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N-[4-(4-Methylpiperazin-1-ylsulfonyl)-phenyl]acetamide monohydrate

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Key indicators

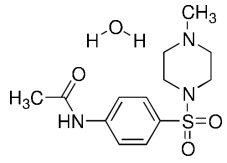
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.131
Data-to-parameter ratio = 16.8

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

The title compound, $C_{13}H_{19}N_3O_3S\cdot H_2O$, is V-shaped and entraps a water molecule. In the crystal structure, N—H···O, O—H···O and O—H···N hydrogen bonds and van der Waals forces stabilize the packing of the molecules.

Comment

Piperazine and its derivatives are important targets for drug discovery. The synthesis and crystal structure reported herein, (I), is part of this study (Guo, 2004).



(I)

The molecular structure of the title compound, (I), is illusrated in Fig. 1. The bond distances and angles are normal, within experimental error. In the crystal structure, symmetry-related molecules are linked by hydrogen bonds (Table 1 and Fig. 2).

Experimental

The title compound was prepared by the reaction of 4-acetamidophenylsulfonyl chloride (4.0 g) with 1-methylpiperazine (2.0 g) under microwave irradiation for 2 min. The resulting product was dispersed in cold water (30 ml), after which 2.5 g of the colorless powder product was separated by filtration. Pure *N*-[4-(4-methylpiperazin-1-ylsulfonyl)phenyl]acetamide (1.5 g) was heated and dissolved in water (20 ml). Single crystals were obtained after 10 h at room temperature.

Crystal data

$C_{13}H_{19}N_3O_3S\cdot H_2O$
M_r = 315.39
Monoclinic, $P2_1/c$
a = 12.851 (6) Å
b = 11.527 (5) Å
c = 10.677 (4) Å
β = 96.251 (7)°
V = 1572.2 (11) Å^3
Z = 4
D_x = 1.332 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 982 reflections
θ = 3.2–26.3°
μ = 0.23 mm^{-1}
T = 293 (2) K
Block, colorless
0.24 × 0.22 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.932, T_{max} = 0.965
8846 measured reflections
3224 independent reflections
2430 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 26.4°
$h = -16 \rightarrow 14$
$k = -14 \rightarrow 14$
$l = -7 \rightarrow 13$

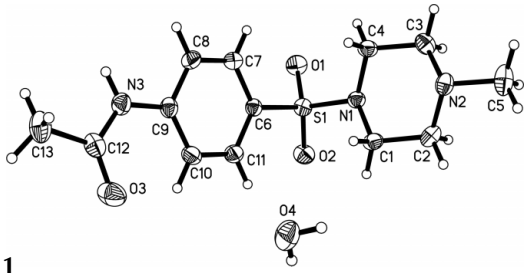


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids.

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0713P)^2 + 0.371P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.039$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.131$	$\Delta\rho_{max} = 0.38$ e Å^{-3}
$S = 1.09$	$\Delta\rho_{min} = -0.23$ e Å^{-3}
3224 reflections	
192 parameters	
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O4^{i}	0.86	2.07	2.915 (3)	167
O4—H4C···O3^{ii}	0.85	2.10	2.915 (3)	162
O4—H4D···N2^{iii}	0.85	2.12	2.914 (3)	156

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

The H atoms of the water molecule were found in a difference Fourier map. However, during refinement, they were fixed at O—H distances of 0.85 Å and their U_{iso} values were set at $1.2U_{eq}$(O). The H atoms of the NH and CH groups were treated as riding, with N—H = 0.86 Å and C—H = 0.93–0.97 Å. For the H atoms attached to atom C5 or C13, U~iso~ (H) = 1.5 U~eq~ (C5,C13), otherwise U_{iso}(H) = $1.2U_{eq}$(N, C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

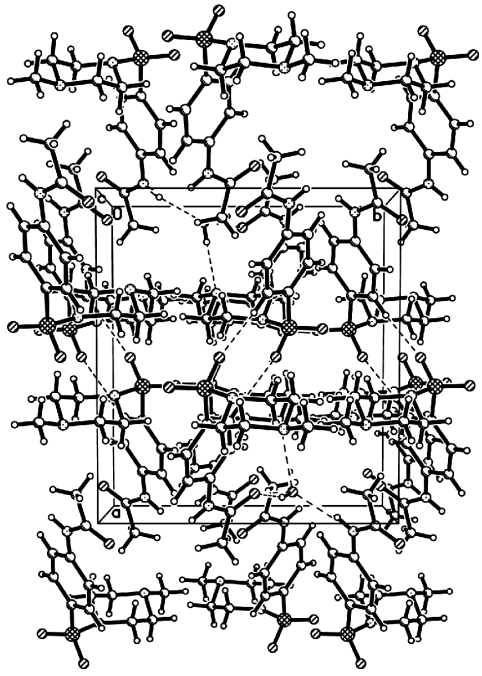


Figure 2
Packing diagram, showing the hydrogen-bond interactions as dashed lines.

References

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