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# 2-Chloro-4,6-dimorpholino-1,3,5-triazine

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**Key indicators**

Single-crystal X-ray study
$T$ = 294 K
Mean $\sigma$(Wae) = 0.000 Å
$R$ factor = 0.026
$wR$ factor = 0.066
Data-to-parameter ratio = 11.7

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

The molecule of the title compound, $C_{11}H_{18}ClN_5O_2$, possesses an approximate mirror plane and both morpholine rings adopt chair conformations.

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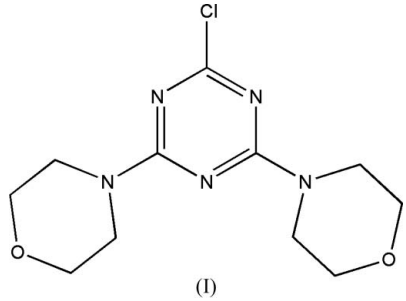
## Comment

Derivatives of 2,4,6-trichloro-1,3,5-triazine has been used as starting materials for drugs and light stabilizers (Azev *et al.*, 2003; Steffensen & Simanek, 2003). The structure of the title compound, (I), is shown in Fig. 1.




(I)

Compound (I) contains an approximate mirror plane, with atoms Cl1, C1 and N3 on the plane. Both morpholine rings adopt chair conformations. The bond lengths and angles (Table 1) compare well with those of the similar compound 2,4-dichloro-6-morpholino-1,3,5-triazine (Dong *et al.*, 2005).

## Experimental

The title compound was prepared from 2,4-dichloro-6-morpholino-1,3,5-triazine and morpholine in tetrahydrofuran (THF). $Na_2CO_3$ (11.77 g, 0.111 mol) and 2,4-dichloro-6-morpholino-1,3,5-triazine (26.09 g, 0.111 mol) were added, with stirring, to THF (120 ml) at 333 K. A solution of morpholine (9.41 g, 0.108 mol) in THF (30 ml) was then added dropwise for 1 h. The reaction mixture was stirred at 330–333 K for a further 3 h. The solvent THF was removed by vacuum evaporation at 317 K, the precipitate was filtered off, washed by water and dried at 318 K. The product (26.52 g) was obtained in a yield of 84.3%. Suitable crystals (m.p. 443–445 K) were obtained by slow evaporation of a solution in a mixture of dichloromethane and ethanol (4:1 *v*/*v*).

*Crystal data*

$C_{11}H_{16}ClN_5O_2$
$M_r$ = 285.74
Monoclinic, *Cc*
$a$ = 23.081 (4) Å
$b$ = 4.5554 (8) Å
$c$ = 13.069 (2) Å
$\beta$ = 108.741 (2)°
$V$ = 1301.3 (4) Å$^3$
$Z$ = 4
$D_x$ = 1.458 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 2215 reflections
$\theta$ = 3.3–26.3°
$\mu$ = 0.30 mm$^{-1}$
$T$ = 294 (2) K
Block, colourless
0.26 × 0.22 × 0.20 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.910, $T_{max}$ = 0.942
3462 measured reflections
2014 independent reflections
1903 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.014
$\theta_{max}$ = 26.4°
$h = -19 \rightarrow 28$
$k = -5 \rightarrow 5$
$l = -16 \rightarrow 14$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.066
$S$ = 1.05
2014 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0382P)^2 + 0.1478P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.11 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$
Absolute structure: Flack (1983), 674 Friedel pairs
Flack parameter: 0.01 (5)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cl1—C1 | 1.7535 (18) | N4—C7 | 1.464 (2) |
| O1—C5 | 1.423 (2) | N5—C2 | 1.348 (2) |
| O2—C10 | 1.417 (3) | N5—C8 | 1.459 (3) |
| N4—C3 | 1.347 (3) | C6—C7 | 1.497 (3) |
| | | | |
| C5—O1—C6 | 109.79 (16) | C2—N5—C8 | 123.12 (15) |
| C10—O2—C9 | 110.28 (15) | N4—C4—H4*A* | 109.6 |
| C1—N1—C3 | 111.87 (15) | O2—C9—C8 | 112.68 (17) |
| C3—N4—C4 | 122.40 (16) | O2—C10—C11 | 112.13 (17) |
| C4—N4—C7 | 114.12 (15) | | |
| | | | |
| C3—N1—C1—Cl1 | −177.96 (11) | C2—N3—C3—N1 | −0.3 (2) |
| C11—N5—C2—N3 | 3.5 (2) | C1—N1—C3—N4 | 178.08 (16) |

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

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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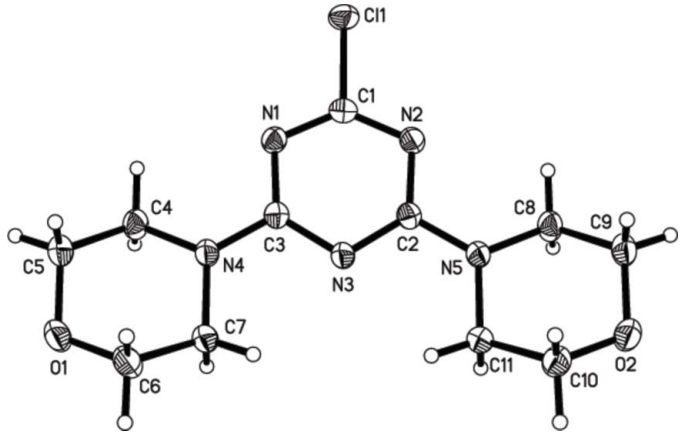


**Figure 1**
A view of the molecule of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

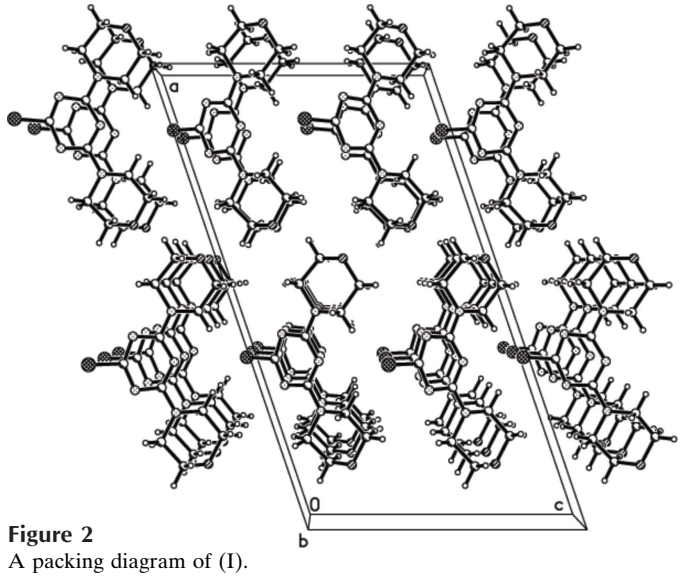


**Figure 2**
A packing diagram of (I).


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