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1,2-Bis[amino(pyrimidin-2-yl)methylene]-hydrazine dihydrate

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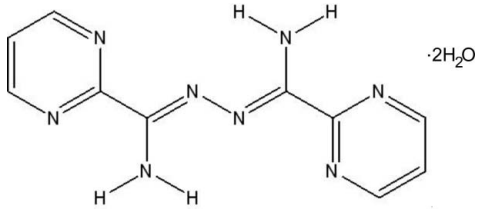
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.102; data-to-parameter ratio = 9.7.

The centrosymmetric organic molecule in the title compound, $C_{10}H_{10}N_8\cdot 2H_2O$, is essentially flat and has a *trans* configuration. The molecules are linked by intermolecular O—H···N, N—H···O and N—H···N hydrogen bonds to form a linear chain structure.

Related literature

For related structures, see: Armstrong *et al.* (1998); Case (1965); Thompson *et al.* (1998); Xu *et al.* (1997, 1998, 2000, 2001).



Experimental

Crystal data

$C_{10}H_{10}N_8\cdot 2H_2O$
M_r = 278.15
Triclinic, $P\overline{1}$
a = 6.109 (2) Å
b = 7.502 (3) Å
c = 7.588 (3) Å
α = 105.112 (6)°
β = 106.975 (7)°
γ = 99.193 (6)°
V = 310.41 (19) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 (2) K
0.48 × 0.22 × 0.18 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.949, T_{max} = 0.980
1526 measured reflections
1036 independent reflections
778 reflections with $I > 2\sigma(I)$
R_{int} = 0.008

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.102
S = 1.04
1036 reflections
107 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···N1^{ii}	0.85 (2)	2.59 (2)	3.276 (2)	138.5 (16)
N3—H3C···O1W^{iii}	0.89 (2)	2.17 (3)	3.043 (3)	166.7 (19)
O1W—H1WA···N2^{iv}	0.79 (3)	2.20 (3)	2.979 (2)	168 (3)
O1W—H1WB···N4	0.91 (3)	2.16 (3)	3.055 (2)	172 (2)

Symmetry codes: (ii) $-x+2, -y+2, -z+2$; (iii) $x+1, y, z$; (iv) $-x, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT-Plus* and *SHELXTL* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; 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: NG2403).

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supporting information

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1,2-Bis[amino(pyrimidin-2-yl)methylene]hydrazine dihydrate

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S1. Comment

The title compound, (I) (Fig. 1), can be regarded as a dihydrazidine. It is formed as the major product from mixing 2-cyanopyrimidine and hydrazine in ethanol (Case, 1965) and the minor product is Pyrimidine-2-carboxamide hydrazone, (II)(Scheme. 1). Compound (I) has now been shown to have *trans* geometry (Fig. 1), with all atoms essentially coplanar. The overall *trans* configuration is therefore due mainly to steric repulsion effects. The title compound contains a single N—N bond, presents several possible mononucleating and dinucleating coordination modes and, also, the potential for free rotation about the N—N bond. The flexible geometries result from the ability of the systems to rotate freely about the single N—N bond of the diazine fragment of the compound.

S2. Refinement

All H atoms were placed in geometrically positions and constrained to ride on their parent atoms, with N—H distances in the range 0.85—0.89 Å and C—H = 0.93 Å, and with U_{iso}(H) = 1.2Ueq(C or N) for all H atoms.

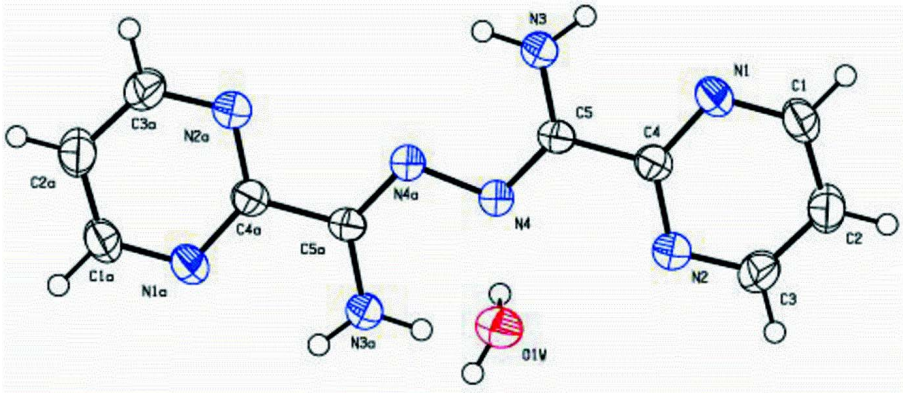

Figure 1

The molecular structure of (I), with atom labels.

1,2-Bis[amino(pyrimidin-2-yl)methylene]hydrazine dihydrate

Crystal data

$C_{10}H_{10}N_8·2H_2O$
M_r = 278.15
Triclinic, $P\overline{1}$
a = 6.109 (2) Å
b = 7.502 (3) Å
c = 7.588 (3) Å
α = 105.112 (6)°
β = 106.975 (7)°
γ = 99.193 (6)°
V = 310.41 (19) Å^3
Z = 1
F(000) = 146
D_x = 1.489 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

μ = 0.11 mm^{-1}
T = 293 K

Prism, yellow
0.48 × 0.22 × 0.18 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.949, T_{max} = 0.980

1526 measured reflections
1036 independent reflections
778 reflections with $I > 2\sigma(I)$
R_{int} = 0.008
θ_{max} = 25.0°, θ_{min} = 2.9°
h = −7→7
k = −8→8
l = −9→8

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.102
S = 1.04
1036 reflections
107 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0576P)^2 + 0.0469P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.6787 (3)	0.9111 (3)	1.2198 (3)	0.0443 (5)
H1A	0.7942	1.0004	1.3310	0.053*
C2	0.4674 (4)	0.8331 (3)	1.2312 (3)	0.0452 (5)
H2A	0.4367	0.8673	1.3468	0.054*
C3	0.3041 (4)	0.7028 (3)	1.0649 (3)	0.0440 (5)
H3A	0.1575	0.6498	1.0681	0.053*
C4	0.5561 (3)	0.7320 (2)	0.9025 (2)	0.0309 (4)
C5	0.6110 (3)	0.6704 (2)	0.7210 (2)	0.0307 (4)
N1	0.7253 (3)	0.8640 (2)	1.0550 (2)	0.0382 (4)
N2	0.3437 (3)	0.6477 (2)	0.8988 (2)	0.0385 (4)
N3	0.8159 (3)	0.7655 (3)	0.7217 (3)	0.0469 (5)
H3B	0.900 (3)	0.857 (3)	0.825 (3)	0.042 (6)*
H3C	0.856 (4)	0.732 (3)	0.617 (3)	0.052 (6)*

N4	0.4600 (2)	0.5260 (2)	0.5788 (2)	0.0334 (4)
O1W	0.0384 (3)	0.6771 (2)	0.4092 (2)	0.0477 (4)
H1WA	−0.074 (5)	0.593 (4)	0.338 (4)	0.079 (10)*
H1WB	0.153 (5)	0.624 (4)	0.462 (4)	0.088 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0481 (12)	0.0404 (11)	0.0308 (11)	−0.0017 (9)	0.0107 (9)	0.0008 (9)
C2	0.0579 (13)	0.0404 (11)	0.0357 (11)	0.0055 (10)	0.0225 (10)	0.0069 (9)
C3	0.0444 (11)	0.0439 (11)	0.0446 (12)	0.0037 (9)	0.0236 (9)	0.0112 (10)
C4	0.0288 (10)	0.0301 (9)	0.0312 (10)	0.0067 (7)	0.0086 (8)	0.0085 (8)
C5	0.0248 (9)	0.0309 (9)	0.0318 (10)	0.0033 (7)	0.0087 (8)	0.0066 (8)
N1	0.0375 (9)	0.0355 (9)	0.0317 (9)	0.0005 (7)	0.0088 (7)	0.0036 (7)
N2	0.0336 (8)	0.0403 (9)	0.0355 (9)	0.0017 (7)	0.0132 (7)	0.0055 (7)
N3	0.0373 (10)	0.0480 (11)	0.0388 (11)	−0.0092 (8)	0.0184 (8)	−0.0062 (9)
N4	0.0295 (8)	0.0374 (9)	0.0285 (8)	0.0037 (7)	0.0114 (7)	0.0043 (7)
O1W	0.0387 (9)	0.0457 (9)	0.0505 (9)	0.0026 (8)	0.0134 (7)	0.0097 (8)

Geometric parameters (Å, º)

C1—N1	1.335 (2)	C4—C5	1.487 (2)
C1—C2	1.366 (3)	C5—N4	1.296 (2)
C1—H1A	0.9300	C5—N3	1.336 (2)
C2—C3	1.361 (3)	N3—H3B	0.85 (2)
C2—H2A	0.9300	N3—H3C	0.89 (2)
C3—N2	1.325 (3)	N4—N4^{i}	1.407 (3)
C3—H3A	0.9300	O1W—H1WA	0.79 (3)
C4—N1	1.328 (2)	O1W—H1WB	0.91 (3)
C4—N2	1.339 (2)		
N1—C1—C2	122.40 (17)	N2—C4—C5	117.39 (15)
N1—C1—H1A	118.8	N4—C5—N3	125.86 (17)
C2—C1—H1A	118.8	N4—C5—C4	117.26 (15)
C3—C2—C1	116.68 (18)	N3—C5—C4	116.84 (16)
C3—C2—H2A	121.7	C4—N1—C1	116.03 (16)
C1—C2—H2A	121.7	C3—N2—C4	115.50 (16)
N2—C3—C2	123.30 (19)	C5—N3—H3B	116.4 (13)
N2—C3—H3A	118.4	C5—N3—H3C	119.7 (14)
C2—C3—H3A	118.4	H3B—N3—H3C	123.9 (19)
N1—C4—N2	126.04 (17)	C5—N4—N4^{i}	111.67 (16)
N1—C4—C5	116.56 (15)	H1WA—O1W—H1WB	108 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*B*···N1^{ii}	0.85 (2)	2.59 (2)	3.276 (2)	138.5 (16)

N3—H3*C*···O1*W*^{iii}	0.89 (2)	2.17 (3)	3.043 (3)	166.7 (19)
O1*W*—H1*WA*···N2^{iv}	0.79 (3)	2.20 (3)	2.979 (2)	168 (3)
O1*W*—H1*WB*···N4	0.91 (3)	2.16 (3)	3.055 (2)	172 (2)

Symmetry codes: (ii) $-x+2, -y+2, -z+2$; (iii) $x+1, y, z$; (iv) $-x, -y+1, -z+1$.