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N-(4-Chloro-6-morpholino-1,3,5-triazin-2-yl)-aniline

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.104
Data-to-parameter ratio = 15.3

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

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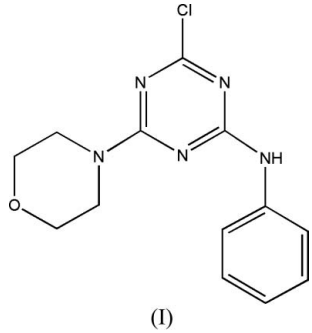
The title compound, $C_{13}H_{14}ClN_5O$, was synthesized from 2,4-dichloro-6-morpholino-1,3,5-triazine and aniline. In the crystal structure, there are intermolecular N—H···O hydrogen bonds which propagate infinite chains parallel to the *c* axis. The morpholine ring adopts a chair conformation.

Comment

1,3,5-Triazine derivatives are of great interest because of their importance as constituents of active dyes and many hindered amine light stabilizers (Goi, 1960; Degussa, 1968; Manasek & Hrdlovik, 1990). The molecular structure of (I) is shown in Fig. 1. In the crystal structure, molecules are linked by N—H···O hydrogen bonds parallel to the *c* axis. There is also an intermolecular contact which indicates a weak C—H···Cl interaction. The morpholine ring adopts a chair conformation, as expected (see Table 1 and Fig. 2).



(I)

Experimental

The title compound was prepared from 2,4-dichloro-6-morpholino-1,3,5-triazine and aniline. 2,4-Dichloro-6-morpholino-1,3,5-triazine was synthesized according to the method described by Dong *et al.* (2005). 2,4-Dichloro-6-morpholino-1,3,5-triazine (23.5 g, 0.1 mol), Na_2CO_3 (5.51 g, 0.051 mol) and aniline (9.3 g, 0.1 mol) were added to toluene (280 ml), which was stirred at 328–333 K for 5 h. The precipitate was filtered off, the solution was washed with water, and the toluene was evaporated under reduced pressure to give compound (I) in 94.3% yield. Crystals suitable for X-ray diffraction were obtained by slow evaporation of a mixed solution in dichloromethane and ethyl acetate (5:1 *v*/*v*) (m.p. 438–440 K).

Crystal data

$C_{13}H_{14}ClN_5O$
M_r = 291.74
Monoclinic, $P2_1/c$
a = 8.3481 (15) Å
b = 17.667 (3) Å
c = 9.9401 (18) Å
β = 108.860 (3)°
V = 1387.3 (4) Å^3
Z = 4
D_x = 1.397 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 2305 reflections
θ = 2.5–25.7°
μ = 0.28 mm^{-1}
T = 294 (2) K
Block, colourless
0.28 × 0.22 × 0.20 mm

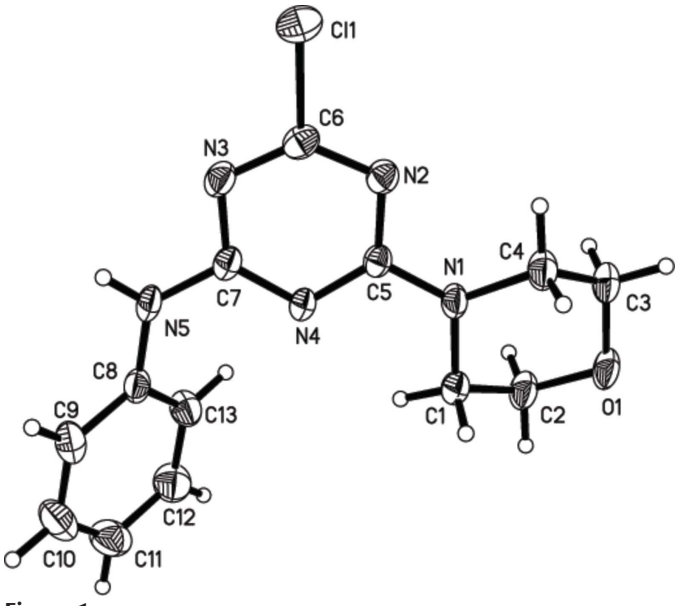


Figure 1
A perspective view of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

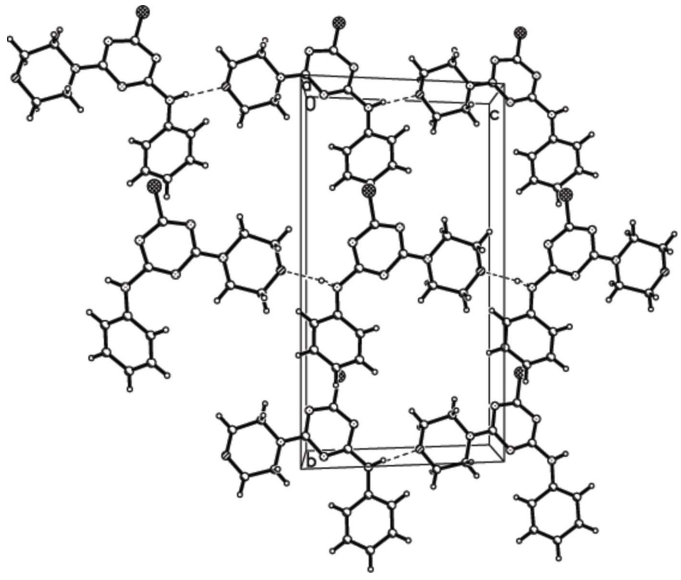


Figure 2
The crystal structure of (I), viewed down the *a* axis. Dashed lines indicate hydrogen-bond interactions.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.920, T_{max} = 0.946
7720 measured reflections
2831 independent reflections
1842 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 26.4°
$h = -8 \rightarrow 10$
$k = -16 \rightarrow 22$
$l = -12 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.104
S = 1.01
2831 reflections
185 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2 + 0.3828P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···O1^{i}	0.84 (2)	2.08 (2)	2.905 (2)	170 (2)

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

The N-bound H atom was located in a difference Fourier map and the N—H distance restrained to 0.84 (2) Å. All other H atoms were positioned geometrically and refined using a riding model, with C—H in the range 0.93–0.97 Å and with U_{iso}(H) = 1.2U_{eq}(C).

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

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