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N-(4,6-Dichloro-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) = 0.005 Å
R factor = 0.054
wR factor = 0.111
Data-to-parameter ratio = 14.5

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

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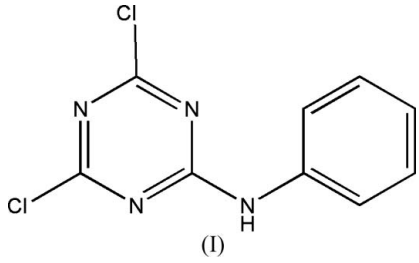
The synthesis of the title compound, $C_9H_6Cl_2N_4$, and its crystal structure are reported in this paper. The crystal structure is stabilized by N—H···Cl and N—H···N hydrogen-bonding interactions.

Comment

The amine derivatives of 2,4,6-trichloro[1,3,5]triazine possess valuable properties, as they are widely used as starting materials for many products, including drugs and light stabilizers (Mathias & Simanek, 1994; Manasek & Hrdlovik, 1990). The title compound, $C_9H_6Cl_2N_4$, (I), has been synthesized from 2,4,6-trichloro-1,3,5-triazine and aniline. The bond lengths and angles are within normal ranges and selected values are given in Table 1. The crystal structure is stabilized by N—H···Cl hydrogen bonds and a weak N—H···N interaction (Fig.2).



(I)

Experimental

2,4,6-Trichloro-1,3,5-triazine (4.61 g, 0.025 mol) and aniline (2.33 g, 0.025 mol) were added to acetone (30 ml), and stirred at 273 K for 2 h. A solution of Na_2CO_3 (1.38 g, 0.013 mol) in water (10 ml) was then added dropwise for 1 h. The reaction mixture was stirred at 273–278 K for a further 3 h. The precipitate was filtered off, and the acetone was evaporated under reduced pressure. The title compound (5.54 g) was obtained in a yield of 92.3%. Suitable crystals (m.p. 407–409 K) were obtained by slow evaporation of a solution in a mixture of dichloromethane and ethyl acetate (6:1 *v*/*v*).

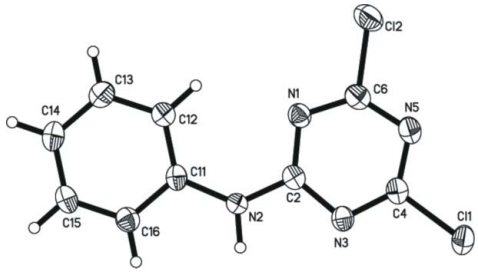


Figure 1
A view of the molecule of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

Crystal data

$C_9H_6Cl_2N_4$
M_r = 241.08
Orthorhombic, *Pbca*
a = 14.114 (3) Å
b = 5.5098 (10) Å
c = 25.621 (5) Å
V = 1992.4 (6) Å^3
Z = 8
D_x = 1.607 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2959 reflections
θ = 3.2–25.9°
μ = 0.62 mm^{-1}
T = 294 (2) K
Block, colourless
0.34 × 0.22 × 0.20 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.800, T_{max} = 0.884
10293 measured reflections
2033 independent reflections
1427 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 26.4°
$h = -17 \rightarrow 15$
$k = -6 \rightarrow 6$
$l = -32 \rightarrow 31$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.111
S = 1.13
2033 reflections
140 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0096P)^2 + 3.9817P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—C4	1.725 (4)	N2—C11	1.413 (4)
N5—C6	1.323 (5)	N2—H2	0.94 (3)
N2—C2	1.346 (4)		
C6—N5—C4	110.9 (3)	C11—N2—H2	118 (2)
C2—N2—C11	131.6 (3)	N3—C4—Cl1	116.0 (3)
C2—N2—H2	110 (2)		
C2—N3—C4—N5	0.8 (5)	C11—N2—C2—N3	174.8 (3)
C2—N3—C4—Cl1	178.7 (2)	C2—N2—C11—C12	−1.4 (6)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N3^{i}	0.94 (3)	2.72 (4)	3.615 (4)	160 (3)
N2—H2···Cl1^{i}	0.94 (3)	2.80 (3)	3.465 (3)	129 (3)

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

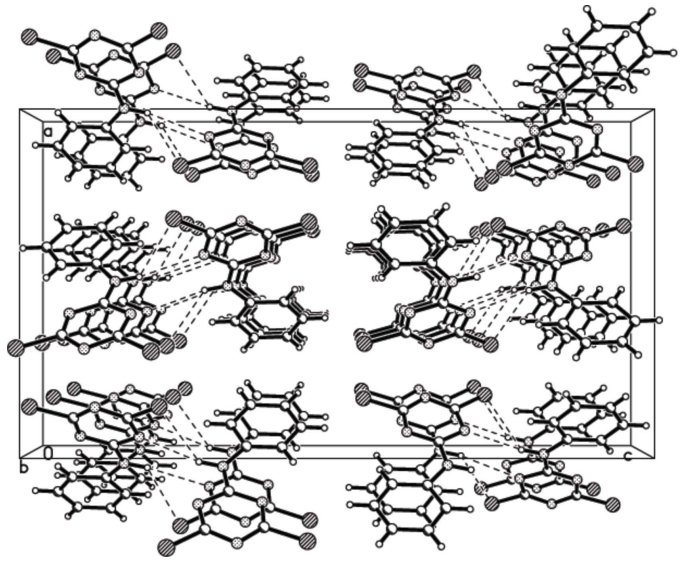


Figure 2
A packing diagram of (I). Dashed lines indicate N—H···Cl and N—H···N interactions.

The H atom of the NH group was initially located in a difference Fourier map and was refined with an N—H distance restraint of 0.94 (3) Å. All other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). In the absence of significant anomalous dispersion effects, Friedel-pair reflections were merged prior to refinement.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); 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*.

References

Bruker (1997). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Manasek, Z. & Hrdlovik, P. (1990). European Patent EP 0377324.
Mathias, P. J. & Simanek, E. E. (1994). *J. Am. Chem. Soc.* **116**, 4326–4340.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.