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N-Cyclohexyl-2-nitrobenzenesulfonamide

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Key indicators

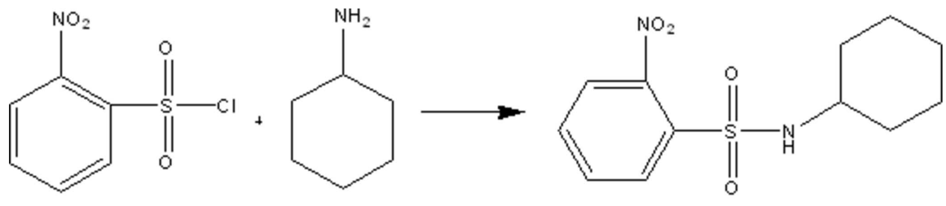
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.105
Data-to-parameter ratio = 20.4

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

The cyclohexane ring of the title compound, $C_{12}H_{16}N_2O_4S$, adopts a chair conformation. The NH group forms a bifurcated hydrogen bond to two O atoms.

Comment

The structure of the title compound, (I), was studied in order to determine its molecular conformation. The cyclohexane ring adopts a chair conformation and the NH group forms a bifurcated hydrogen bond to two O atoms (Table 1).



(I)

Experimental

Compound (I) was prepared according to the procedure of Moore *et al.* (2003), using 2-nitrobenzene-1-sulfonyl chloride (0.01 mol), cyclohexylamine (0.01 mol) and 10% NaOH (33 ml) (2.27 g, 80% yield). Colourless single crystals suitable for X-ray diffraction analysis were obtained by recrystallization from 99% ethanol.

Crystal data

$C_{12}H_{16}N_2O_4S$
M_r = 284.33
Tetragonal, $P4_12_12$
a = 9.6392 (13) Å
c = 31.162 (6) Å
V = 2895.4 (8) Å^3
Z = 8
D_x = 1.305 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 294 (2) K
Prism, colourless
0.24 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.946, T_{max} = 0.977
18343 measured reflections
3598 independent reflections
2528 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 28.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.105
S = 1.02
3598 reflections
176 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 0.3079P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter: −0.06 (10), 1419 Friedel pairs

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1···O3	0.78 (3)	2.45 (3)	3.030 (3)	133 (2)
N1—H1···O1[i]	0.78 (3)	2.31 (3)	2.989 (3)	146 (2)

Symmetry code: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{4}$.

The H atom bonded to nitrogen was located in a difference map and refined freely. All C—H atoms were positioned with an idealized geometry and refined using a riding model, with C—H distances fixed at 0.93 Å for the phenyl group, 0.96 Å for tertiary C atoms and 0.97 Å for methylene C atoms. The *U* values of the carbon-bound H atoms were set at $1.2U_{eq}$(C).

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, 1998); software used to prepare material for publication: *SHELXTL*.

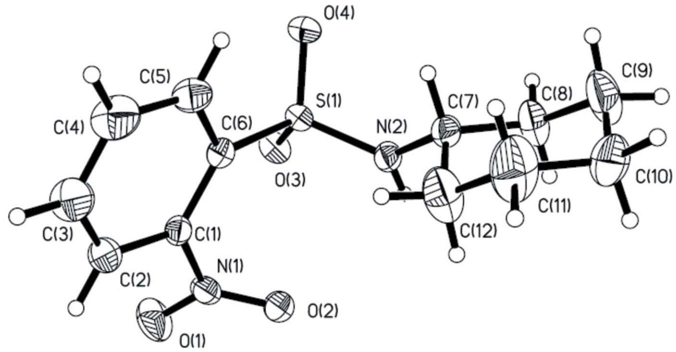


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level.

References

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