Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structure of 4-methyl-*N*-propylbenzenesulfonamide

Brock A. Stenfors,[a] Rachel C. Collins,[a] Jonah R. J. Duran,[a] Richard J. Staples,[b] Shannon M. Biros[a] and Felix N. Ngassa[a]*

[a]Department of Chemistry, Grand Valley State University, 1 Campus Dr., Allendale, MI 49401, USA, and [b]Center for Crystallographic Research, Department of Chemistry, Michigan State University, East Lansing, MI 48824, USA. *Correspondence e-mail: ngassaf@gvsu.edu

Received 26 May 2020
Accepted 6 June 2020

Edited by M. Weil, Vienna University of Technology, Austria

Keywords: crystal structure; sulfonamide; intermolecular N—H···O hydrogen bonding; intermolecular C—H···O hydrogen bonding.

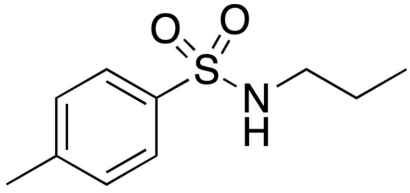
CCDC reference: 2008411

Supporting information: this article has supporting information at journals.iucr.org/e

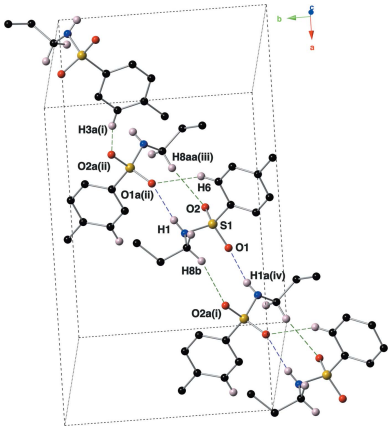
The crystal structure of the title sulfonamide, $C_{10}H_{15}NO_2S$, comprises two molecules in the asymmetric unit. The S=O bond lengths of the sulfonamide functional group range from 1.428 (2) to 1.441 (2) Å, with S—C bond lengths of 1.766 (3) Å (for both molecules in the asymmetric unit), and S—N bond lengths of 1.618 (2) and 1.622 (3) Å, respectively. When both molecules are viewed down the N—S bond, the propyl group is *gauche* to the toluene moiety. In the crystal structure, molecules of the title compound are arranged in an intricate three-dimensional network that is formed *via* intermolecular C—H···O and N—H···O hydrogen bonds. The crystal structure was refined from a crystal twinned by inversion.

1. Chemical context

Molecules containing the sulfonamide moiety are found among a variety of biologically significant compounds, and have been used to inhibit a variety of enzymes to improve or repair biological functions. Commonly referred to as 'sulfa drugs', these molecules have been in clinical use since 1968 (Connor, 1998). Since then, many sulfonamides have been recognized as effective inhibitors of the zinc enzyme carbonic anhydrase (Gul *et al.*, 2018). Several interesting anticancer properties are exhibited upon inhibition of this enzyme (Supuran *et al.*, 2001).



The title compound, 4-methyl-*N*-propylbenzenesulfonamide, is structurally similar to a variety of biologically significant compounds. In particular, tacrine-*p*-toluenesulfonamide derivatives containing the 4-methyl-*N*-propylbenzenesulfonamide moiety have proven to be effective acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) inhibitors (Makhaeva *et al.*, 2019; Fig. 1). The AChE cholinesterase enzyme catalyzes the hydrolysis of acetylcholine (ACh), a neurotransmitter with the ability to coordinate neural responses in the brain (Picciotto *et al.*, 2012). The inhibition of AChE decreases the extent of ACh hydrolysis and enhances cholinergic transmission. AChE inhibition treats the symptoms of neuron deterioration characteristic of



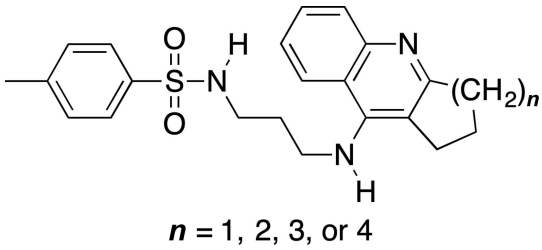


Figure 1
Acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) inhibitors containing the *N*-propyl-4-methylbenzenesulfonamide moiety.

Alzheimer's disease (García-Ayllón *et al.*, 2011). While BChE and AChE both regulate the cholinergic system, the effects of BChE are more prevalent in the blood than the nervous system (Pohanka, 2014). BChE is, however, found in the central nervous system and is involved in the formation or growth of β-amyloid plaques (Kim *et al.*, 2016). The inhibition of both AChE and BChE improves cognitive function and minimizes the accumulation of β-amyloid and is a viable strategy for treating Alzheimer's disease.

A facile synthesis of sulfonamides is necessary to produce a variety of compounds with the potential to improve human health. A review of the current literature suggests that nucleophilic substitution of sulfonyl halides or sulfonic acids with an amine is an efficient method for the synthesis of sulfonamides (Mukherjee *et al.*, 2018; De Luca & Giacomelli, 2008). The title compound was synthesized by reacting *p*-toluenesulfonyl chloride with propylamine in the presence of pyridine. The reaction was carried out in an inert atmosphere, using dichloromethane as the solvent. These reaction conditions resulted in a poor yield and slow reaction time. To work toward a facile synthesis of sulfonamides, a more efficient and environmentally benign method was recently developed. By substituting pyridine and dichloromethane with aqueous potassium carbonate and tetrahydrofuran, a significant increase in the yield and rate of the reaction was observed. The products formed under these reaction conditions are easily isolated upon acidification of the reaction mixture. Furthermore, the solvent combination supports a broader range of nitrogen nucleophiles. In our ongoing efforts to synthesize and characterize sulfonamide products, the synthesis and crystal structure of 4-methyl-*N*-propylbenzenesulfonamide is reported here.

2. Structural commentary

The title compound comprises two equivalents of the molecule in the asymmetric unit, as shown in Fig. 2 (suffix '*A*' for all atomic labels used for the second molecule). The S=O bond lengths of the sulfonamide functional group range from

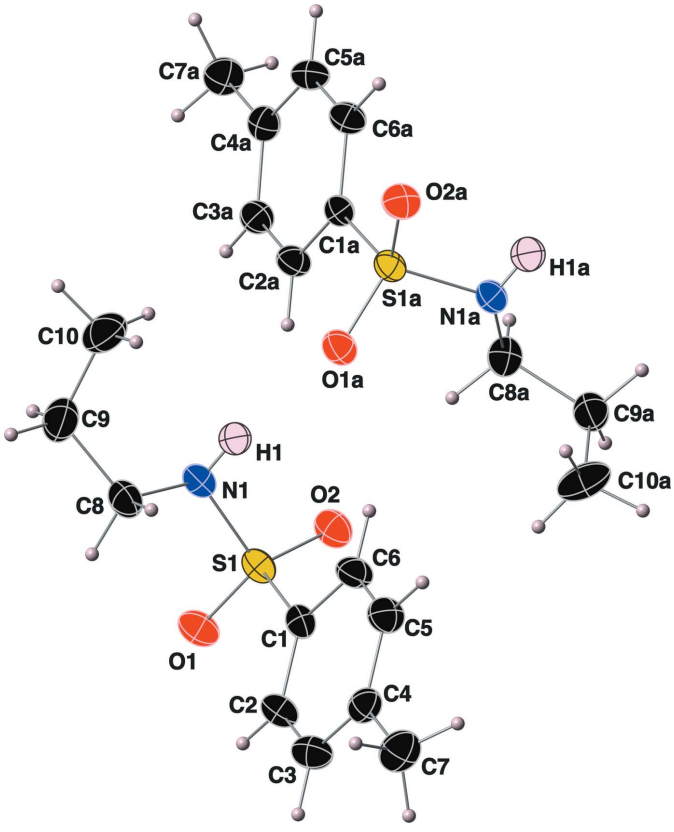


Figure 2
The structures of the two molecules in the asymmetric unit of the title compound, with the atom-labeling scheme. Displacement ellipsoids are shown at the 40% probability level using standard CPK colors.

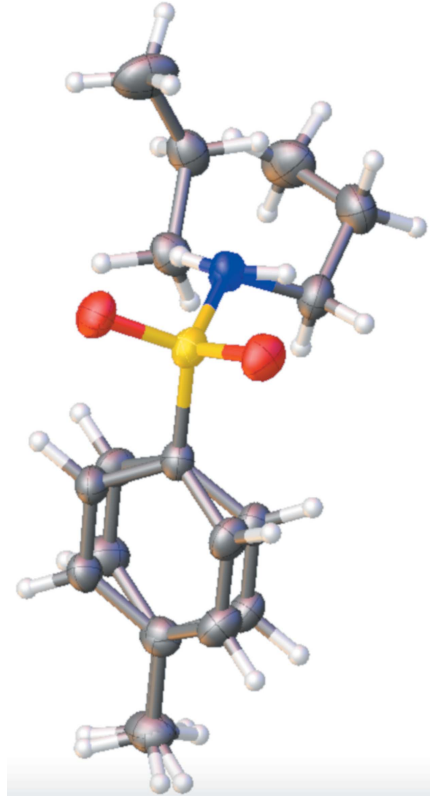


Figure 3
Overlay plot of the two independent molecules in the title compound, with grouping of the atoms C1—S1—-N1 and C1*A*—S1*A*—N1*A*, and the molecule oriented so as to view it down the S—N bond. Displacement ellipsoids are as in Fig. 2.

1.428 (2) to 1.441 (2) Å, which fall within expected values. The S—C bond lengths are 1.766 (3) Å for both molecules, and the S—N bond lengths are 1.618 (2) and 1.622 (3) Å. The O—S—O bond angles are 119.49 (13) and 118.26 (13)°, with N—S—C bond angles of 106.86 (13) and 108.27 (13)°. The two independent molecules differ in the orientation of the propyl chain and the H atom attached to the N atom, however, in each case with the propyl chain being *gauche* to a sulfonamide oxygen atom and to the toluene moiety when the molecules are viewed down the N1—S1 bond (Fig. 3). The torsion angles between the first carbon atom of the propyl chain (C8 or C8*A*) and the sulfonamide oxygen atom O1 or O1*A* are 60.5 (3) and 57.3 (2)°, respectively. The groups bonded to the sulfur atom of both sulfonamide groups adopt slightly distorted tetrahedral environments with fourfold coordination τ_4 descriptors of 0.94 for both S1 and S1*A* (ideal values are 0 for square-planar, 0.85 for trigonal pyramidal, and 1 for tetrahedral coordinations; Yang *et al.*, 2007).

3. Supramolecular features

Hydrogen-bonding interactions, both N—H···O and C—H···O, hold molecules of the title compound together in the crystal structure (Table 1, Fig. 4). The intermolecular N—H···O interactions are between the sulfonamide N(H) atoms and the oxygen (O1 or O1*A*) atoms of a nearby molecule. These classic hydrogen-bonding interactions form ribbons of the title compound that lie parallel to the *ab* plane. These interactions have *D*···*A* distances of 2.925 (3) and 2.968 (3) Å, with *D*—H···*A* angles of 161 (3) and 172 (3)°.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3*A*—H3*A*···O2*A*^{i}	0.95	2.53	3.399 (4)	153
C6—H6···O1*A*^{ii}	0.95	2.59	3.474 (4)	156
C8—H8*B*···O2*A*^{i}	0.99	2.56	3.489 (4)	156
C8*A*—H8*AA*···O2^{iii}	0.99	2.61	3.594 (4)	170
N1*A*—H1*A*···O1^{iv}	0.82 (3)	2.14 (3)	2.925 (3)	161 (3)
N1—H1···O1*A*^{ii}	0.85 (3)	2.13 (4)	2.968 (3)	172 (3)

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

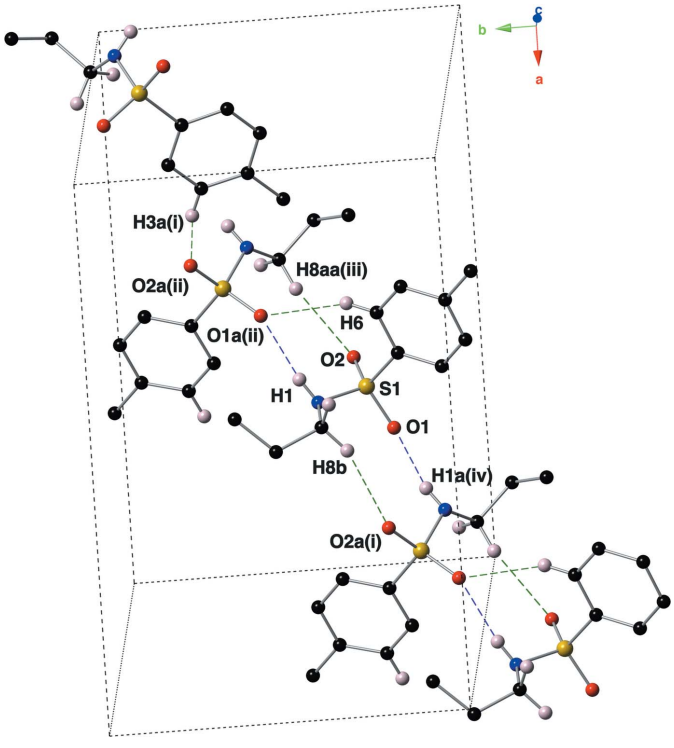


Figure 4
A diagram showing the specific hydrogen-bonding interactions (N—H···O: purple dashed lines, C—H···O: green dashed lines) present in the title compound, using a ball-and-stick model with standard CPK colors. Hydrogen atoms bonded to parent atoms that are not involved in a non-covalent interaction have been omitted for clarity. [Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x, -y+1, z+\frac{1}{2}$; (iii) $x, -y+1, z-\frac{1}{2}$; (iv) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$].

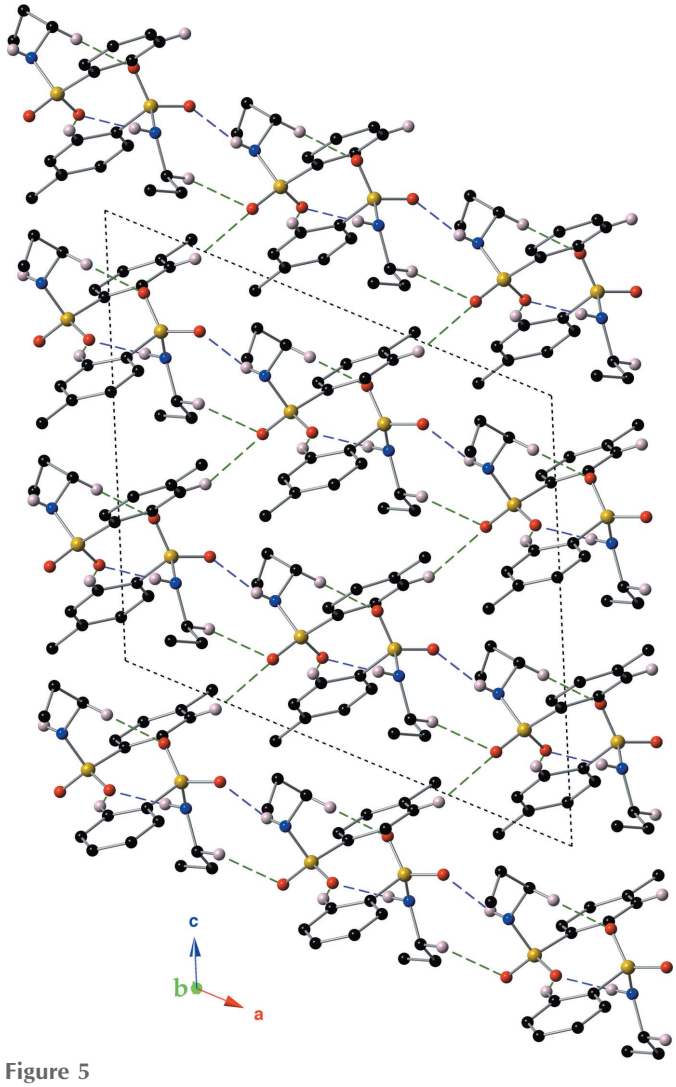


Figure 5
A packing diagram of the title compound viewed down the *b* axis. Intermolecular hydrogen bonds are shown with dashed lines (N—H···O: purple, C—H···O: green). This figure was drawn using a ball and stick model with standard CPK colors. Hydrogen atoms bonded to parent atoms that are not involved in a non-covalent interaction have been omitted for clarity.

The intermolecular C—H···O hydrogen bonding interactions (Sutor, 1958, 1962, 1963; Steiner, 1996) have, as expected, longer $D\cdots A$ distances ranging from 3.399 (4) to 3.594 (4) Å, and D—H···A angles ranging from 152.8 to 170.2°. Specifically, the C8(H8*B*)···O2*A*, C8*A*(H8*AA*)···O2 and C6(H6)···O1*A* interactions contribute to the stabilization of the supramolecular ribbons. The interaction between C3*A*(H3*A*) and O2*A* links the supramolecular ribbons into an intricate three-dimensional network (Fig. 5).

4. Database survey

A search for structures containing the *p*-methylbenzenesulfonamide entity in the Cambridge Structural Database (CSD, Version 5.41, November, 2019; Groom *et al.*, 2016), where the nitrogen atom bears one carbon-containing group, resulted in over 2,200 hits. A few structures with relatively simple, yet interesting, –*R* groups bonded to the sulfonamide nitrogen atom are BOLPOH (Germain *et al.*, 1983), AZUQUI (Rehman *et al.*, 2011), AYURUI and AYURUI01 (Khan *et al.*, 2011; Akyıldız *et al.*, 2018), and ATOVIO (Muller *et al.*, 2004). In the structures of BOLPOH and AZUQUI, the –*R* groups are both aromatic systems with a quinoline ring and a 4-aminobenzene ring, respectively. The structures of AYURUI and AYURUI01 contain two *p*-methylbenzenesulfonamide groups linked *via* a propane chain. Lastly, the –*R* group in ATOVIO is a tricycloheptyl ring system.

5. Synthesis and crystallization

The title compound was prepared by the dropwise addition of 0.59 *M* aqueous potassium carbonate (10 ml, 5.90 mmol) to a stirring mixture of propylamine (0.49 ml, 5.90 mmol) and *p*-toluenesulfonyl chloride (1.00 g, 5.25 mmol) in 10 ml of tetrahydrofuran. The reaction mixture was stirred at room temperate for 24 h under a nitrogen atmosphere. After acidification with 5 *M* HCl and dilution with 15 ml of dichloromethane, the organic layer was washed with water and brine. The aqueous layers were back extracted with 10 ml of dichloromethane. The combined organic layers were then combined, dried over anhydrous sodium sulfate, and evaporated to dryness. The liquid residue was triturated with diethyl ether, placed in a freezer for 48 h and, after isolation *via* vacuum filtration, the product was obtained as colorless crystals (59%; m.p. 335–337 K).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystal under investigation was twinned by inversion, with a refined Flack parameter of 0.443 (19) (Parsons *et al.*, 2013). For this structure, hydrogen atoms bonded to carbon atoms were placed in calculated positions and refined to ride on their parent atoms: C—H = 0.95–1.00 Å with U_{iso}(H) = 1.2U_{eq}(C) for methylene groups and aromatic hydrogen atoms, and U_{iso}(H) = 1.5U_{eq}(C) for methyl groups. Hydrogen atoms bonded to nitrogen atoms were located using electron density difference maps, and were refined freely.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{10}H_{15}NO_2S$
M_r	213.29
Crystal system, space group	Monoclinic, *Cc*
Temperature (K)	173
a, *b*, *c* (Å)	15.9353 (9), 10.3526 (6), 14.8486 (9)
β (°)	115.1347 (6)
V (Å^3)	2217.7 (2)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.27
Crystal size (mm)	0.45 × 0.40 × 0.39
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.684, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18931, 4554, 4422
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.626
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.031, 0.083, 1.02
No. of reflections	4554
No. of parameters	265
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.20
Absolute structure	Flack *x* determined using 2140 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.443 (19)

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009; Bourhis *et al.*, 2015) and *CrystalMaker* (Palmer, 2007).

Acknowledgements

The authors are grateful to Pfizer, Inc. for the donation of a Varian INOVA 400 FT NMR.

Funding information

Funding for this research was provided by: National Science Foundation, Directorate for Mathematical and Physical Sciences (grant No. MRI CHE-1725699; grant No. MRI CHE-1919817); GVSU Chemistry Department's Weldon Fund.

References

Akyıldız, F., Alyar, S., Bilkan, M. T. & Alyar, H. (2018). *J. Mol. Struct.* **1174**, 160–170.
Bourhis, L. J., Dolomanov, O. V., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2015). *Acta Cryst.* A**71**, 59–75.
Bruker (2013). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc. Madison, Wisconsin, USA.
Connor, E. E. (1998). *Elsevier Science Inc.* **5**, 32–35.
De Luca, L. & Giacomelli, G. (2008). *J. Org. Chem.* **73**, 3967–3969.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
García-Ayllón, M., Small, D. H., Avila, J. & Sáez-Valero, J. (2011). *Front. Mol. Neurosci.* **4**, 22.
Germain, G., Declercq, J.-P., Castresana, J. M., Elizalde, M. P. & Arrieta, J. M. (1983). *Acta Cryst.* C**39**, 230–232.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Gul, H. I., Yamali, C., Sakagami, H., Angeli, A., Leitans, J., Kazaks, A., Tars, K., Ozgun, D. O. & Supuran, C. T. (2018). *Bioorg. Chem.* **77**, 411–419.
Khan, I. U., Sheikh, T. A., Ejaz & Harrison, W. T. A. (2011). *Acta Cryst.* E**67**, o2371.
Kim, J. H., Lee, S., Lee, H. W., Sun, Y. N., Jang, W., Yang, S., Jang, H. & Kim, Y. H. (2016). *Int. J. Biol. Macromol.* **91**, 1033–1039.
Makhaeva, G. F., Rudakova, E. V., Kovaleva, N. V., Lushchekina, S. V., Boltneva, N. P., Proshin, A. N., Shchegolkov, E. V., Burgart, Y. V. & Saloutin, V. I. (2019). *Russ. Chem. Bull.* **68**, 967–984.
Mukherjee, P., Woroch, C. P., Cleary, L., Rusznak, M., Franzese, R. W., Reese, M. R., Tucker, J. W., Humphrey, J. M., Etuk, S. M., Kwan, S. C., am Ende, C. W. & Ball, N. D. (2018). *Org. Lett.* **20**, 3943–3947.
Müller, P., Riegert, D. & Bernardinelli, G. (2004). *Helv. Chim. Acta*, **87**, 227–239.
Palmer, D. (2007). *CrystalMaker*. CrystalMaker Software, Bicester, Oxfordshire, England.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Picciotto, M. R., Higley, M. J. & Mineur, Y. S. (2012). *Neuron*, **76**, 116–129.
Pohanka, M. (2014). *Int. J. Mol. Sci.* **15**, 9809–9825.
Rehman, J., **Ejaz** , Khan, I. U. & Harrison, W. T. A. (2011). *Acta Cryst.* E**67**, o2709.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Steiner, T. (1996). *Crystallogr. Rev.* **6**, 157–305.
Supuran, C. T., Briganti, F., Tilli, S., Chegwidden, W. R. & Scozzafava, A. (2001). *Bioorg. Med. Chem.* **9**, 703–714.
Sutor, D. J. (1958). *Acta Cryst.* **11**, 453–458.
Sutor, D. J. (1962). *Nature*, **195**, 68–69.
Sutor, D. J. (1963). *J. Chem. Soc.* pp. 1105–1110.
Yang, L., Powell, D. R. & Houser, R. P. (2007). *Dalton Trans.* pp. 955–964.

supporting information

Acta Cryst. (2020). E**76**, 1070-1074 [https://doi.org/10.1107/S2056989020007756]

Crystal structure of 4-methyl-*N*-propylbenzenesulfonamide

Brock A. Stenfors, Rachel C. Collins, Jonah R. J. Duran, Richard J. Staples, Shannon M. Biros and Felix N. Ngassa

Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009; Bourhis *et al.*, 2015); software used to prepare material for publication: *CrystalMaker* (Palmer, 2007).

4-Methyl-*N*-propylbenzenesulfonamide

Crystal data

$C_{10}H_{15}NO_2S$
$M_r = 213.29$
Monoclinic, *Cc*
$a = 15.9353$ (9) Å
$b = 10.3526$ (6) Å
$c = 14.8486$ (9) Å
$\beta = 115.1347$ (6)°
$V = 2217.7$ (2) Å^3
$Z = 8$
$F(000) = 912$
$D_x = 1.278$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9996 reflections
$\theta = 2.4$–26.4°
$\mu = 0.27$ mm^{-1}
$T = 173$ K
Block, colourless
0.45 × 0.40 × 0.39 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
$T_{min} = 0.684$, $T_{max} = 0.745$
18931 measured reflections
4554 independent reflections
4422 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.4°$
$h = -19 \rightarrow 19$
$k = -12 \rightarrow 12$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.083$
$S = 1.02$
4554 reflections
265 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 0.9882P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}
Absolute structure: Flack *x* determined using 2140 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.443 (19)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1A	0.40337 (4)	0.32398 (6)	0.21849 (4)	0.02809 (16)
S1	0.61545 (4)	0.30322 (7)	0.77858 (4)	0.03083 (17)
O2A	0.33689 (14)	0.2460 (2)	0.14206 (15)	0.0368 (5)
C1A	0.48935 (19)	0.2218 (3)	0.3034 (2)	0.0266 (5)
C5	0.3803 (2)	0.1709 (3)	0.5601 (3)	0.0388 (7)
H5	0.3189	0.2015	0.5231	0.047*
C3A	0.6417 (2)	0.1911 (3)	0.4327 (2)	0.0325 (6)
H3A	0.7009	0.2249	0.4749	0.039*
C1	0.5341 (2)	0.2024 (3)	0.6871 (2)	0.0300 (6)
C6	0.4440 (2)	0.2486 (3)	0.6334 (2)	0.0366 (7)
H6	0.4267	0.3316	0.6470	0.044*
C4	0.4047 (2)	0.0488 (3)	0.5397 (2)	0.0347 (6)
C2A	0.5763 (2)	0.2713 (3)	0.3643 (2)	0.0324 (6)
H2A	0.5905	0.3593	0.3590	0.039*
N1	0.62264 (18)	0.4342 (2)	0.72284 (18)	0.0328 (5)
O2	0.58027 (16)	0.3406 (2)	0.84936 (15)	0.0400 (5)
C4A	0.6225 (2)	0.0614 (3)	0.4409 (2)	0.0319 (6)
O1A	0.45006 (14)	0.4257 (2)	0.19202 (16)	0.0362 (5)
C2	0.5590 (2)	0.0820 (3)	0.6681 (2)	0.0370 (7)
H2	0.6204	0.0514	0.7050	0.044*
C3	0.4942 (2)	0.0052 (3)	0.5949 (2)	0.0418 (7)
H3	0.5115	−0.0784	0.5825	0.050*
N1A	0.34797 (17)	0.3914 (2)	0.27586 (19)	0.0332 (5)
C5A	0.5348 (2)	0.0145 (3)	0.3788 (2)	0.0350 (6)
H5A	0.5204	−0.0736	0.3837	0.042*
C8	0.6443 (2)	0.4213 (3)	0.6357 (2)	0.0399 (7)
H8A	0.5885	0.3916	0.5774	0.048*
H8B	0.6936	0.3558	0.6499	0.048*
C9A	0.3349 (2)	0.5714 (3)	0.3760 (2)	0.0421 (7)
H9AA	0.2776	0.5292	0.3720	0.051*
H9AB	0.3659	0.6119	0.4425	0.051*
C6A	0.4685 (2)	0.0937 (3)	0.3105 (2)	0.0338 (6)
H6A	0.4090	0.0604	0.2688	0.041*
O1	0.70368 (15)	0.2382 (2)	0.81488 (17)	0.0411 (5)
C7	0.3343 (3)	−0.0346 (3)	0.4595 (3)	0.0480 (8)
H7A	0.3372	−0.0177	0.3960	0.072*
H7B	0.2720	−0.0144	0.4535	0.072*
H7C	0.3480	−0.1259	0.4772	0.072*
C7A	0.6943 (2)	−0.0253 (3)	0.5154 (2)	0.0420 (7)

H7AA	0.7558	0.0133	0.5359	0.063*
H7AB	0.6928	−0.1099	0.4851	0.063*
H7AC	0.6810	−0.0358	0.5737	0.063*
C8A	0.3984 (2)	0.4693 (3)	0.3654 (2)	0.0377 (6)
H8AA	0.4523	0.5114	0.3608	0.045*
H8AB	0.4219	0.4127	0.4248	0.045*
C10	0.6052 (3)	0.6546 (4)	0.5879 (3)	0.0575 (10)
H10D	0.5466	0.6260	0.5343	0.086*
H10E	0.6273	0.7319	0.5666	0.086*
H10F	0.5953	0.6747	0.6472	0.086*
C9	0.6761 (3)	0.5489 (4)	0.6120 (3)	0.0535 (9)
H9A	0.7334	0.5760	0.6696	0.064*
H9B	0.6916	0.5370	0.5546	0.064*
C10A	0.3090 (3)	0.6751 (4)	0.2977 (3)	0.0613 (11)
H10A	0.2820	0.6352	0.2316	0.092*
H10B	0.3645	0.7240	0.3061	0.092*
H10C	0.2636	0.7335	0.3044	0.092*
H1A	0.307 (2)	0.343 (3)	0.277 (2)	0.034 (9)*
H1	0.576 (2)	0.481 (3)	0.713 (2)	0.030 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0225 (3)	0.0303 (3)	0.0288 (3)	−0.0027 (3)	0.0082 (3)	0.0011 (3)
S1	0.0278 (3)	0.0362 (3)	0.0270 (3)	0.0067 (3)	0.0102 (3)	−0.0013 (3)
O2A	0.0286 (10)	0.0384 (11)	0.0336 (10)	−0.0029 (9)	0.0039 (9)	−0.0020 (9)
C1A	0.0250 (13)	0.0287 (13)	0.0257 (13)	−0.0013 (10)	0.0104 (11)	0.0008 (11)
C5	0.0275 (15)	0.0389 (17)	0.0436 (18)	0.0017 (12)	0.0088 (14)	−0.0004 (13)
C3A	0.0274 (14)	0.0338 (16)	0.0327 (15)	−0.0037 (11)	0.0094 (13)	−0.0031 (11)
C1	0.0281 (14)	0.0353 (14)	0.0289 (14)	0.0030 (11)	0.0143 (12)	0.0011 (11)
C6	0.0304 (14)	0.0304 (15)	0.0451 (17)	0.0054 (12)	0.0124 (14)	−0.0022 (12)
C4	0.0403 (16)	0.0338 (15)	0.0327 (14)	−0.0044 (12)	0.0180 (13)	−0.0004 (12)
C2A	0.0275 (14)	0.0305 (14)	0.0362 (15)	−0.0043 (11)	0.0106 (12)	0.0009 (11)
N1	0.0309 (12)	0.0334 (12)	0.0349 (12)	0.0048 (10)	0.0147 (10)	−0.0028 (10)
O2	0.0442 (12)	0.0468 (12)	0.0318 (10)	0.0060 (10)	0.0188 (9)	−0.0014 (9)
C4A	0.0348 (15)	0.0362 (15)	0.0263 (13)	0.0020 (12)	0.0143 (12)	0.0023 (11)
O1A	0.0305 (10)	0.0367 (11)	0.0405 (11)	−0.0013 (8)	0.0141 (9)	0.0073 (9)
C2	0.0347 (15)	0.0360 (15)	0.0392 (16)	0.0100 (12)	0.0147 (13)	0.0005 (13)
C3	0.0485 (19)	0.0360 (16)	0.0412 (17)	0.0063 (14)	0.0193 (15)	−0.0034 (13)
N1A	0.0244 (11)	0.0343 (13)	0.0404 (13)	−0.0051 (10)	0.0133 (10)	−0.0042 (10)
C5A	0.0417 (17)	0.0272 (14)	0.0353 (14)	−0.0046 (12)	0.0156 (13)	0.0016 (11)
C8	0.0415 (16)	0.0430 (16)	0.0420 (16)	0.0048 (14)	0.0243 (14)	−0.0015 (14)
C9A	0.0377 (16)	0.0497 (19)	0.0421 (17)	−0.0032 (14)	0.0199 (14)	−0.0107 (14)
C6A	0.0323 (14)	0.0337 (14)	0.0323 (14)	−0.0075 (12)	0.0105 (12)	−0.0024 (11)
O1	0.0334 (11)	0.0448 (13)	0.0379 (11)	0.0111 (9)	0.0083 (9)	0.0001 (9)
C7	0.051 (2)	0.0457 (18)	0.0440 (18)	−0.0119 (15)	0.0171 (16)	−0.0088 (15)
C7A	0.0437 (18)	0.0407 (17)	0.0381 (16)	0.0047 (13)	0.0139 (14)	0.0081 (13)
C8A	0.0321 (15)	0.0457 (16)	0.0323 (14)	−0.0014 (13)	0.0109 (12)	−0.0053 (13)

C10	0.079 (3)	0.0418 (19)	0.060 (2)	−0.0037 (19)	0.038 (2)	0.0091 (16)
C9	0.053 (2)	0.058 (2)	0.062 (2)	−0.0094 (17)	0.0365 (19)	−0.0031 (18)
C10A	0.082 (3)	0.042 (2)	0.051 (2)	0.0113 (19)	0.021 (2)	−0.0126 (16)

Geometric parameters (Å, º)

S1A—O2A	1.428 (2)	N1A—C8A	1.469 (4)
S1A—C1A	1.766 (3)	N1A—H1A	0.82 (3)
S1A—O1A	1.437 (2)	C5A—H5A	0.9500
S1A—N1A	1.622 (3)	C5A—C6A	1.381 (4)
S1—C1	1.766 (3)	C8—H8A	0.9900
S1—N1	1.618 (3)	C8—H8B	0.9900
S1—O2	1.438 (2)	C8—C9	1.509 (5)
S1—O1	1.441 (2)	C9A—H9AA	0.9900
C1A—C2A	1.392 (4)	C9A—H9AB	0.9900
C1A—C6A	1.382 (4)	C9A—C8A	1.518 (4)
C5—H5	0.9500	C9A—C10A	1.505 (6)
C5—C6	1.387 (5)	C6A—H6A	0.9500
C5—C4	1.393 (4)	C7—H7A	0.9800
C3A—H3A	0.9500	C7—H7B	0.9800
C3A—C2A	1.381 (4)	C7—H7C	0.9800
C3A—C4A	1.394 (4)	C7A—H7AA	0.9800
C1—C6	1.397 (4)	C7A—H7AB	0.9800
C1—C2	1.374 (4)	C7A—H7AC	0.9800
C6—H6	0.9500	C8A—H8AA	0.9900
C4—C3	1.385 (5)	C8A—H8AB	0.9900
C4—C7	1.512 (4)	C10—H10D	0.9800
C2A—H2A	0.9500	C10—H10E	0.9800
N1—C8	1.481 (4)	C10—H10F	0.9800
N1—H1	0.85 (3)	C10—C9	1.503 (6)
C4A—C5A	1.394 (4)	C9—H9A	0.9900
C4A—C7A	1.505 (4)	C9—H9B	0.9900
C2—H2	0.9500	C10A—H10A	0.9800
C2—C3	1.389 (5)	C10A—H10B	0.9800
C3—H3	0.9500	C10A—H10C	0.9800
O2A—S1A—C1A	108.49 (13)	N1—C8—H8A	109.5
O2A—S1A—O1A	119.48 (13)	N1—C8—H8B	109.5
O2A—S1A—N1A	105.96 (13)	N1—C8—C9	110.6 (3)
O1A—S1A—C1A	107.43 (13)	H8A—C8—H8B	108.1
O1A—S1A—N1A	106.77 (13)	C9—C8—H8A	109.5
N1A—S1A—C1A	108.27 (13)	C9—C8—H8B	109.5
N1—S1—C1	106.86 (13)	H9AA—C9A—H9AB	107.8
O2—S1—C1	109.52 (13)	C8A—C9A—H9AA	109.0
O2—S1—N1	106.43 (13)	C8A—C9A—H9AB	109.0
O2—S1—O1	118.26 (13)	C10A—C9A—H9AA	109.0
O1—S1—C1	107.03 (13)	C10A—C9A—H9AB	109.0
O1—S1—N1	108.23 (14)	C10A—C9A—C8A	113.1 (3)

C2A—C1A—S1A	120.0 (2)	C1A—C6A—H6A	120.3
C6A—C1A—S1A	119.4 (2)	C5A—C6A—C1A	119.5 (3)
C6A—C1A—C2A	120.6 (3)	C5A—C6A—H6A	120.3
C6—C5—H5	119.4	C4—C7—H7A	109.5
C6—C5—C4	121.2 (3)	C4—C7—H7B	109.5
C4—C5—H5	119.4	C4—C7—H7C	109.5
C2A—C3A—H3A	119.4	H7A—C7—H7B	109.5
C2A—C3A—C4A	121.2 (3)	H7A—C7—H7C	109.5
C4A—C3A—H3A	119.4	H7B—C7—H7C	109.5
C6—C1—S1	118.5 (2)	C4A—C7A—H7AA	109.5
C2—C1—S1	120.8 (2)	C4A—C7A—H7AB	109.5
C2—C1—C6	120.7 (3)	C4A—C7A—H7AC	109.5
C5—C6—C1	118.8 (3)	H7AA—C7A—H7AB	109.5
C5—C6—H6	120.6	H7AA—C7A—H7AC	109.5
C1—C6—H6	120.6	H7AB—C7A—H7AC	109.5
C5—C4—C7	120.5 (3)	N1A—C8A—C9A	110.1 (2)
C3—C4—C5	118.7 (3)	N1A—C8A—H8AA	109.6
C3—C4—C7	120.8 (3)	N1A—C8A—H8AB	109.6
C1A—C2A—H2A	120.4	C9A—C8A—H8AA	109.6
C3A—C2A—C1A	119.2 (3)	C9A—C8A—H8AB	109.6
C3A—C2A—H2A	120.4	H8AA—C8A—H8AB	108.2
S1—N1—H1	108 (2)	H10D—C10—H10E	109.5
C8—N1—S1	117.7 (2)	H10D—C10—H10F	109.5
C8—N1—H1	115 (2)	H10E—C10—H10F	109.5
C3A—C4A—C5A	118.3 (3)	C9—C10—H10D	109.5
C3A—C4A—C7A	120.8 (3)	C9—C10—H10E	109.5
C5A—C4A—C7A	120.9 (3)	C9—C10—H10F	109.5
C1—C2—H2	120.1	C8—C9—H9A	108.9
C1—C2—C3	119.7 (3)	C8—C9—H9B	108.9
C3—C2—H2	120.1	C10—C9—C8	113.5 (3)
C4—C3—C2	120.9 (3)	C10—C9—H9A	108.9
C4—C3—H3	119.5	C10—C9—H9B	108.9
C2—C3—H3	119.5	H9A—C9—H9B	107.7
S1A—N1A—H1A	111 (2)	C9A—C10A—H10A	109.5
C8A—N1A—S1A	120.07 (19)	C9A—C10A—H10B	109.5
C8A—N1A—H1A	117 (2)	C9A—C10A—H10C	109.5
C4A—C5A—H5A	119.4	H10A—C10A—H10B	109.5
C6A—C5A—H5A	119.4	H10A—C10A—H10C	109.5
C6A—C5A—H5A	119.4	H10B—C10A—H10C	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3*A*—H3*A*···O2*A*^{i}	0.95	2.53	3.399 (4)	153
C6—H6···O1*A*^{ii}	0.95	2.59	3.474 (4)	156
C8—H8*B*···O2*A*^{i}	0.99	2.56	3.489 (4)	156
C8*A*—H8*AA*···O2^{iii}	0.99	2.61	3.594 (4)	170

N1*A*—H1*A*···O1^{iv}	0.82 (3)	2.14 (3)	2.925 (3)	161 (3)
N1—H1···O1*A*^{ii}	0.85 (3)	2.13 (4)	2.968 (3)	172 (3)

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