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4-Hydrazino-1-methylpyrazolo[3,4-*d*]-pyrimidine

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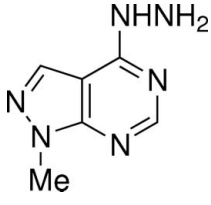
Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.006 Å; R factor = 0.065; wR factor = 0.159; data-to-parameter ratio = 7.1.

The title compound, $C_6H_8N_6$, crystallizes as an N—H···N hydrogen-bond-linked dimer of two almost identical molecules in the asymmetric unit. Both of the molecules are almost planar (rms deviations of 0.0186 and 0.0296 Å in the two molecules) and their hydrazino groups are turned towards the pyrazole rings. The dimers are arranged into chains *via* intermolecular N—H···N hydrogen bonds between the hydrazino groups and the N atoms of the pyrimidine rings of both types of the molecules, linking the molecules into a $C(7)$ graph-set motif along [100]. The methyl groups and the N atoms of the pyrazole rings form weak C—H···N hydrogen bonds, which connect chains of the dimers in a $C(4)$ motif parallel to [100].

Related literature

For recent reviews on the synthesis and biological activity of pyrazolo[3,4-*d*]pyrimidines, see: Caravatti *et al.* (2001); Dang (2002); Schenone *et al.* (2007); Schenone *et al.* (2008). The synthesis of the title compound was performed according to the procedure reported by Taylor & Loeffler (1960). For the crystal structure of 1-methyl-4-(2-methylhydrazino)pyrazolo-[3,4-*d*]pyrimidine, see: Hosmane *et al.* (1988). For the graph-set analysis of hydrogen bonding, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_6H_8N_6$
M_r = 164.18
Orthorhombic, $Pna2_1$
a = 14.086 (4) Å
b = 3.8756 (12) Å
c = 27.271 (8) Å
V = 1488.8 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 223 K
0.58 × 0.26 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.943, T_{max} = 0.990
8939 measured reflections
1715 independent reflections
1652 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.065
$wR(F^2)$ = 0.159
S = 1.21
1715 reflections
243 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12*B*···N1^{i}	0.97	2.65	3.297 (7)	124
C6—H6*C*···N7^{ii}	0.97	2.54	3.410 (7)	150
N11—H11*N*···N4	0.85 (6)	2.11 (6)	2.948 (6)	170 (5)
N5—H5*N*···N10	0.84 (7)	2.13 (7)	2.961 (6)	170 (5)
N12—H12*E*···N9^{iii}	0.97 (7)	2.56 (6)	3.125 (5)	117 (4)
N12—H12*D*···N9^{iv}	0.91 (6)	2.24 (6)	3.125 (6)	166 (5)
N6—H6*NB*···N3^{v}	0.89 (7)	2.59 (6)	3.251 (6)	131 (5)
N6—H6*NA*···N3^{vi}	0.86 (7)	2.30 (7)	3.149 (6)	168 (7)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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: JH2082).

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supplementary materials

Acta Cryst. (2009). E**65**, o1720-o1721 [**doi:10.1107/S1600536809023952**]

4-Hydrazino-1-methylpyrazolo[3,4-*d*]pyrimidine

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Comment

The pyrazolo[3,4-*d*]pyrimidine heterocyclic system is known to be a bioisoster of purine. Therefore, chemistry of pyrazolo[3,4-*d*]pyrimidines has received significant attention, particularly for the development of new biologically active substances (Caravatti *et al.*, 2001; Dang, 2002; Schenone *et al.*, 2007; Schenone *et al.*, 2008).

Herein, we report the crystal structure of 4-hydrazino-1-methylpyrazolo[3,4-*d*]pyrimidine, which was prepared *via* a reaction of 4-cyano-5-[(ethoxymethylene)amino]-1-methylpyrazole with hydrazine according to Taylor and Loeffler (1960) (Fig. 1). Theoretically, the compound might be involved in tautomerism with three tautomeric forms (Fig. 2). However, only one tautomeric form, similarly to previously reported 1-methyl-4-(2-methylhydrazino)pyrazolo[3,4-*d*]pyrimidine (Hosmane *et al.*, 1988), was found in the crystal.

The title compound crystallizes in asymmetric unit as a dimer of two almost identical molecules (Fig. 3). Both molecules are essentially planar except for the hydrazino groups, which are turned towards pyrazole ring making the torsion angles C2—C5—N5—N6 and C8—C11—N11—N12 equal to 4.1 (7)° and 4.0 (7)°, respectively. The geometry of the molecule as well as 1.348 (6) Å and 1.332 (5) Å distances of C5—N5 and C11—N11 bonds indicate delocalization of the electron pairs of N5 and N11 with the pyrazolo[3,4-*d*]pyrimidine aromatic system.

In the crystal, the dimer molecules are linked in a $R^2_2(8)$ graph-set motif (Bernstein *et al.*, 1995) by the N—H···N hydrogen bonds (Fig. 4, Table 1). The dimers are arranged into chains *via* intermolecular N—H···N hydrogen bonds between the hydrazino groups and the nitrogen atoms of the pyrimidine rings of both type of the molecules linking them with symmetry-related molecules in a *C*(7) graph-set motif along the [100] direction. The interactions between pyrimidine rings and hydrazino groups make a $R^4_4(14)$ hydrogen bond motif of the fourth order. The methyl groups and the nitrogen atoms of the pyrazole rings form weak C—H···N hydrogen bonds connecting chains of the dimers in a *C*(4) motif parallel to the [100]) direction.

Experimental

4-Hydrazino-1-methylpyrazolo[3,4-*d*]pyrimidine was synthesized by cyclocondensation of 4-cyano-5-[(ethoxymethylene)amino]-1-methylpyrazole with hydrazine according to the procedure reported by Taylor and Loeffler (1960). Single crystals suitable for crystallographic analysis were grown by recrystallization from ethanol.

Refinement

All the H atoms attached to the carbon atoms were constrained in a riding motion approximation [0.94 Å for C_{aryl}—H and 0.97 Å for methyl groups; $U_{iso}(H) = 1.2U_{eq}(C_{aryl})$ and $U_{iso}(H) = 1.5U_{eq}(C_{methyl})$] while the N-bound H atoms were located in a difference map and refined freely. Friedel pairs were merged.

Figures

Fig. 1. The synthesis of 4-hydrazino-1-methylpyrazolo[3,4-*d*]pyrimidine

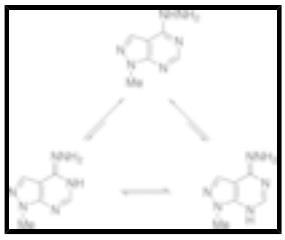

Fig. 2. The hydrazino-hydrazono tautomerism in the title compound

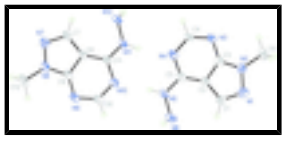

Fig. 3. The molecular structure of 4-hydrazino-1-methylpyrazolo[3,4-*d*]pyrimidine with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

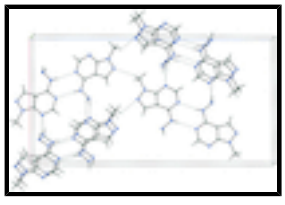

Fig. 4. Molecular parking in the crystal, viewed along the *b* axis.

4-Hydrazino-1-methylpyrazolo[3,4-*d*]pyrimidine

Crystal data

$C_6H_8N_6$	D_x = 1.465 Mg m^{-3}
M_r = 164.18	Melting point: 514 K
Orthorhombic, *Pna*2$_1$	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: P 2c -2n	Cell parameters from 3657 reflections
a = 14.086 (4) Å	θ = 2.9–27.2º
b = 3.8756 (12) Å	μ = 0.10 mm^{-1}
c = 27.271 (8) Å	*T* = 223 K
V = 1488.8 (8) Å^3	Block, colourless
Z = 8	0.58 × 0.26 × 0.10 mm
F_{000} = 688	

Data collection

Bruker SMART APEX CCD diffractometer	1715 independent reflections
Radiation source: fine-focus sealed tube	1652 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.051
T = 223 K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	*h* = −18→18

T_{min} = 0.943, T_{max} = 0.990
8939 measured reflections
$k = -5 \rightarrow 4$
$l = -24 \rightarrow 35$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.159$
$S = 1.21$
1715 reflections
243 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0699P)^2 + 1.3392P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
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 $F^2 > \sigma(F^2)$ 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	0.4891 (3)	0.4783 (12)	0.43889 (16)	0.0351 (9)
N2	0.4203 (3)	0.6408 (11)	0.46578 (15)	0.0307 (9)
N3	0.3922 (2)	0.8124 (10)	0.54938 (15)	0.0273 (9)
N4	0.5189 (3)	0.6416 (10)	0.60298 (15)	0.0281 (8)
N5	0.6553 (3)	0.3740 (12)	0.57903 (17)	0.0321 (9)
H5N	0.668 (4)	0.343 (14)	0.609 (2)	0.030 (14)*
N6	0.7119 (3)	0.2094 (13)	0.54313 (18)	0.0348 (10)
H6NA	0.764 (5)	0.32 (2)	0.549 (3)	0.05 (2)*
H6NB	0.731 (4)	0.007 (19)	0.555 (2)	0.037 (16)*
N7	0.7580 (3)	0.6324 (11)	0.84251 (15)	0.0335 (9)
N8	0.8271 (3)	0.4576 (10)	0.81702 (14)	0.0297 (9)
N9	0.8504 (2)	0.2236 (10)	0.73690 (15)	0.0274 (9)
N10	0.7183 (3)	0.3347 (11)	0.68245 (15)	0.0281 (8)
N11	0.5809 (2)	0.5994 (12)	0.70605 (16)	0.0300 (9)

H11N	0.566 (4)	0.587 (14)	0.676 (2)	0.025 (13)*
N12	0.5243 (3)	0.7763 (12)	0.74061 (17)	0.0292 (9)
H12D	0.469 (4)	0.656 (15)	0.743 (2)	0.030 (14)*
H12E	0.518 (4)	1.019 (18)	0.732 (2)	0.037 (15)*
C1	0.5567 (3)	0.3971 (14)	0.47002 (17)	0.0310 (10)
H1	0.6128	0.2804	0.4616	0.037*
C2	0.5337 (3)	0.5087 (12)	0.51798 (17)	0.0242 (9)
C3	0.4448 (3)	0.6664 (12)	0.51286 (17)	0.0247 (9)
C4	0.4345 (3)	0.7879 (13)	0.59211 (18)	0.0280 (10)
H4	0.4016	0.8853	0.6187	0.034*
C5	0.5701 (3)	0.5040 (12)	0.56624 (17)	0.0253 (9)
C6	0.3354 (4)	0.7825 (17)	0.4417 (2)	0.0425 (13)
H6A	0.3540	0.9659	0.4195	0.064*
H6B	0.2925	0.8736	0.4663	0.064*
H6C	0.3038	0.6013	0.4234	0.064*
C9	0.7999 (3)	0.3896 (12)	0.77082 (18)	0.0242 (9)
C7	0.6873 (3)	0.6765 (13)	0.81121 (18)	0.0309 (10)
H7	0.6305	0.7923	0.8187	0.037*
C8	0.7076 (3)	0.5295 (12)	0.76570 (18)	0.0239 (9)
C10	0.8039 (3)	0.2142 (13)	0.69443 (18)	0.0282 (10)
H10	0.8367	0.1051	0.6687	0.034*
C11	0.6678 (3)	0.4953 (12)	0.71848 (16)	0.0242 (9)
C12	0.9129 (4)	0.3412 (17)	0.8420 (2)	0.0430 (14)
H12A	0.9554	0.2352	0.8184	0.065*
H12B	0.8962	0.1739	0.8670	0.065*
H12C	0.9442	0.5369	0.8571	0.065*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0288 (19)	0.046 (2)	0.031 (2)	−0.0051 (18)	0.0019 (17)	−0.0057 (19)
N2	0.0226 (18)	0.042 (2)	0.027 (2)	−0.0047 (16)	−0.0017 (15)	0.0028 (18)
N3	0.0193 (16)	0.030 (2)	0.032 (2)	0.0040 (15)	−0.0007 (16)	−0.0014 (16)
N4	0.0202 (18)	0.034 (2)	0.030 (2)	−0.0008 (15)	−0.0005 (14)	−0.0005 (17)
N5	0.0208 (17)	0.046 (3)	0.029 (2)	0.0086 (17)	−0.0004 (16)	0.0020 (19)
N6	0.0206 (19)	0.036 (3)	0.048 (3)	0.0011 (18)	0.0044 (18)	−0.001 (2)
N7	0.0301 (19)	0.039 (2)	0.031 (2)	0.0009 (18)	−0.0001 (16)	0.0056 (18)
N8	0.0227 (17)	0.035 (2)	0.031 (2)	−0.0009 (15)	−0.0055 (16)	0.0078 (17)
N9	0.0163 (16)	0.0300 (19)	0.036 (2)	−0.0027 (15)	0.0012 (15)	0.0041 (17)
N10	0.0222 (17)	0.035 (2)	0.0272 (19)	0.0039 (15)	−0.0023 (15)	0.0049 (17)
N11	0.0158 (17)	0.046 (2)	0.028 (2)	0.0042 (16)	−0.0029 (15)	−0.0013 (18)
N12	0.0126 (16)	0.036 (2)	0.039 (2)	0.0009 (16)	−0.0018 (15)	−0.0010 (19)
C1	0.023 (2)	0.043 (3)	0.027 (2)	−0.005 (2)	0.0039 (19)	0.002 (2)
C2	0.0166 (18)	0.028 (2)	0.029 (2)	−0.0044 (17)	0.0037 (16)	0.0003 (18)
C3	0.020 (2)	0.025 (2)	0.029 (2)	−0.0086 (16)	−0.0021 (17)	0.0052 (18)
C4	0.0210 (19)	0.035 (3)	0.029 (2)	0.0055 (18)	0.0048 (18)	0.0001 (18)
C5	0.0191 (17)	0.024 (2)	0.033 (2)	−0.0056 (15)	0.0011 (16)	0.0043 (17)
C6	0.032 (3)	0.058 (4)	0.037 (3)	0.001 (2)	−0.015 (2)	−0.001 (3)

C9	0.0162 (17)	0.023 (2)	0.033 (2)	−0.0034 (16)	−0.0032 (17)	0.0062 (18)
C7	0.0192 (19)	0.039 (3)	0.035 (2)	−0.0018 (18)	−0.0007 (19)	0.006 (2)
C8	0.0158 (17)	0.025 (2)	0.031 (2)	−0.0027 (15)	0.0003 (17)	0.0072 (18)
C10	0.022 (2)	0.035 (2)	0.028 (2)	−0.0029 (18)	0.0048 (18)	0.0010 (19)
C11	0.0145 (17)	0.031 (2)	0.027 (2)	−0.0012 (16)	−0.0001 (16)	0.0029 (18)
C12	0.029 (2)	0.056 (3)	0.044 (3)	0.005 (2)	−0.018 (2)	0.010 (3)

Geometric parameters (Å, °)

N1—C1	1.314 (7)	N11—C11	1.332 (5)
N1—N2	1.369 (6)	N11—N12	1.412 (6)
N2—C3	1.333 (6)	N11—H11N	0.85 (6)
N2—C6	1.470 (6)	N12—H12D	0.91 (6)
N3—C4	1.312 (6)	N12—H12E	0.97 (7)
N3—C3	1.364 (6)	C1—C2	1.415 (7)
N4—C5	1.345 (6)	C1—H1	0.9400
N4—C4	1.350 (6)	C2—C3	1.401 (6)
N5—C5	1.348 (6)	C2—C5	1.413 (6)
N5—N6	1.415 (6)	C4—H4	0.9400
N5—H5N	0.84 (7)	C6—H6A	0.9700
N6—H6NA	0.86 (7)	C6—H6B	0.9700
N6—H6NB	0.89 (7)	C6—H6C	0.9700
N7—C7	1.322 (6)	C9—C8	1.415 (5)
N7—N8	1.375 (6)	C7—C8	1.395 (7)
N8—C9	1.343 (6)	C7—H7	0.9400
N8—C12	1.458 (6)	C8—C11	1.411 (6)
N9—C10	1.331 (6)	C10—H10	0.9400
N9—C9	1.332 (6)	C12—H12A	0.9700
N10—C10	1.334 (6)	C12—H12B	0.9700
N10—C11	1.364 (6)	C12—H12C	0.9700
C1—N1—N2	106.1 (4)	N3—C4—N4	128.7 (4)
C3—N2—N1	111.5 (4)	N3—C4—H4	115.7
C3—N2—C6	127.8 (4)	N4—C4—H4	115.7
N1—N2—C6	120.5 (4)	N4—C5—N5	115.7 (4)
C4—N3—C3	111.9 (4)	N4—C5—C2	119.6 (4)
C5—N4—C4	118.4 (4)	N5—C5—C2	124.7 (4)
C5—N5—N6	119.4 (4)	N2—C6—H6A	109.5
C5—N5—H5N	120 (4)	N2—C6—H6B	109.5
N6—N5—H5N	119 (4)	H6A—C6—H6B	109.5
N5—N6—H6NA	97 (5)	N2—C6—H6C	109.5
N5—N6—H6NB	108 (4)	H6A—C6—H6C	109.5
H6NA—N6—H6NB	97 (6)	H6B—C6—H6C	109.5
C7—N7—N8	105.7 (4)	N9—C9—N8	126.4 (4)
C9—N8—N7	111.6 (4)	N9—C9—C8	127.3 (4)
C9—N8—C12	127.8 (4)	N8—C9—C8	106.2 (4)
N7—N8—C12	120.2 (4)	N7—C7—C8	111.6 (4)
C10—N9—C9	110.8 (4)	N7—C7—H7	124.2
C10—N10—C11	117.1 (4)	C8—C7—H7	124.2
C11—N11—N12	119.7 (4)	C7—C8—C11	140.2 (4)

C11—N11—H11N	118 (3)	C7—C8—C9	104.9 (4)
N12—N11—H11N	122 (4)	C11—C8—C9	114.8 (4)
N11—N12—H12D	107 (4)	N9—C10—N10	130.4 (5)
N11—N12—H12E	111 (4)	N9—C10—H10	114.8
H12D—N12—H12E	116 (5)	N10—C10—H10	114.8
N1—C1—C2	111.0 (4)	N11—C11—N10	115.7 (4)
N1—C1—H1	124.5	N11—C11—C8	124.7 (4)
C2—C1—H1	124.5	N10—C11—C8	119.5 (4)
C3—C2—C5	115.0 (4)	N8—C12—H12A	109.5
C3—C2—C1	104.2 (4)	N8—C12—H12B	109.5
C5—C2—C1	140.7 (4)	H12A—C12—H12B	109.5
N2—C3—N3	126.4 (4)	N8—C12—H12C	109.5
N2—C3—C2	107.2 (4)	H12A—C12—H12C	109.5
N3—C3—C2	126.4 (4)	H12B—C12—H12C	109.5
C1—N1—N2—C3	1.0 (5)	C3—C2—C5—N5	−178.1 (4)
C1—N1—N2—C6	177.0 (4)	C1—C2—C5—N5	3.4 (9)
C7—N7—N8—C9	−0.8 (5)	C10—N9—C9—N8	−177.2 (4)
C7—N7—N8—C12	−175.0 (4)	C10—N9—C9—C8	2.7 (6)
N2—N1—C1—C2	−0.6 (6)	N7—N8—C9—N9	−179.8 (4)
N1—C1—C2—C3	0.1 (6)	C12—N8—C9—N9	−6.0 (7)
N1—C1—C2—C5	178.6 (5)	N7—N8—C9—C8	0.3 (5)
N1—N2—C3—N3	−179.7 (4)	C12—N8—C9—C8	174.0 (5)
C6—N2—C3—N3	4.7 (8)	N8—N7—C7—C8	1.0 (6)
N1—N2—C3—C2	−0.9 (5)	N7—C7—C8—C11	−177.1 (5)
C6—N2—C3—C2	−176.6 (5)	N7—C7—C8—C9	−0.8 (6)
C4—N3—C3—N2	178.0 (4)	N9—C9—C8—C7	−179.7 (4)
C4—N3—C3—C2	−0.5 (6)	N8—C9—C8—C7	0.3 (5)
C5—C2—C3—N2	−178.5 (4)	N9—C9—C8—C11	−2.3 (7)
C1—C2—C3—N2	0.5 (5)	N8—C9—C8—C11	177.7 (4)
C5—C2—C3—N3	0.3 (6)	C9—N9—C10—N10	−1.5 (7)
C1—C2—C3—N3	179.3 (4)	C11—N10—C10—N9	0.0 (7)
C3—N3—C4—N4	−0.3 (7)	N12—N11—C11—N10	−178.3 (4)
C5—N4—C4—N3	1.3 (8)	N12—N11—C11—C8	4.0 (7)
C4—N4—C5—N5	177.5 (4)	C10—N10—C11—N11	−177.1 (4)
C4—N4—C5—C2	−1.5 (6)	C10—N10—C11—C8	0.6 (6)
N6—N5—C5—N4	176.9 (4)	C7—C8—C11—N11	−6.0 (9)
N6—N5—C5—C2	−4.1 (7)	C9—C8—C11—N11	177.9 (4)
C3—C2—C5—N4	0.8 (6)	C7—C8—C11—N10	176.4 (5)
C1—C2—C5—N4	−177.7 (6)	C9—C8—C11—N10	0.4 (6)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12B···N1^{i}	0.97	2.65	3.297 (7)	124
C6—H6C···N7^{ii}	0.97	2.54	3.410 (7)	150
N11—H11N···N4	0.85 (6)	2.11 (6)	2.948 (6)	170 (5)
N5—H5N···N10	0.84 (7)	2.13 (7)	2.961 (6)	170 (5)
N12—H12E···N9^{iii}	0.97 (7)	2.56 (6)	3.125 (5)	117 (4)

N12—H12D···N9^{iv}	0.91 (6)	2.24 (6)	3.125 (6)	166 (5)
N6—H6NB···N3^{v}	0.89 (7)	2.59 (6)	3.251 (6)	131 (5)
N6—H6NA···N3^{vi}	0.86 (7)	2.30 (7)	3.149 (6)	168 (7)

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

Fig. 1

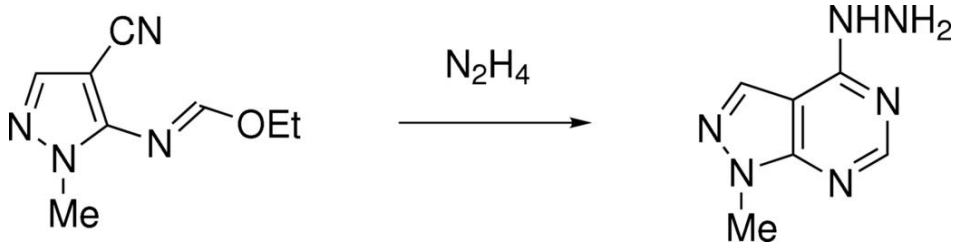

Fig. 2

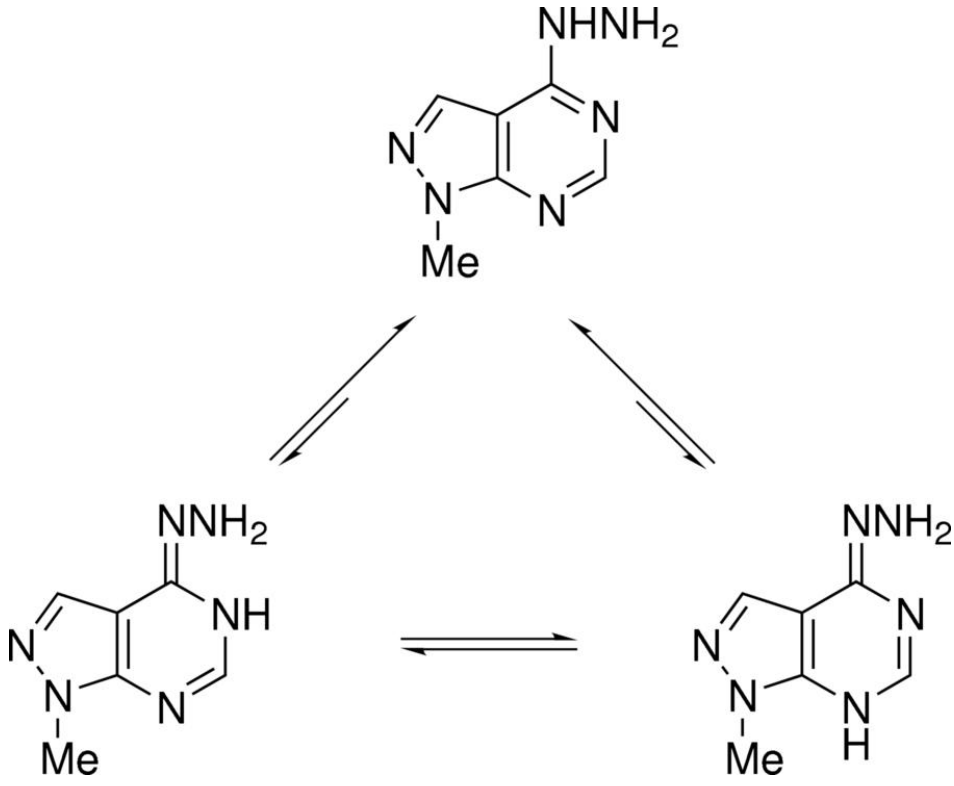

Fig. 3

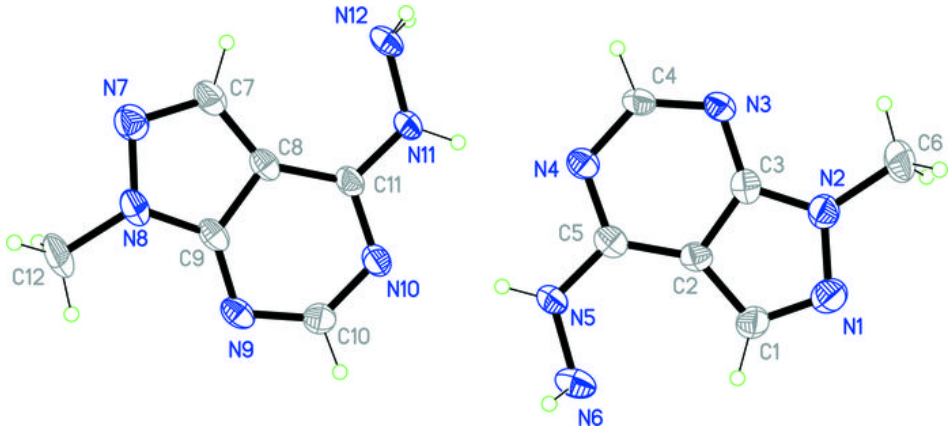
N12
N7
C7
C8
N11
C11
N8
C9
N10
C12
N9
C10
C4
N3
C6
N4
C3
N2
C5
C2
N5
N1
C1
N6

Fig. 4