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5,6-Dimethyl-1,2,4-triazin-3-amine

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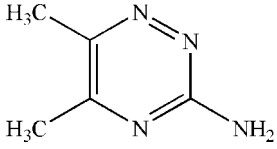
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.048; wR factor = 0.157; data-to-parameter ratio = 10.6.

In the crystal structure of the title compound, $C_5H_8N_4$, adjacent molecules are connected through N—H···N hydrogen bonds, resulting in a zigzag chain along [100]. The amino groups and heterocyclic N atoms are involved in further N—H···N hydrogen bonds, forming $R_2^2(8)$ motifs.

Related literature

For the biological and medical applications of triazine, see: Anderson *et al.*(2003); Gavai *et al.* (2009); Hunt *et al.* (2004). For the structures of complexes containing triazine, see: Drew *et al.* (2001); Li *et al.* (2009); Machura *et al.* (2008). For the structures of complexes containing the title compound, see: Jiang *et al.* (2011); Self *et al.* (1991); Wu *et al.* (2011). For the structures of compounds containing $R_2^2(8)$-type hydrogen bonds, see: Etter (1990); Glidewell *et al.* (2003).



Experimental

Crystal data

$C_5H_8N_4$
M_r = 124.14
Orthorhombic, *Pnma*
a = 7.4877 (8) Å
b = 6.7530 (7) Å
c = 12.6615 (13) Å
V = 640.22 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.50 × 0.39 × 0.38 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.960, T_{max} = 0.969
2997 measured reflections
614 independent reflections
421 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.157
S = 1.11
614 reflections
58 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···N3^{i}	0.86	2.19	3.045 (4)	179
N4—H4B···N2^{ii}	0.86	2.09	2.947 (4)	176

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RN2097).

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5,6-Dimethyl-1,2,4-triazin-3-amine

Man-Hua Wu, Qi-Ming Qiu, Sen Gao, Qiong-Hua Jin and Cun-Lin Zhang

S1. Comment

The heterocyclic nitrogen compounds containing 1,2,4-triazine moieties have drawn much attention in recent years, owing to their interesting biological and medicinal properties (Anderson *et al.*, 2003; Gavai *et al.*, 2009; Hunt *et al.*,2004). They usually act as efficient ligands in supramolecular compounds (Drew *et al.*, 2001; Li *et al.*, 2009; Machura *et al.*, 2008). The title compound (I) has been used as a multidentate ligand to form poly-nuclear complexes (Self *et al.*, 1991). In (I), hydrogen bonds are formed between the NH groups of amino group and the N atoms.

We are interested in synthesizing new transition metal complexes containing (I) (Jiang *et al.*, 2011; Wu *et al.*, 2011). The title compound was unexpectedly obtained in the course of synthesizing Cu(I) complexes.

In the title compound, adjacent molecules are connected by intermolecular N—H···N hydrogen bonds to form a zigzag structure (Fig. 2). In the crystal structure, the amino groups and heterocyclic N atoms are involved in hydrogen bonds,forming $R_2^2(8)$ type hydrogen bonds (Etter, 1990; Glidewell *et al.*, 2003).

S2. Experimental

A mixture of CuCN and ADMT (ADMT=3-amino-5,6-dimethyl- 1,2,4-triazine) in molar ratio of 1:1 in the mixed solution of CH_3CN (7 ml)/ CH_3OH (3 ml) was stirred for 3 h,then filtered. Pale yellow crystals were obtained from the filtrate after standing at room temperature for several days.

S3. Refinement

The final refinements were performed with isotropic thermal parameters. All hydrogen atoms were located in the calculated sites and included in the final refinement in the riding model approximation with displacement parameters derived from the parent atoms to which they were bonded. The ratios of H atom U_{iso} to C atom U_{eq} are 1.5. The ratios of H atom U_{iso} to N atom U_{eq} are 1.2.

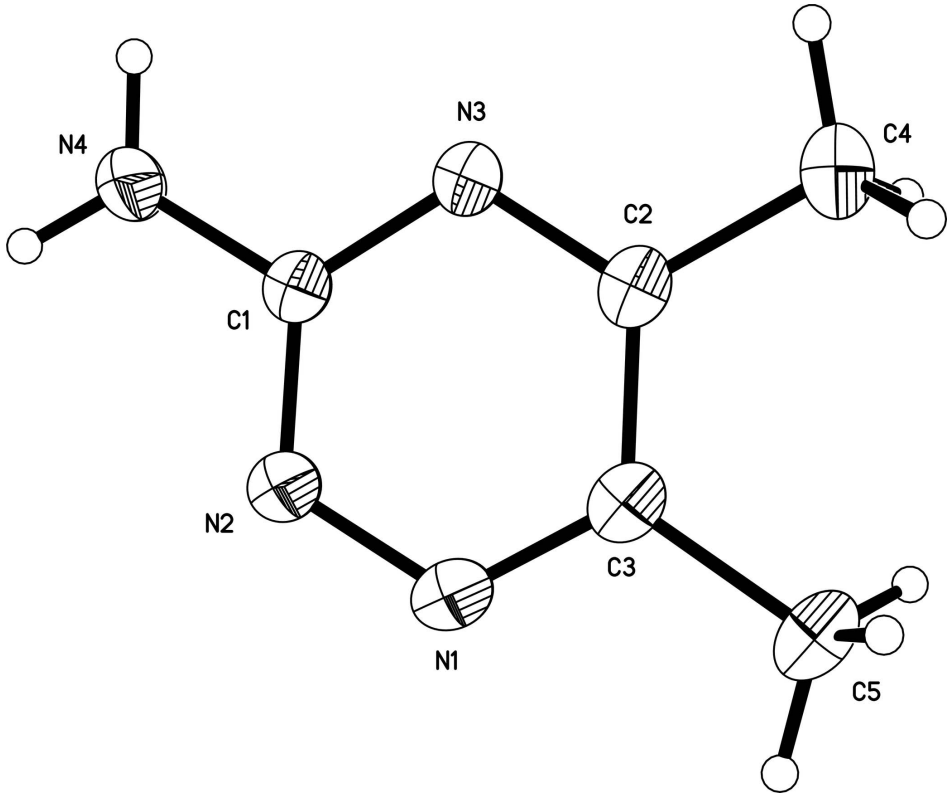

Figure 1

Molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level.

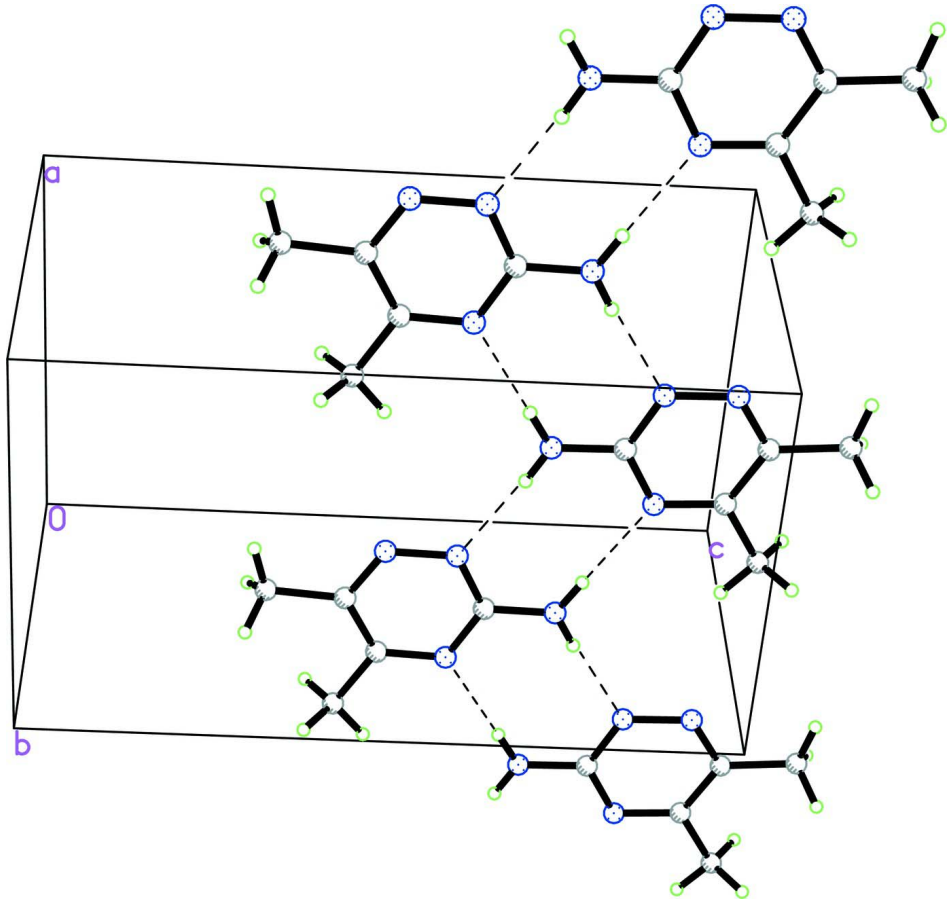

Figure 2

Crystal packing for (I) with hydrogen bonds shown as dashed lines.

5,6-Dimethyl-1,2,4-triazin-3-amine

Crystal data

$C_5H_8N_4$
M_r = 124.14
Orthorhombic, *Pnma*
a = 7.4877 (8) Å
b = 6.7530 (7) Å
c = 12.6615 (13) Å
V = 640.22 (12) Å^3
Z = 4
F(000) = 264
D_x = 1.278 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1029 reflections
θ = 2.7–28.0°
μ = 0.08 mm^{-1}
T = 293 K
Block, yellow
0.50 × 0.39 × 0.38 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.960, T_{max} = 0.969
2997 measured reflections
614 independent reflections
421 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 25.0°, θ_{min} = 3.2°
h = −7→8
k = −8→7
l = −14→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.157$
$S = 1.11$
614 reflections
58 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0627P)^2 + 0.3625P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
N1	1.0561 (4)	0.2500	0.5062 (2)	0.0514 (9)	
N2	1.0506 (4)	0.2500	0.6123 (2)	0.0499 (8)	
N3	0.7314 (4)	0.2500	0.60746 (19)	0.0466 (8)	
N4	0.8858 (4)	0.2500	0.7657 (2)	0.0609 (10)	
H4A	0.9838	0.2500	0.8011	0.073*	
H4B	0.7850	0.2500	0.7982	0.073*	
C1	0.8903 (4)	0.2500	0.6589 (2)	0.0447 (9)	
C2	0.7407 (5)	0.2500	0.5030 (2)	0.0469 (9)	
C3	0.9072 (5)	0.2500	0.4511 (2)	0.0477 (9)	
C4	0.5682 (5)	0.2500	0.4422 (3)	0.0678 (12)	
H4C	0.5720	0.3512	0.3890	0.102*	0.50
H4D	0.4708	0.2755	0.4896	0.102*	0.50
H4E	0.5516	0.1233	0.4093	0.102*	0.50
C5	0.9233 (5)	0.2500	0.3332 (2)	0.0624 (11)	
H5A	0.8506	0.1461	0.3044	0.094*	0.50
H5B	1.0456	0.2286	0.3137	0.094*	0.50
H5C	0.8839	0.3753	0.3060	0.094*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0485 (19)	0.063 (2)	0.0425 (16)	0.000	0.0087 (13)	0.000
N2	0.0412 (17)	0.069 (2)	0.0395 (16)	0.000	0.0016 (12)	0.000
N3	0.0431 (16)	0.062 (2)	0.0346 (15)	0.000	−0.0012 (11)	0.000
N4	0.0382 (16)	0.105 (3)	0.0391 (16)	0.000	−0.0064 (12)	0.000

C1	0.0417 (19)	0.057 (2)	0.0350 (17)	0.000	−0.0008 (13)	0.000
C2	0.054 (2)	0.050 (2)	0.0374 (19)	0.000	−0.0014 (14)	0.000
C3	0.055 (2)	0.049 (2)	0.0397 (19)	0.000	0.0031 (16)	0.000
C4	0.060 (2)	0.097 (3)	0.047 (2)	0.000	−0.0118 (17)	0.000
C5	0.075 (3)	0.074 (3)	0.0376 (19)	0.000	0.0075 (18)	0.000

Geometric parameters (Å, º)

N1—C3	1.315 (4)	C2—C4	1.503 (5)
N1—N2	1.344 (4)	C3—C5	1.498 (4)
N2—C1	1.338 (4)	C4—H4C	0.9600
N3—C2	1.325 (4)	C4—H4D	0.9600
N3—C1	1.356 (4)	C4—H4E	0.9600
N4—C1	1.353 (4)	C5—H5A	0.9600
N4—H4A	0.8600	C5—H5B	0.9600
N4—H4B	0.8600	C5—H5C	0.9600
C2—C3	1.409 (5)		
C3—N1—N2	120.2 (3)	C2—C3—C5	122.4 (3)
C1—N2—N1	117.9 (3)	C2—C4—H4C	109.5
C2—N3—C1	115.7 (3)	C2—C4—H4D	109.5
C1—N4—H4A	120.0	H4C—C4—H4D	109.5
C1—N4—H4B	120.0	C2—C4—H4E	109.5
H4A—N4—H4B	120.0	H4C—C4—H4E	109.5
N2—C1—N4	117.6 (3)	H4D—C4—H4E	109.5
N2—C1—N3	125.2 (3)	C3—C5—H5A	109.5
N4—C1—N3	117.3 (3)	C3—C5—H5B	109.5
N3—C2—C3	120.8 (3)	H5A—C5—H5B	109.5
N3—C2—C4	117.7 (3)	C3—C5—H5C	109.5
C3—C2—C4	121.5 (3)	H5A—C5—H5C	109.5
N1—C3—C2	120.2 (3)	H5B—C5—H5C	109.5
N1—C3—C5	117.4 (3)		
C3—N1—N2—C1	0.0	N2—N1—C3—C2	0.0
N1—N2—C1—N4	180.0	N2—N1—C3—C5	180.0
N1—N2—C1—N3	0.000 (1)	N3—C2—C3—N1	0.0
C2—N3—C1—N2	0.000 (1)	C4—C2—C3—N1	180.0
C2—N3—C1—N4	180.0	N3—C2—C3—C5	180.0
C1—N3—C2—C3	0.0	C4—C2—C3—C5	0.0
C1—N3—C2—C4	180.0		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···N3^{i}	0.86	2.19	3.045 (4)	179
N4—H4*B*···N2^{ii}	0.86	2.09	2.947 (4)	176

Symmetry codes: (i) *x*+1/2, *y*, −*z*+3/2; (ii) *x*−1/2, *y*, −*z*+3/2.