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N-[4-(Propylsulfamoyl)phenyl]acetamide

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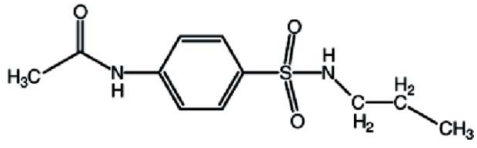
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.057; wR factor = 0.173; data-to-parameter ratio = 18.9.

In the title compound, $C_{11}H_{16}N_2O_3S$, the S atom has a distorted tetrahedral geometry [maximum deviation: O—S—O = 119.48 (15)°]. The dihedral angles between the benzene ring and its propylsulfonamide and methylamide substituents are 71.8 (2) and 5.8 (1)°, respectively. In the crystal, molecules are linked by N_m—H···O_s (m = methylamide and s = sulfonamide) hydrogen bonds, forming $C(8)$ chains along the a axis. The two molecule chains are connected by N—H···O hydrogen bonds, generating $R_3^2(18)$ rings. The crystal packing is further stabilized by weak intermolecular C—H···O hydrogen bonds.

Related literature

For background to sulfonamides, see: Adams (2001); Ahrens (1996); Betts *et al.* (2003); Faryal *et al.* (2011); Mayers (2009); Root (1999). For related structures, see: Faryal *et al.* (2011); Ahmad *et al.* (2011*a*,*b*). For computation of ring patterns formed by hydrogen bonds in crystal structures, see: Etter *et al.* (1990); Bernstein *et al.* (1995); Motherwell *et al.* (1999).



Experimental

Crystal data

$C_{11}H_{16}N_2O_3S$
M_r = 256.33
Orthorhombic, *Pbca*
a = 8.7791 (6) Å
b = 14.1747 (11) Å
c = 20.1577 (14) Å
V = 2508.5 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 296 K
0.13 × 0.12 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
22013 measured reflections
3103 independent reflections
1579 reflections with $I > 2\sigma(I)$
R_{int} = 0.077

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.173
S = 1.01
3103 reflections
164 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O3^{i}	0.86 (2)	2.07 (2)	2.904 (3)	165 (2)
N2—H2*N*···O2^{ii}	0.85 (2)	2.25 (2)	3.075 (3)	164 (2)
C9—H9···O1^{iii}	0.93	2.59	3.308 (3)	135

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+1$; (ii) $x+1, y, z$; (iii) $x+\frac{1}{2}, y, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5426).

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N-[4-(Propylsulfamoyl)phenyl]acetamide

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S1. Comment

Sulfonamides are derivatives of *p*-aminobenzene sulfonic acid (Ahrens, 1996) belong to the oldest group of antibiotics which are also being used now-a-days. These are white crystalline powder derived from azo dye (Adams, 2001) and have weak organic acid characteristics with a structural resemblance to *p*-aminobenzoic acid which is an intermediate required for the synthesis of folic acid in bacteria (Ahrens, 1996). The sensitivity of sulfonamides is dependent on the mode in which organisms fulfill their folic acid requirements. Sulfonamides are considered as bacteriostatic drugs (Mayers, 2009 & Betts *et al.*, 2003) which are used for the treatment of systematic infections and are absorbed in the gastrointestinal tract (Root, 1999).

As part of our ongoing studies (Faryal *et al.*, 2011, Ahmad *et al.* (2011*a*,*b*), we synthesized the title compound, (I), and report herein its crystal structure.

In the title compound, (Fig. 1), the dihedral angles between the benzene ring (C4—C9) and the propylsulfonamide (C1,C2,C3,N1,S1) and methylamide (N2,C10,O3,C11) moieties are 71.8 (1) and 5.8 (1)°, respectively. The S atom has a distorted tetrahedral geometry [maximum deviation: O—S—O = 119.48 (15)°]. The C—S—N—C torsion angles are 66.1 (2)°.

In the crystal, the molecules are linked by N_m—H···O_s (m = methylamide, s = sulfonamide) hydrogen bonds, forming C(8) chains along the *a* axis (Table1, Fig. 2). The two molecule chains also connect by N—H···O hydrogen bonds, generating $R_3^2(18)$ rings (Bernstein *et al.*, 1995; Etter *et al.*, 1990; Motherwell *et al.*, 1999; Table 1, Fig. 2). The crystal packing is further stabilized by the intermolecular C—H···O hydrogen bonds.

S2. Experimental

10 m*M* of 4-acetamido benzene sulfonyl chloride was taken in the reaction flask and about 20 ml distilled water was added in it. Mixed it well. Then 10 m*M* of propylamine hydrochloride was added in it. 3% Na_2CO_3 was used to maintain the pH at 8–10. The reaction was stirred for about 2 h to get the maximum yield. Precipitates obtained was filtered and dried. They are recrystallized in the mixture of methanol and ethyl acetate 1:1. The reaction was monitored by TLC.

S3. Refinement

The N-bound H atoms were located in difference Fourier maps and isotropically refined with the N–H distance restraint [0.86 (1) Å)]. The C-bound H atoms were geometrically placed using a riding model with C—H = 0.93 - 0.97 Å, and U_{iso}(H)= 1.2U_{eq}($C_{aromatic}$, $C_{methylene}$) and U_{iso}(H) = 1.5U_{eq}(C_{methyl}).

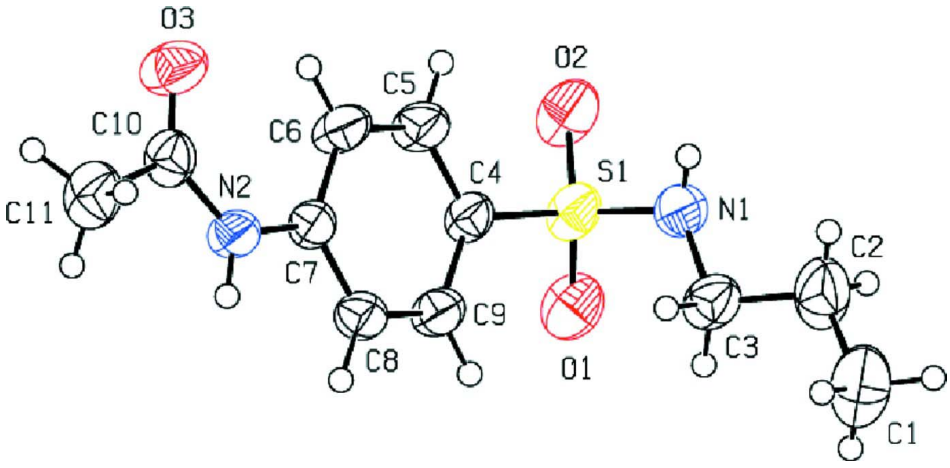

Figure 1

View of the title compound (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

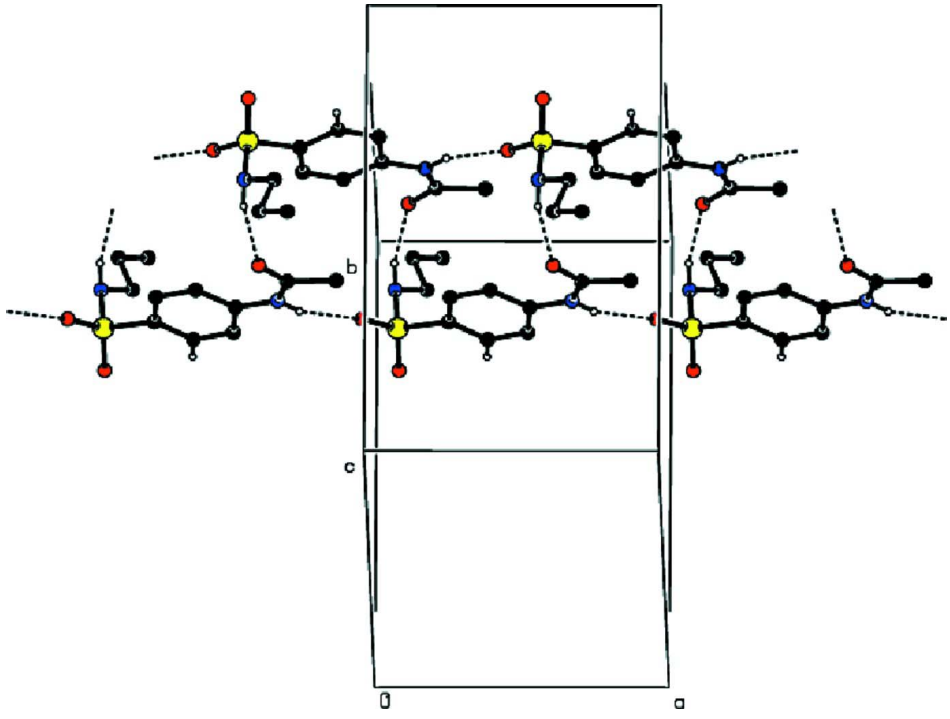

Figure 2

View of the molecules linked by N—H···O hydrogen bonds as the $R_3^2(18)$ ring motifs. H atoms not involved in hydrogen bonds (dashed lines) and C—H···O intreractions have been omitted for clarity.

N-[4-(Propylsulfamoyl)phenyl]acetamide

Crystal data

$C_{11}H_{16}N_2O_3S$
M_r = 256.33
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab

a = 8.7791 (6) Å
b = 14.1747 (11) Å
c = 20.1577 (14) Å
V = 2508.5 (3) Å^3

$Z = 8$
$F(000) = 1088$
$D_x = 1.357$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1934 reflections

$\theta = 2.9$–$21.9°$
$\mu = 0.26$ mm^{-1}
$T = 296$ K
Block, colourless
0.13 × 0.12 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
22013 measured reflections
3103 independent reflections

1579 reflections with $I > 2\sigma(I)$
$R_{int} = 0.077$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.0°$
$h = -10 \rightarrow 11$
$k = -18 \rightarrow 18$
$l = -26 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.173$
$S = 1.01$
3103 reflections
164 parameters
2 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0795P)^2 + 0.2926P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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}
S1	0.08384 (8)	0.62424 (6)	0.34117 (4)	0.0520 (3)
O1	0.0871 (3)	0.55742 (16)	0.28801 (9)	0.0662 (8)
O2	−0.0349 (2)	0.61902 (17)	0.38968 (11)	0.0702 (9)
O3	0.6209 (3)	0.63450 (16)	0.58686 (10)	0.0681 (9)
N1	0.0734 (3)	0.7275 (2)	0.30872 (12)	0.0530 (9)
N2	0.6813 (3)	0.61300 (18)	0.47900 (11)	0.0492 (9)
C1	0.2273 (4)	0.8744 (3)	0.1670 (2)	0.0893 (16)
C2	0.1289 (4)	0.8443 (3)	0.22353 (19)	0.0803 (16)
C3	0.1785 (3)	0.7554 (2)	0.25581 (13)	0.0557 (10)
C4	0.2588 (3)	0.61648 (19)	0.38364 (13)	0.0431 (10)
C5	0.2664 (3)	0.6361 (2)	0.45047 (14)	0.0532 (10)

C6	0.4031 (3)	0.6343 (2)	0.48376 (14)	0.0546 (10)
C7	0.5362 (3)	0.61413 (19)	0.44927 (13)	0.0419 (9)
C8	0.5275 (3)	0.5935 (2)	0.38184 (13)	0.0474 (10)
C9	0.3906 (3)	0.5945 (2)	0.34959 (13)	0.0492 (10)
C10	0.7159 (4)	0.6219 (2)	0.54421 (15)	0.0494 (11)
C11	0.8829 (3)	0.6153 (2)	0.56009 (17)	0.0667 (14)
H1A	0.32730	0.88930	0.18310	0.1340*
H1B	0.18390	0.92900	0.14620	0.1340*
H1C	0.23410	0.82410	0.13520	0.1340*
H1N	0.071 (3)	0.7722 (14)	0.3372 (10)	0.047 (9)*
H2A	0.12780	0.89410	0.25650	0.0960*
H2B	0.02550	0.83630	0.20750	0.0960*
H2N	0.754 (2)	0.604 (2)	0.4517 (12)	0.060 (10)*
H3A	0.18360	0.70560	0.22290	0.0670*
H3B	0.27970	0.76380	0.27420	0.0670*
H5	0.17760	0.65070	0.47350	0.0640*
H6	0.40650	0.64660	0.52910	0.0660*
H8	0.61580	0.57900	0.35850	0.0570*
H9	0.38620	0.58020	0.30460	0.0590*
H11A	0.92890	0.67640	0.55550	0.1000*
H11B	0.93090	0.57180	0.53010	0.1000*
H11C	0.89560	0.59340	0.60480	0.1000*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0345 (4)	0.0769 (6)	0.0447 (4)	−0.0061 (4)	−0.0052 (3)	0.0085 (4)
O1	0.0641 (15)	0.0778 (16)	0.0568 (12)	−0.0094 (12)	−0.0178 (11)	−0.0047 (12)
O2	0.0343 (12)	0.116 (2)	0.0604 (13)	−0.0096 (12)	0.0010 (10)	0.0234 (13)
O3	0.0522 (14)	0.1056 (19)	0.0465 (12)	−0.0005 (12)	−0.0017 (11)	−0.0090 (12)
N1	0.0418 (15)	0.0712 (19)	0.0461 (14)	0.0069 (13)	−0.0014 (12)	0.0017 (13)
N2	0.0309 (14)	0.0773 (18)	0.0395 (13)	0.0056 (12)	0.0018 (11)	0.0019 (12)
C1	0.051 (2)	0.117 (3)	0.100 (3)	−0.003 (2)	0.003 (2)	0.049 (2)
C2	0.055 (2)	0.103 (3)	0.083 (3)	0.014 (2)	0.008 (2)	0.037 (2)
C3	0.0451 (18)	0.075 (2)	0.0471 (16)	−0.0035 (17)	0.0025 (14)	0.0057 (16)
C4	0.0339 (16)	0.0585 (19)	0.0370 (14)	−0.0018 (13)	−0.0012 (11)	0.0061 (13)
C5	0.0311 (16)	0.085 (2)	0.0436 (16)	0.0025 (15)	0.0065 (13)	0.0038 (15)
C6	0.0385 (17)	0.092 (2)	0.0334 (14)	0.0001 (16)	0.0019 (13)	0.0000 (14)
C7	0.0328 (15)	0.0541 (18)	0.0388 (14)	0.0023 (13)	0.0016 (12)	0.0059 (13)
C8	0.0353 (16)	0.063 (2)	0.0438 (16)	0.0039 (14)	0.0058 (12)	0.0025 (14)
C9	0.0422 (18)	0.069 (2)	0.0363 (15)	0.0029 (14)	0.0004 (13)	−0.0001 (14)
C10	0.0410 (18)	0.056 (2)	0.0512 (18)	−0.0010 (15)	−0.0058 (14)	0.0038 (14)
C11	0.043 (2)	0.092 (3)	0.065 (2)	−0.0018 (17)	−0.0138 (16)	0.0075 (18)

Geometric parameters (Å, º)

S1—O1	1.431 (2)	C8—C9	1.367 (4)
S1—O2	1.431 (2)	C10—C11	1.504 (4)

S1—N1	1.606 (3)	C1—H1A	0.9600
S1—C4	1.762 (3)	C1—H1B	0.9600
O3—C10	1.211 (4)	C1—H1C	0.9600
N1—C3	1.465 (4)	C2—H2A	0.9700
N2—C7	1.408 (4)	C2—H2B	0.9700
N2—C10	1.355 (4)	C3—H3A	0.9700
N1—H1N	0.86 (2)	C3—H3B	0.9700
N2—H2N	0.85 (2)	C5—H5	0.9300
C1—C2	1.492 (5)	C6—H6	0.9300
C2—C3	1.484 (5)	C8—H8	0.9300
C4—C9	1.381 (4)	C9—H9	0.9300
C4—C5	1.377 (4)	C11—H11A	0.9600
C5—C6	1.375 (4)	C11—H11B	0.9600
C6—C7	1.389 (4)	C11—H11C	0.9600
C7—C8	1.392 (4)		

O1—S1—O2	119.48 (15)	C2—C1—H1C	109.00
O1—S1—N1	107.43 (13)	H1A—C1—H1B	109.00
O1—S1—C4	107.77 (14)	H1A—C1—H1C	109.00
O2—S1—N1	106.49 (14)	H1B—C1—H1C	109.00
O2—S1—C4	107.44 (13)	C1—C2—H2A	109.00
N1—S1—C4	107.73 (13)	C1—C2—H2B	109.00
S1—N1—C3	120.5 (2)	C3—C2—H2A	109.00
C7—N2—C10	127.9 (3)	C3—C2—H2B	109.00
S1—N1—H1N	113.8 (13)	H2A—C2—H2B	108.00
C3—N1—H1N	107.7 (16)	N1—C3—H3A	109.00
C7—N2—H2N	113.9 (15)	N1—C3—H3B	109.00
C10—N2—H2N	118.2 (15)	C2—C3—H3A	109.00
C1—C2—C3	114.1 (3)	C2—C3—H3B	109.00
N1—C3—C2	111.3 (2)	H3A—C3—H3B	108.00
C5—C4—C9	119.4 (2)	C4—C5—H5	119.00
S1—C4—C5	120.3 (2)	C6—C5—H5	119.00
S1—C4—C9	120.2 (2)	C5—C6—H6	120.00
C4—C5—C6	121.1 (3)	C7—C6—H6	120.00
C5—C6—C7	119.6 (3)	C7—C8—H8	120.00
N2—C7—C6	123.4 (2)	C9—C8—H8	120.00
N2—C7—C8	117.6 (2)	C4—C9—H9	120.00
C6—C7—C8	119.1 (2)	C8—C9—H9	120.00
C7—C8—C9	120.7 (2)	C10—C11—H11A	109.00
C4—C9—C8	120.2 (2)	C10—C11—H11B	109.00
O3—C10—C11	122.0 (3)	C10—C11—H11C	109.00
N2—C10—C11	114.8 (3)	H11A—C11—H11B	109.00
O3—C10—N2	123.2 (3)	H11A—C11—H11C	109.00
C2—C1—H1A	110.00	H11B—C11—H11C	109.00
C2—C1—H1B	110.00		

O1—S1—N1—C3	−49.8 (3)	C7—N2—C10—O3	−1.6 (5)
O2—S1—N1—C3	−178.9 (2)	C1—C2—C3—N1	−177.3 (3)

C4—S1—N1—C3	66.1 (2)	S1—C4—C5—C6	−177.2 (2)
N1—S1—C4—C9	−82.9 (3)	S1—C4—C9—C8	176.5 (2)
N1—S1—C4—C5	94.4 (2)	C5—C4—C9—C8	−0.9 (4)
O1—S1—C4—C5	−149.9 (2)	C9—C4—C5—C6	0.1 (4)
O2—S1—C4—C5	−20.0 (3)	C4—C5—C6—C7	1.2 (4)
O1—S1—C4—C9	32.8 (3)	C5—C6—C7—N2	178.4 (3)
O2—S1—C4—C9	162.8 (2)	C5—C6—C7—C8	−1.8 (4)
S1—N1—C3—C2	167.9 (2)	N2—C7—C8—C9	−179.2 (3)
C10—N2—C7—C6	6.5 (5)	C6—C7—C8—C9	1.1 (4)
C7—N2—C10—C11	178.6 (3)	C7—C8—C9—C4	0.3 (4)
C10—N2—C7—C8	−173.2 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O3^{i}	0.86 (2)	2.07 (2)	2.904 (3)	165 (2)
N2—H2*N*···O2^{ii}	0.85 (2)	2.25 (2)	3.075 (3)	164 (2)
C9—H9···O1^{iii}	0.93	2.59	3.308 (3)	135

Symmetry codes: (i) *x*−1/2, −*y*+3/2, −*z*+1; (ii) *x*+1, *y*, *z*; (iii) *x*+1/2, *y*, −*z*+1/2.