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N-Cyclohexyl-4-methylbenzenesulfonamide

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The title compound, $C_{13}H_{19}NO_2S$, is a new potent herbicide. X-ray analysis reveals the cyclohexane ring to be disordered, which results in the two conformers, both of which adopt a chair conformation. An N—H···O═S hydrogen bond [2.915 (4) Å] and its centrosymmetric equivalent connect two molecules into a dimer.

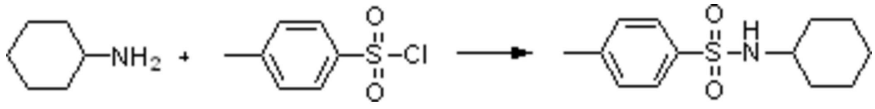
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
Disorder in main residue
R factor = 0.054
wR factor = 0.166
Data-to-parameter ratio = 13.6

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

Comment

The preparation and properties of a large variety of *N*-alkyl and *N*-aryl monosubstituted sulfamides have been reported (Kort *et al.*, 2004). *N*-aryl mono-substituted sulfamides have long been used in the analysis of amines (Pasto *et al.*, 1969), as protective groups for amines (Hendrickson *et al.*, 1970) and in pharmacology (Welnstein, 1965).



(I)

The title compound, (I), has a disordered cyclohexane ring (Fig. 1), the two conformers having occupancies of 0.852 (4) and 0.148 (4). Both conformers exhibit chair conformations. The differences between them are illustrated by the values of two torsion angles: C8—C9—C10—C11 = −57.6 (7)° and C11—C12—C13—C8 = 54.7 (7)°; C8′—C9′—C10′—C11′ = −59.0 (19)° and C11′—C12′—C13′—C8′ = 48 (3)°. The S1—N1 bond length [1.609 (4) Å] is equal to the reported value (Creaser *et al.*, 2001). Two crystallographically equivalent N—H···O═S hydrogen bonds connect two molecules into a dimer (Table 1 and Fig. 2).

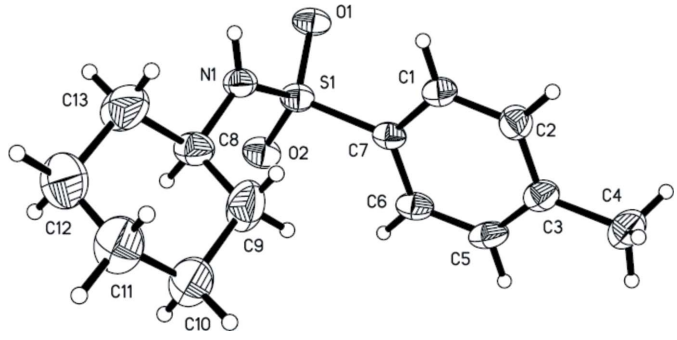


Figure 1
View of the title compound, (I), with displacement ellipsoids drawn at the 30% probability level. The minor disorder component is not shown.

Experimental

Compound (I) was prepared according to the procedure of Moore *et al.* (2003) using 4-methylbenzene-1-sulfonyl chloride (0.01 mol), cyclohexanamine (0.01 mol) and 10% NaOH (33 ml) (2.02 g, 80% yield). Colourless single crystals suitable for X-ray structure analysis were obtained by recrystallization from ethanol.

Crystal data

$C_{13}H_{19}NO_2S$
$M_r = 253.35$
Monoclinic, $P2_1/c$
$a = 9.812$ (5) Å
$b = 12.927$ (7) Å
$c = 11.095$ (6) Å
$\beta = 102.294$ (9)°
$V = 1375.1$ (13) Å^3
$Z = 4$
$D_x = 1.224$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.23$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
0.30 × 0.26 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1990)
$T_{min} = 0.935$, $T_{max} = 0.952$
6797 measured reflections
2428 independent reflections
1396 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.166$
$S = 1.01$
2428 reflections
178 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0804P)^2 + 0.4445P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.76 (3)	2.20 (4)	2.951 (4)	172 (4)

Symmetry code: (i) $-x+1, -y, -z+1$.

The H atom attached to nitrogen was located in a difference map and refined freely. All C-bound H atoms were generated using a riding model, with C—H distances fixed at 0.93 (phenyl group), 0.98 (methyl group) and 0.97 Å (methylene group) and U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C). The cyclohexyl ring was treated as disordered over two positions with refined occupancies of 0.852 (4) and 0.148 (4)

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

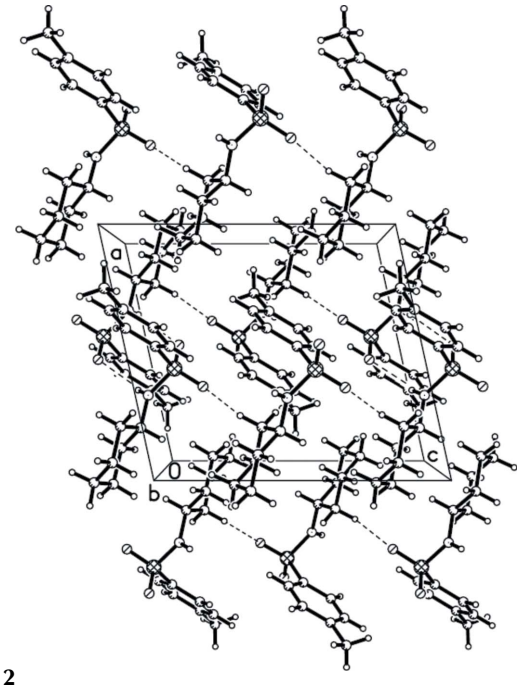


Figure 2
The crystal packing of the title compound, showing the dimers, with hydrogen bonds represented by dashed lines. The major disorder component is shown.].

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