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N,N-Bis(trifluoromethylsulfonyl)aniline

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Key indicators

Single-crystal X-ray study
T = 143 K
Mean σ(C–C) = 0.001 Å
R factor = 0.026
wR factor = 0.069
Data-to-parameter ratio = 25.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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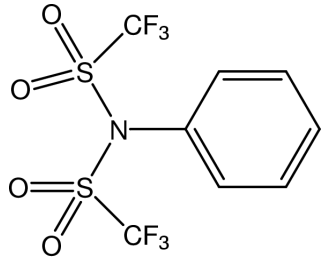
The title molecule, $C_8H_5F_6NO_4S_2$, has crystallographic twofold symmetry. The crystal packing consists of three intermolecular C—H···O contacts, resulting in a two-dimensional network. In the third direction, only a very weak C—H···F interaction, with an H···F distance of 2.83 Å, is found.

Comment

The crystal structure determination of the title compound, (I), was undertaken to study the influence of the F atoms on the crystal packing.



(I)

The molecule (Fig. 1) has *C*2 symmetry: atoms N, C1, C4 and H4 lie on a crystallographic twofold axis. This twofold symmetry results in an exact planarity of the N atom. The angle between the plane defined by the N atom and the plane of the phenyl group is 80.08 (3)°. The molecule shows no short intramolecular contacts. A very similar almost *C*2-symmetrical molecular conformation, with an angle of 85.2° between the planes defined by the N atom and the phenyl group, has been reported for *N,N*-bis(methylsulfonyl)aniline (Jones *et al.*, 1995).

The crystal packing (Fig. 2 and Table 1) shows three intermolecular C—H···O interactions. The C4—H4 bond donates a bifurcated weak hydrogen bond in the **c** direction to O atoms of two symmetry-related molecules. The molecules are connected in the **b** direction by a C2—H2···O2 interaction. No short intermolecular contacts are found which connect the molecules in the **a** direction. The shortest interaction found in this direction is a C3—H3···F3(1/4−*x*, 3/4+*y*, *z*−1/4) contact, with an H···F distance of 2.83 Å. This contact is very long and thus should be rather weak.

Experimental

A commercial sample of (I) (Aldrich Chemical Co.) was recrystallized from ether at 293 K.

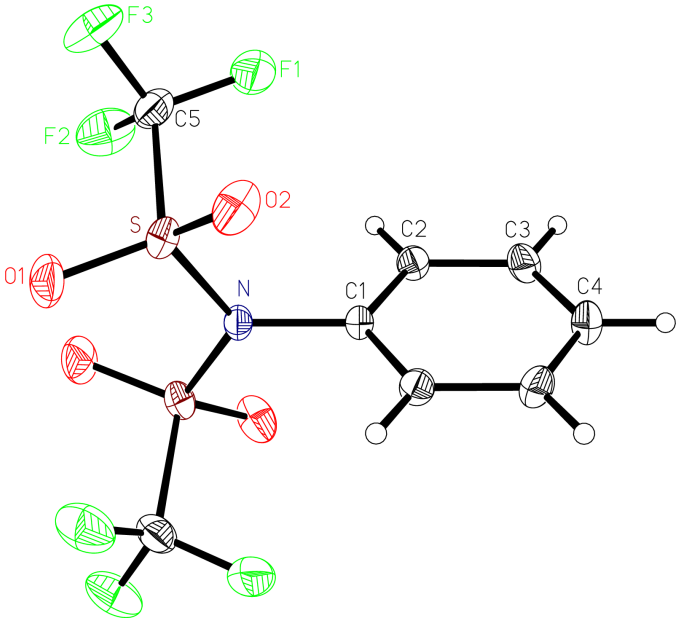


Figure 1
The structure of (I), with 50% probability displacement ellipsoids.

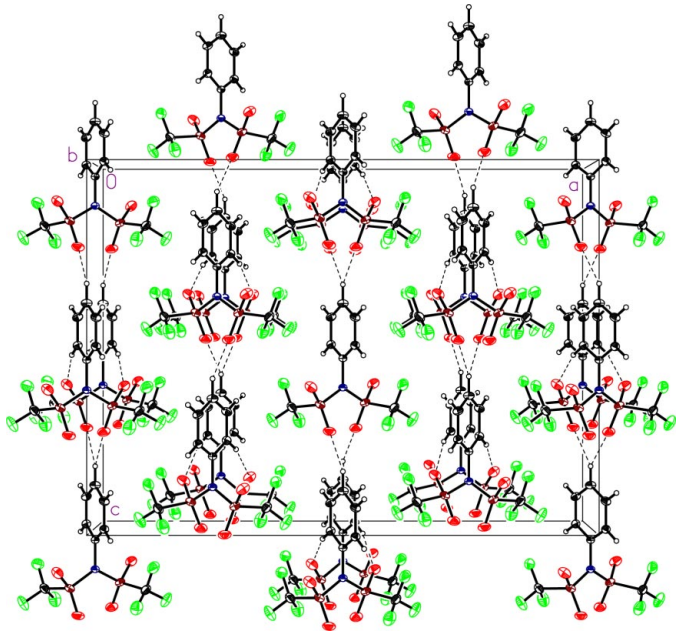


Figure 2
The crystal packing of (I), viewed down *b*.

Crystal data

$C_8H_5F_6NO_4S_2$
M_r = 357.25
Orthorhombic, *Fdd*2
a = 24.871 (4) Å
b = 5.6208 (6) Å
c = 18.2216 (19) Å
V = 2547.3 (6) Å^3
Z = 8
D_x = 1.863 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 234 reflections
θ = 3–36°
μ = 0.51 mm^{-1}
T = 143 (2) K
Rod, colorless
0.50 × 0.18 × 0.12 mm

Data collection

Siemens SMART CCD diffractometer
ω scans
Absorption correction: numerical (*SHELXTL*; Sheldrick, 1996)
T_{min} = 0.823, T_{max} = 0.946
13534 measured reflections
2529 independent reflections
2334 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 35.0°
h = −33 → 39
k = −8 → 9
l = −28 → 26
205 standard reflections
frequency: 600 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.069
S = 1.20
2529 reflections
98 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.00060 (14)
Absolute structure: Flack (1983); 1139 Friedel pairs
Flack parameter = 0.00 (5)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O2^{i}	0.95	2.53	3.458 (2)	167
C4—H4···O1^{ii}	0.95	2.51	3.267 (2)	137

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

The H atoms were taken from a difference Fourier synthesis. They were refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C)], using a riding model with fixed distances (H—C = 0.95 Å).

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 1996); software used to prepare material for publication: *SHELXL*97.

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