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2,4-Diamino-1,3,5-triazine (guanamine)

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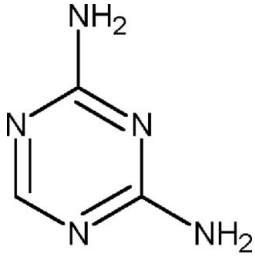
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(N–C) = 0.001 Å; R factor = 0.042; wR factor = 0.128; data-to-parameter ratio = 18.1.

Molecules of 2,4-diamino-1,3,5-triazine (guanamine), $C_3H_5N_5$, are associated in the crystal structure *via* four independent N—H···N hydrogen bonds to form a three-dimensional framework. The hydrogen-bonding scheme involves all hydrogen donor/acceptor sites. The molecular geometry of the aromatic ring conforms to C_{2v} symmetry within experimental error.

Related literature

For related literature describing crystalline adducts of DNA/RNA pyrimidine bases coupled with amino derivatives of aromatic *N*-heterocycles *via* multiple hydrogen bonds to mimic the base-pairing of nucleic acids, see: Portalone *et al.* (1999, 2002); Brunetti *et al.* (2000, 2002); Portalone & Colapietro (2004*a*,*b*, 2006, 2007*a*,*b*,*c*,*d*).



Experimental

Crystal data

$C_3H_5N_5$
M_r = 111.12
Monoclinic, $P2_1/c$
a = 9.8631 (9) Å
b = 3.7180 (3) Å
c = 12.9609 (9) Å
β = 99.643 (9)°
V = 468.57 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 298 (2) K
0.15 × 0.12 × 0.10 mm

Data collection

Huber CS four-circle diffractometer
Absorption correction: none
2088 measured reflections
1684 independent reflections
1450 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
3 standard reflections
every 97 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.128
S = 1.07
1684 reflections
93 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N7—H71···N3^{i}	0.866 (16)	2.549 (16)	3.1811 (10)	130.7 (13)
N7—H72···N5^{ii}	0.903 (18)	2.113 (18)	3.0106 (12)	172.3 (14)
N8—H81···N1^{iii}	0.893 (17)	2.123 (17)	3.0150 (11)	176.6 (14)
N8—H82···N3^{iv}	0.851 (16)	2.310 (15)	3.0962 (11)	153.9 (14)

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

Data collection: *XCS* (Colapietro *et al.*, 1992); cell refinement: *XCS*; data reduction: *XCS*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2037).

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supplementary materials

Acta Cryst. (2007). E**63**, o3232 [**doi:10.1107/S1600536807027407**]

2,4-Diamino-1,3,5-triazine (guanamine)

G. Portalone

Comment

As a part of our continuing study of crystal adducts of DNA/RNA pyrimidine bases coupled with amino-derivatives of aromatic *N*-heterocycles *via* multiple hydrogen bonds to mimic the base-pairing of nucleic acids (Portalone *et al.*, 1999; Brunetti *et al.*, 2000, 2002; Portalone *et al.*, 2002; Portalone & Colapietro, 2004*a*,b; Portalone & Colapietro, 2006; Portalone & Colapietro, 2007*a*,b,c,d) we became interested in guanamine (I), as a good candidate to be associated in the crystal with pyrimidinic nucleobases.

The asymmetric unit of (I) comprises a planar molecule and is shown in Fig. 1. With regard to the aromatic ring, the bond lengths and angles are normal and conform within experimental error to C_{2v} symmetry (Table 1). The H-bonding scheme involves all H atoms of the NH_2 groups (Fig. 2) and consists entirely of N—H··· N intermolecular interactions (Table 2). These interactions delineate patterns in which rings are the most prominent features. Besides the intermolecular N—H··· N hydrogen bonds, two small rings of descriptor $R^2_2(8)$ are formed by centrosymmetric molecules. Infinite $C^2_2(6)$ chains are then generated by the 2_1 screw axis running along the b direction,

Experimental

Guanamine was purchased from Sigma Aldrich (99% purity). and used as obtained. Crystals of guanamine were grown from a hot water solution (0.25 mmol in *ca* 10 ml) by slow evaporation of the solvent.

Refinement

All H atoms were found in a difference Fourier map. Positional and isotropic displacement parameters of all H atoms were independently refined (C—H = 0.972 (13) Å, N—H = 0.851 (16)–0.903 (18) Å).

Figures

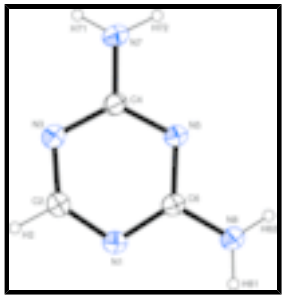

Fig. 1. The crystallographic asymmetric unit in guanamine, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

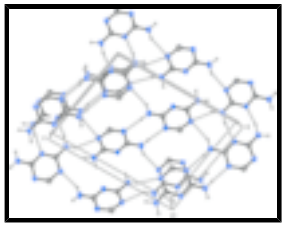

Fig. 2. Packing diagram of guanamine viewed down the crystallographic *b* axis. For the sake of clarity, only H atoms involved in hydrogen bonding are shown as small spheres of arbitrary radii. Displacements ellipsoids are drawn at the 50% probability level. Hydrogen bonding is indicated by dashed lines.

2,4-diamino-1,3,5-triazine

Crystal data

$C_3H_5N_5$	F_{000} = 232
M_r = 111.12	D_x = 1.575 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71069 Å
Hall symbol: -P 2ybc	Cell parameters from 87 reflections
a = 9.8631 (9) Å	θ = 21–27º
b = 3.7180 (3) Å	μ = 0.12 mm^{-1}
c = 12.9609 (9) Å	T = 298 (2) K
β = 99.643 (9)º	Tablet, colourless
V = 468.57 (7) Å^3	0.15 × 0.12 × 0.10 mm
Z = 4	

Data collection

Huber CS four-circle diffractometer	R_{int} = 0.026
Radiation source: X-Ray tube	θ_{max} = 32.5º
Monochromator: graphite	θ_{min} = 2.1º
T = 298(2) K	h = 0→14
ω scans	k = 0→5
Absorption correction: none	l = −19→19
2088 measured reflections	3 standard reflections
1684 independent reflections	every 97 reflections
1450 reflections with $I > 2\sigma(I)$	intensity decay: 1%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.042	All H-atom parameters refined
$wR(F^2)$ = 0.128	$w = 1/[\sigma^2(F_o^2) + (0.0865P)^2 + 0.0407P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.001
1684 reflections	$\Delta\rho_{max}$ = 0.35 e Å^{-3}

93 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.61517 (7)	0.0133 (2)	0.89333 (5)	0.02784 (18)
N3	0.79107 (7)	0.0531 (2)	0.78800 (5)	0.02702 (18)
N5	0.83121 (7)	0.2817 (2)	0.96284 (5)	0.02508 (18)
N7	0.99658 (8)	0.3212 (2)	0.85938 (6)	0.03028 (19)
N8	0.66293 (9)	0.2167 (3)	1.06320 (6)	0.0387 (2)
C2	0.66676 (8)	−0.0349 (3)	0.80627 (6)	0.02765 (19)
C4	0.87077 (8)	0.2155 (2)	0.87067 (6)	0.02206 (17)
C6	0.70459 (8)	0.1707 (2)	0.97155 (6)	0.02440 (18)
H2	0.6089 (13)	−0.151 (3)	0.7476 (10)	0.032 (3)*
H71	1.0272 (14)	0.261 (4)	0.8030 (12)	0.048 (4)*
H72	1.0486 (19)	0.421 (4)	0.9162 (13)	0.049 (4)*
H81	0.5800 (17)	0.144 (4)	1.0735 (12)	0.043 (3)*
H82	0.7201 (16)	0.298 (4)	1.1143 (12)	0.051 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0212 (3)	0.0393 (4)	0.0235 (3)	−0.0077 (3)	0.0052 (2)	−0.0031 (2)
N3	0.0238 (3)	0.0369 (4)	0.0211 (3)	−0.0032 (3)	0.0061 (2)	−0.0024 (2)
N5	0.0201 (3)	0.0352 (4)	0.0210 (3)	−0.0061 (2)	0.0063 (2)	−0.0026 (2)
N7	0.0219 (3)	0.0442 (4)	0.0269 (4)	−0.0066 (3)	0.0102 (3)	−0.0025 (3)
N8	0.0279 (4)	0.0668 (6)	0.0238 (4)	−0.0178 (4)	0.0114 (3)	−0.0114 (3)
C2	0.0238 (4)	0.0368 (4)	0.0223 (3)	−0.0054 (3)	0.0036 (3)	−0.0037 (3)
C4	0.0200 (3)	0.0259 (3)	0.0209 (3)	−0.0007 (2)	0.0054 (2)	0.0020 (2)
C6	0.0209 (3)	0.0320 (4)	0.0212 (3)	−0.0046 (3)	0.0060 (3)	−0.0009 (2)

Geometric parameters (Å, °)

N1—C2	1.3254 (10)	N7—H71	0.866 (16)
N1—C6	1.3597 (10)	N7—H72	0.903 (18)

N3—C2	1.3280 (11)	N8—C6	1.3313 (10)
N3—C4	1.3596 (10)	N8—H81	0.893 (17)
N5—C6	1.3378 (10)	N8—H82	0.851 (16)
N5—C4	1.3401 (9)	C2—H2	0.972 (13)
N7—C4	1.3329 (10)		
C2—N1—C6	113.55 (7)	N1—C2—N3	128.02 (7)
C2—N3—C4	113.46 (7)	N1—C2—H2	117.9 (8)
C6—N5—C4	115.72 (7)	N3—C2—H2	114.1 (8)
C4—N7—H71	118.6 (10)	N7—C4—N5	117.34 (7)
C4—N7—H72	116.3 (11)	N7—C4—N3	118.06 (7)
H71—N7—H72	124.3 (14)	N5—C4—N3	124.59 (7)
C6—N8—H81	121.4 (10)	N8—C6—N5	117.89 (7)
C6—N8—H82	118.5 (11)	N8—C6—N1	117.51 (7)
H81—N8—H82	119.7 (15)	N5—C6—N1	124.60 (7)
C6—N1—C2—N3	−0.52 (15)	C2—N3—C4—N5	0.49 (13)
C4—N3—C2—N1	−0.82 (15)	C4—N5—C6—N8	177.18 (8)
C6—N5—C4—N7	−179.75 (7)	C4—N5—C6—N1	−2.70 (14)
C6—N5—C4—N3	1.13 (13)	C2—N1—C6—N8	−177.48 (9)
C2—N3—C4—N7	−178.62 (8)	C2—N1—C6—N5	2.40 (13)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N7—H71···N3^{i}	0.866 (16)	2.549 (16)	3.1811 (10)	130.7 (13)
N7—H72···N5^{ii}	0.903 (18)	2.113 (18)	3.0106 (12)	172.3 (14)
N8—H81···N1^{iii}	0.893 (17)	2.123 (17)	3.0150 (11)	176.6 (14)
N8—H82···N3^{iv}	0.851 (16)	2.310 (15)	3.0962 (11)	153.9 (14)

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

Fig. 1

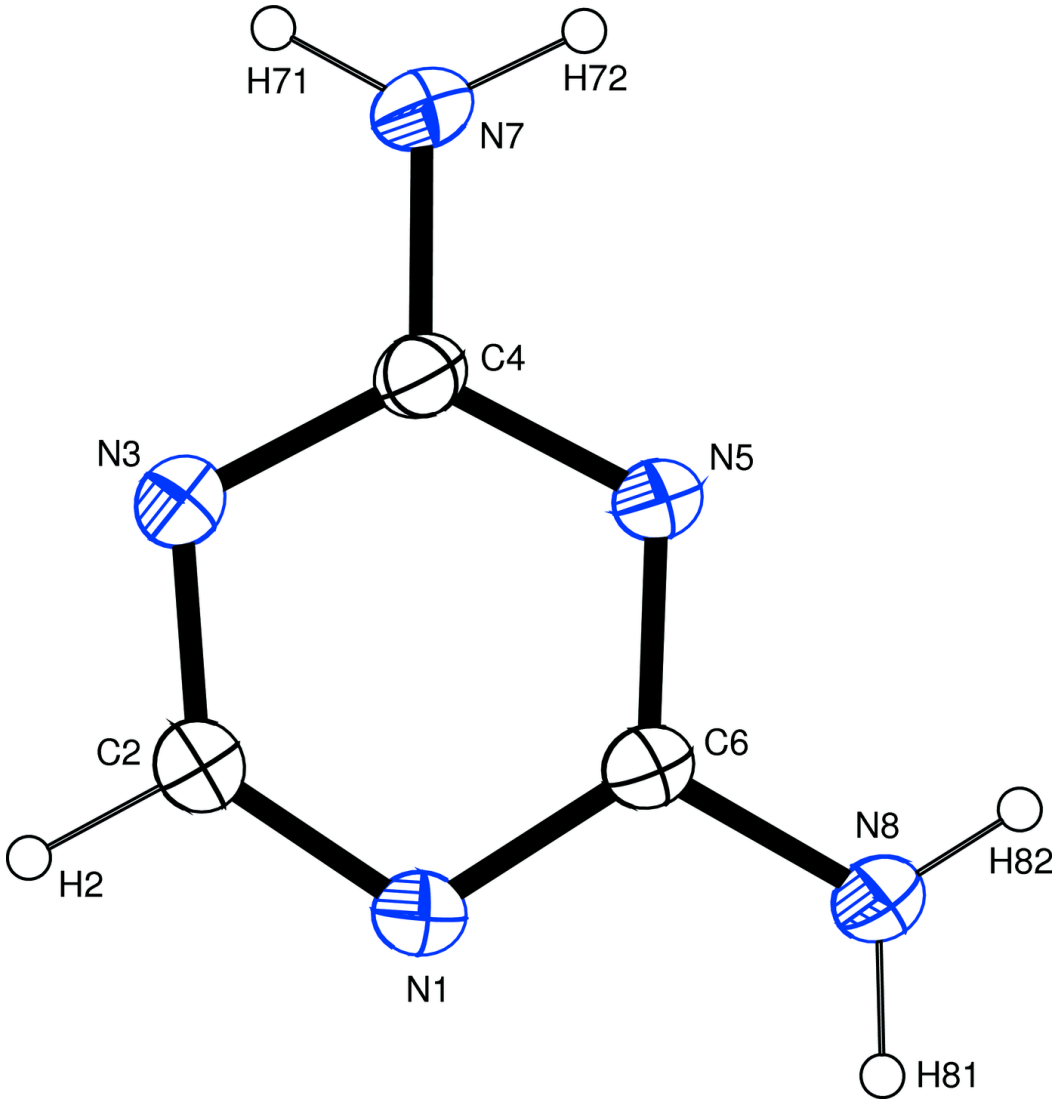

Fig. 2