZO (Otwinowski & Minor, 1997) and COLLECT; data reduction: DENZO and COLLECT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997) and DIAMOND (Brandenburg, 2006); software used to prepare material for publication: pubCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5319).

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supplementary materials

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N-(4-Chlorophenyl)-1,1,1-trifluoro-*N*-(trifluoromethylsulfonyl)methanesulfonamide

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Comment

N,N-Bis(trifluoromethanesulfonyl)aniline derivatives find use in synthetic chemistry such as mild triflating reagents (Zeller, 2001; Wulff *et al.*, 1986). Following a literature procedure to *p*-ClC₆H₄NHSO₂CF₃, using *p*-ClC₆H₄NH₂, (F₃CSO₂)O and Et₃N in CH₂Cl₂ at 213 K, a little of the di-substituted compound, *p*-ClC₆H₄(NSO₂CF₃), (I), was isolated as a side-product (Greenfield & Crosanu, 2008; Deprez *et al.*, 1995). Compound (I) has been reported previously (Laali *et al.*, 2007) and the X-ray structure determination is reported herein.

In (I), the SO₂CF₃ groups occupy approximately orthogonal positions to either side of the aromatic ring: the C3/C4/N1/S1, S2 torsion angles are 77.44 (17) and -101.55 (15) °, respectively; the dihedral angle formed between the benzene ring and NS₂ group is 78.13 (6) °. The CF₃ groups lie to either side of the molecule and fold back over the benzene ring so that, overall, the molecule has non-crystallographic 2-fold symmetry when viewed down the C11–C1–C4–N1 axis.

Supramolecular aggregation in (I) is dominated by C–H···O interactions that lead to the formation of a sequence of 12-membered {···HC₂NSO}₂ synthons aligned along [1 0 1], Fig. 2 and Table 1. Chains are connected into layers through the agency of C–Cl···π interactions between centrosymmetrically related residues [C1–C11···ring centroid(C1–C6)]ⁱ = 3.4592 (8) Å with angle at C11 = 92.46 (6) ° for *i*: 2-*x*, 2-*y*, 1-*z*]. The layers thus formed stack along the *b* axis with the closest contacts between successive layers being of the type C–F···π [C8–F4···ring centroid(C1–C6)]ⁱⁱ = 3.4708 (16) Å with angle at F4 = 122.83 (11) ° for *ii*: *x*, 3/2-*y*, 1/2+*z*].

Experimental

To a cooled (213 K) solution of *p*-ClC₆H₄NH₂ (11.5 g, 9.0 mmol) and triethylamine (1.50 ml; 10.8 mmol, 1.20 eq.) in CH₂Cl₂ (40 ml) was slowly added a solution of trifluoromethanesulfonic anhydride (2.40 ml; 13.5 mmol, 1.50 eq.) in CH₂Cl₂ (40 ml). After the mixture was stirred at 213–223 K for 1 h, water (30 ml) was added. The mixture was allowed to warm to room temperature, and the organic layer was decanted, washed with water, dried, and evaporated. The products, *N*-(4-chlorophenyl)trifluoromethylsulfonamide and *N*-(4-chlorophenyl)-bis-trifluoromethylsulfonamide, (I), were purified by chromatography on silica gel with hexane as eluent. Products were recrystallized from hexane. Characterisation data for (I): m.pt. 346–348 K, ¹H-NMR (500 MHz, CDCl₃) δ: 7.34 (2*H*), 7.50 (2*H*) p.p.m. ¹³C-NMR (125 MHz, CDCl₃) δ: 119.36 (q, ¹J(C,F) = 325 Hz), 125.17 (C3), 130.06, 132.18, 138.84 p.p.m. ¹⁹F-NMR (376 MHz, CDCl₃) δ: 71.11 p.p.m.

Refinement

The C-bound H atoms were geometrically placed (C–H = 0.95 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C).

Figures

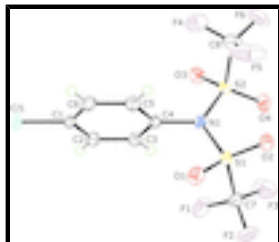


Fig. 1. The molecular structure of (I) showing displacement ellipsoids at the 50% probability level.

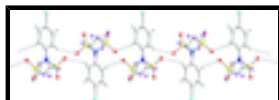


Fig. 2. A view of the supramolecular chain in (I) aligned along [1 0 1] and mediated by C–H...O interactions (blue dashed lines). Colour code: Cl, cyan; S, yellow; F, pink; O, red; N, blue; C, grey; and H, green.

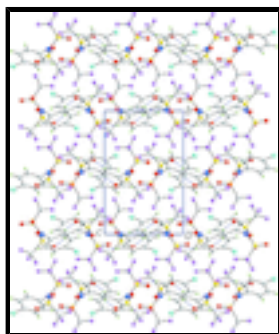


Fig. 3. View of the stacking of layers in (I). The C–H...O interactions are shown as blue dashed lines. Colour code: Cl, cyan; S, yellow; F, pink; O, red; N, blue; C, grey; and H, green.

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Crystal data

$C_8H_4ClF_6NO_4S_2$

$M_r = 391.70$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 11.5998$ (3) Å

$b = 13.4423$ (4) Å

$c = 9.0548$ (2) Å

$\beta = 108.014$ (2)°

$V = 1342.69$ (6) Å³

$Z = 4$

$F(000) = 776$

$D_x = 1.938$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2983 reflections

$\theta = 2.9$ – 27.5 °

$\mu = 0.68$ mm⁻¹

$T = 120$ K

Block, colourless

$0.40 \times 0.25 \times 0.25$ mm

Data collection

Nonius KappaCCD area-detector diffractometer

3047 independent reflections

Radiation source: Enraf Nonius FR591 rotating anode

2806 reflections with $I > 2\sigma(I)$

10 cm confocal mirrors

$R_{int} = 0.023$

Detector resolution: 9.091 pixels mm⁻¹

$\theta_{max} = 27.5$ °, $\theta_{min} = 2.9$ °

φ and ω scans

$h = -15 \rightarrow 15$

Absorption correction: multi-scan
(SADABS; Sheldrick, 2007) $k = -17 \rightarrow 17$
 $T_{\min} = 0.821$, $T_{\max} = 1.000$ $l = -11 \rightarrow 11$
17100 measured reflections

Refinement

Refinement on F^2 Primary atom site location: structure-invariant direct methods
Least-squares matrix: full Secondary atom site location: difference Fourier map
 $R[F^2 > 2\sigma(F^2)] = 0.031$ Hydrogen site location: inferred from neighbouring sites
 $wR(F^2) = 0.082$ H-atom parameters constrained
 $S = 1.04$ $w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 1.1662P]$
where $P = (F_o^2 + 2F_c^2)/3$
3047 reflections $(\Delta/\sigma)_{\max} = 0.001$
199 parameters $\Delta\rho_{\max} = 0.62 \text{ e } \text{\AA}^{-3}$
0 restraints $\Delta\rho_{\min} = -0.41 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.97286 (4)	0.86092 (3)	0.34987 (5)	0.02733 (12)
S1	0.78053 (4)	1.09197 (3)	0.91222 (4)	0.01889 (11)
S2	0.59031 (4)	0.94255 (3)	0.78741 (5)	0.01943 (11)
F1	0.70006 (16)	1.20000 (9)	0.66292 (14)	0.0497 (4)
F2	0.75847 (13)	1.28200 (9)	0.87505 (16)	0.0449 (3)
F3	0.58975 (12)	1.20628 (11)	0.8139 (2)	0.0551 (4)
F4	0.69058 (14)	0.77016 (10)	0.86879 (18)	0.0525 (4)
F5	0.71980 (16)	0.87281 (11)	1.05802 (17)	0.0663 (5)
F6	0.54674 (13)	0.80495 (10)	0.96076 (16)	0.0478 (3)
O1	0.90194 (11)	1.10259 (10)	0.91208 (15)	0.0280 (3)
O2	0.74816 (13)	1.08338 (10)	1.04986 (15)	0.0293 (3)
O3	0.54372 (11)	0.89593 (10)	0.64061 (14)	0.0254 (3)
O4	0.52094 (12)	1.00882 (11)	0.84680 (16)	0.0308 (3)
N1	0.72049 (12)	0.99798 (10)	0.79108 (15)	0.0167 (3)

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C1	0.89885 (15)	0.90047 (12)	0.4795 (2)	0.0192 (3)
C2	0.79853 (15)	0.96166 (12)	0.42518 (19)	0.0201 (3)
H2	0.7706	0.9812	0.3192	0.024*
C3	0.73954 (14)	0.99385 (12)	0.52852 (18)	0.0182 (3)
H3	0.6704	1.0358	0.4943	0.022*
C4	0.78292 (14)	0.96396 (12)	0.68241 (18)	0.0162 (3)
C5	0.88287 (15)	0.90243 (12)	0.73621 (19)	0.0198 (3)
H5	0.9106	0.8824	0.8420	0.024*
C6	0.94185 (15)	0.87055 (12)	0.6327 (2)	0.0218 (3)
H6	1.0110	0.8286	0.6668	0.026*
C7	0.70024 (18)	1.20199 (13)	0.8072 (2)	0.0258 (4)
C8	0.64203 (18)	0.84073 (14)	0.9298 (2)	0.0301 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0291 (2)	0.0285 (2)	0.0294 (2)	-0.00347 (16)	0.01644 (18)	-0.01089 (17)
S1	0.0231 (2)	0.0187 (2)	0.01481 (19)	-0.00119 (14)	0.00583 (15)	-0.00231 (13)
S2	0.0178 (2)	0.0220 (2)	0.0187 (2)	-0.00101 (14)	0.00585 (15)	0.00126 (14)
F1	0.0996 (12)	0.0286 (6)	0.0236 (6)	0.0191 (7)	0.0229 (7)	0.0060 (5)
F2	0.0691 (9)	0.0188 (5)	0.0461 (7)	-0.0062 (6)	0.0167 (7)	-0.0067 (5)
F3	0.0402 (7)	0.0402 (7)	0.0918 (12)	0.0177 (6)	0.0303 (8)	0.0267 (7)
F4	0.0650 (9)	0.0347 (7)	0.0620 (9)	0.0206 (7)	0.0257 (8)	0.0194 (6)
F5	0.0872 (11)	0.0427 (8)	0.0367 (7)	-0.0277 (8)	-0.0281 (7)	0.0189 (6)
F6	0.0593 (9)	0.0433 (7)	0.0469 (8)	-0.0179 (6)	0.0252 (7)	0.0100 (6)
O1	0.0216 (6)	0.0317 (7)	0.0290 (7)	-0.0046 (5)	0.0053 (5)	-0.0099 (5)
O2	0.0462 (8)	0.0276 (7)	0.0174 (6)	-0.0026 (6)	0.0146 (6)	-0.0025 (5)
O3	0.0211 (6)	0.0313 (7)	0.0216 (6)	-0.0065 (5)	0.0032 (5)	-0.0025 (5)
O4	0.0267 (7)	0.0358 (7)	0.0357 (7)	0.0025 (6)	0.0182 (6)	-0.0020 (6)
N1	0.0178 (6)	0.0171 (6)	0.0158 (6)	-0.0006 (5)	0.0060 (5)	-0.0025 (5)
C1	0.0216 (8)	0.0159 (7)	0.0226 (8)	-0.0044 (6)	0.0105 (6)	-0.0059 (6)
C2	0.0241 (8)	0.0204 (8)	0.0152 (7)	-0.0020 (6)	0.0055 (6)	-0.0020 (6)
C3	0.0182 (7)	0.0175 (7)	0.0171 (7)	0.0018 (6)	0.0027 (6)	0.0002 (6)
C4	0.0163 (7)	0.0166 (7)	0.0160 (7)	-0.0004 (6)	0.0055 (6)	-0.0015 (6)
C5	0.0197 (8)	0.0207 (8)	0.0176 (8)	0.0021 (6)	0.0038 (6)	0.0024 (6)
C6	0.0190 (8)	0.0193 (8)	0.0269 (8)	0.0029 (6)	0.0069 (7)	-0.0003 (6)
C7	0.0371 (10)	0.0185 (8)	0.0244 (9)	0.0017 (7)	0.0134 (7)	0.0002 (6)
C8	0.0360 (10)	0.0247 (9)	0.0258 (9)	-0.0082 (7)	0.0040 (8)	0.0053 (7)

Geometric parameters (\AA , $^\circ$)

C11—C1	1.7380 (16)	F5—C8	1.304 (2)
S1—O2	1.4131 (13)	F6—C8	1.313 (2)
S1—O1	1.4160 (13)	N1—C4	1.4637 (19)
S1—N1	1.6769 (13)	C1—C6	1.381 (2)
S1—C7	1.8470 (18)	C1—C2	1.385 (2)
S2—O4	1.4135 (13)	C2—C3	1.388 (2)
S2—O3	1.4168 (13)	C2—H2	0.9500
S2—N1	1.6749 (14)	C3—C4	1.387 (2)

S2—C8	1.8483 (19)	C3—H3	0.9500
F1—C7	1.306 (2)	C4—C5	1.384 (2)
F2—C7	1.317 (2)	C5—C6	1.388 (2)
F3—C7	1.303 (2)	C5—H5	0.9500
F4—C8	1.309 (3)	C6—H6	0.9500
O2—S1—O1	123.00 (9)	C2—C3—H3	120.5
O2—S1—N1	110.21 (8)	C5—C4—C3	122.06 (15)
O1—S1—N1	106.70 (7)	C5—C4—N1	119.00 (14)
O2—S1—C7	106.88 (8)	C3—C4—N1	118.94 (14)
O1—S1—C7	105.19 (9)	C4—C5—C6	118.75 (15)
N1—S1—C7	103.02 (8)	C4—C5—H5	120.6
O4—S2—O3	122.60 (8)	C6—C5—H5	120.6
O4—S2—N1	109.14 (8)	C1—C6—C5	119.21 (15)
O3—S2—N1	107.18 (7)	C1—C6—H6	120.4
O4—S2—C8	107.55 (9)	C5—C6—H6	120.4
O3—S2—C8	105.91 (8)	F3—C7—F1	110.51 (18)
N1—S2—C8	102.67 (8)	F3—C7—F2	108.18 (16)
C4—N1—S2	118.56 (10)	F1—C7—F2	109.00 (16)
C4—N1—S1	118.91 (10)	F3—C7—S1	110.98 (13)
S2—N1—S1	122.53 (8)	F1—C7—S1	110.08 (12)
C6—C1—C2	122.17 (15)	F2—C7—S1	108.03 (13)
C6—C1—C11	119.27 (13)	F5—C8—F4	110.23 (19)
C2—C1—C11	118.56 (13)	F5—C8—F6	109.09 (18)
C1—C2—C3	118.74 (15)	F4—C8—F6	108.97 (16)
C1—C2—H2	120.6	F5—C8—S2	111.24 (13)
C3—C2—H2	120.6	F4—C8—S2	109.37 (13)
C4—C3—C2	119.07 (15)	F6—C8—S2	107.89 (14)
C4—C3—H3	120.5		
O4—S2—N1—C4	-155.34 (12)	N1—C4—C5—C6	-179.88 (14)
O3—S2—N1—C4	-20.57 (14)	C2—C1—C6—C5	0.1 (3)
C8—S2—N1—C4	90.75 (13)	C11—C1—C6—C5	179.81 (13)
O4—S2—N1—S1	23.61 (12)	C4—C5—C6—C1	-0.4 (2)
O3—S2—N1—S1	158.38 (9)	O2—S1—C7—F3	-40.94 (16)
C8—S2—N1—S1	-90.29 (11)	O1—S1—C7—F3	-173.17 (14)
O2—S1—N1—C4	-151.50 (12)	N1—S1—C7—F3	75.21 (15)
O1—S1—N1—C4	-15.75 (14)	O2—S1—C7—F1	-163.59 (14)
C7—S1—N1—C4	94.75 (13)	O1—S1—C7—F1	64.17 (16)
O2—S1—N1—S2	29.55 (12)	N1—S1—C7—F1	-47.44 (16)
O1—S1—N1—S2	165.30 (9)	O2—S1—C7—F2	77.50 (14)
C7—S1—N1—S2	-84.20 (11)	O1—S1—C7—F2	-54.73 (14)
C6—C1—C2—C3	0.0 (2)	N1—S1—C7—F2	-166.35 (12)
C11—C1—C2—C3	-179.66 (12)	O4—S2—C8—F5	-67.64 (18)
C1—C2—C3—C4	0.1 (2)	O3—S2—C8—F5	159.68 (16)
C2—C3—C4—C5	-0.4 (2)	N1—S2—C8—F5	47.42 (18)
C2—C3—C4—N1	-179.97 (14)	O4—S2—C8—F4	170.36 (13)
S2—N1—C4—C5	-102.12 (15)	O3—S2—C8—F4	37.69 (16)
S1—N1—C4—C5	78.89 (17)	N1—S2—C8—F4	-74.58 (15)
S2—N1—C4—C3	77.44 (17)	O4—S2—C8—F6	51.97 (16)

supplementary materials

S1—N1—C4—C3	-101.55 (15)	O3—S2—C8—F6	-80.71 (15)
C3—C4—C5—C6	0.6 (2)	N1—S2—C8—F6	167.02 (13)

Hydrogen-bond geometry (Å, °)

<i>D—H···A</i>	<i>D—H</i>	<i>H···A</i>	<i>D···A</i>	<i>D—H···A</i>
C3—H3···O3 ⁱ	0.95	2.57	3.496 (2)	164
C5—H5···O1 ⁱⁱ	0.95	2.59	3.385 (2)	141

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $-x+2, -y+2, -z+2$.

Fig. 1

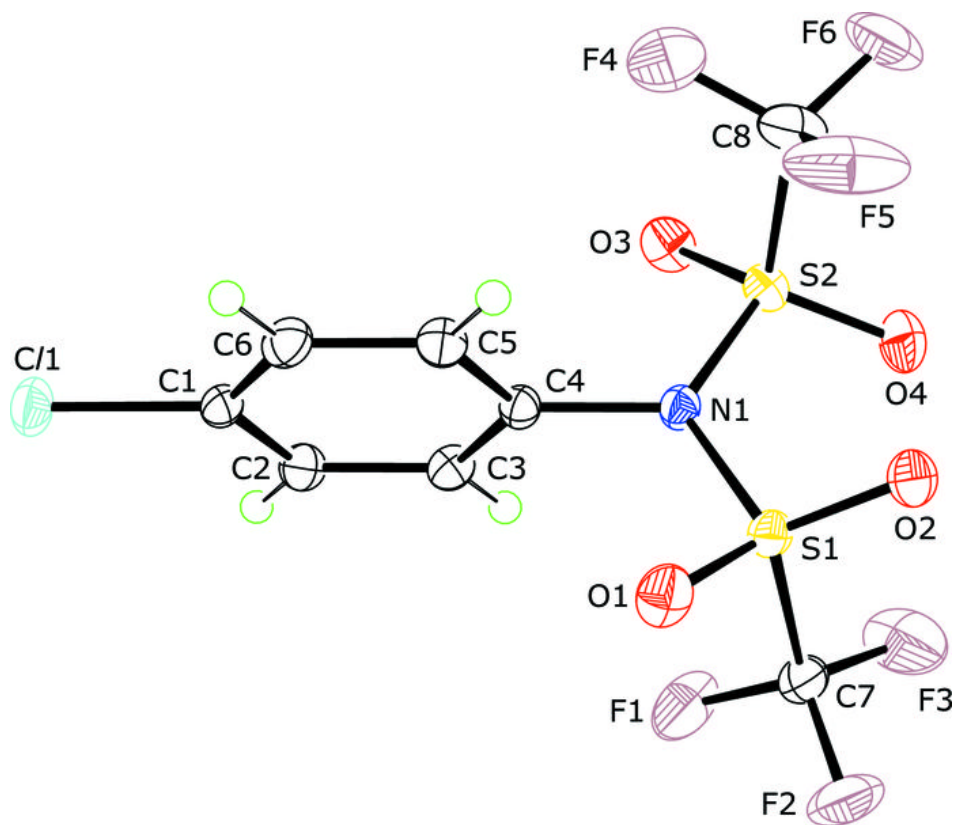


Fig. 3

