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2-(4*H*-1,2,4-Triazol-4-yl)pyrimidine

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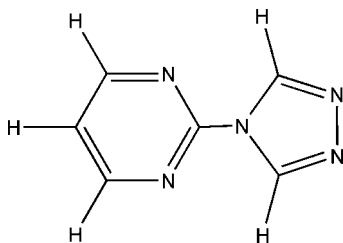
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.035; wR factor = 0.101; data-to-parameter ratio = 11.5.The title compound, $\text{C}_6\text{H}_5\text{N}_5$, is almost planar, the triazole and pyrimidine rings forming a dihedral angle of 2.9 (13)°.

Related literature

For the synthesis of the title compound, see: Wiley & Hart (1953). For properties of related compounds, see: Haasnoot (2000).



Experimental

Crystal data

 $\text{C}_6\text{H}_5\text{N}_5$ $M_r = 147.15$ Triclinic, $P\bar{1}$ $a = 5.6929$ (10) Å $b = 7.7355$ (14) Å $c = 8.6102$ (15) Å $\alpha = 67.233$ (2)° $\beta = 80.755$ (2)° $\gamma = 69.837$ (2)° $V = 328.04$ (10) Å³ $Z = 2$ Mo $K\alpha$ radiation $\mu = 0.10$ mm⁻¹ $T = 293$ K $0.46 \times 0.34 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\min} = 0.954$, $T_{\max} = 0.988$

1803 measured reflections

1154 independent reflections

916 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.010$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.035$ $wR(F^2) = 0.101$ $S = 1.03$

1154 reflections

100 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.11$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.17$ e Å⁻³

Data collection: SMART (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AA2030).

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supplementary materials

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2-(4*H*-1,2,4-Triazol-4-yl)pyrimidine

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Comment

Many molecular compounds exhibit interesting magnetic and luminescent properties (Haasnoot, 2000). One of the requirements for possessing such macroscopic properties is to create interactions between the molecular units and the active sites within the crystal lattices. 1,2,4-Triazole and its derivatives are interesting bridging ligands. In the title compound the triazole and the pyrimidine rings are almost in the same plane, the dihedral angles between them is 2.9 (13)°.

Experimental

A mixture of 1.2 g (0.012 mol) of pyrimidin-2-amine and 2.0 g (0.011 mol) of diformylhydrazine was heated slowly to 160–170 °C for 30 min. The crystals, which separated on cooling, were collected and recrystallized from water and acetonitrile and dried on air. Yield 0.7 g (43%). Anal. Calc. for C₆H₅N₅ (%): C, 50.52; H, 5.30; N 44.18. Found (%): C, 50.59; H, 5.36; N 44.23.

Refinement

Hydrogen atoms were included into calculated positions and refined as riding on the C atoms with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5 U_{\text{eq}}(\text{C})$. Friedel pairs were averaged for the data used on the final cycles of the refinement.

Figures

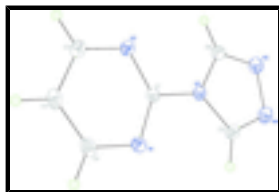


Fig. 1. An ORTEP-3 view of the title compound with the displacement ellipsoids shown on 30% probability level.

2-(4*H*-1,2,4-Triazol-4-yl)pyrimidine

Crystal data

C₆H₅N₅

$M_r = 147.15$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 5.6929$ (10) Å

$Z = 2$

$F(000) = 152$

$D_x = 1.490$ Mg m⁻³

$D_m = 1.490$ Mg m⁻³

D_m measured by not measured

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 786 reflections

supplementary materials

$b = 7.7355 (14) \text{ \AA}$	$\theta = 2.6\text{--}25.9^\circ$
$c = 8.6102 (15) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$\alpha = 67.233 (2)^\circ$	$T = 293 \text{ K}$
$\beta = 80.755 (2)^\circ$	Sheet, colourless
$\gamma = 69.837 (2)^\circ$	$0.46 \times 0.34 \times 0.12 \text{ mm}$
$V = 328.04 (10) \text{ \AA}^3$	

Data collection

Bruker SMART CCD area-detector diffractometer	1154 independent reflections
Radiation source: fine-focus sealed tube graphite	916 reflections with $I > 2\sigma(I)$
phi and ω scans	$R_{\text{int}} = 0.010$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{\text{max}} = 25.0^\circ, \theta_{\text{min}} = 2.6^\circ$
$T_{\text{min}} = 0.954, T_{\text{max}} = 0.988$	$h = -6 \rightarrow 6$
1803 measured reflections	$k = -9 \rightarrow 6$
	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.035$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.101$	H-atom parameters constrained
$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.0595P)^2 + 0.0336P]$
1154 reflections	where $P = (F_o^2 + 2F_c^2)/3$
100 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.11 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 (\AA^2)

x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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N1	0.5226 (2)	0.81660 (19)	0.85375 (15)	0.0447 (4)
N2	0.2458 (2)	0.66148 (18)	0.82287 (15)	0.0450 (4)
N3	0.20693 (19)	0.75348 (16)	1.05328 (14)	0.0371 (3)
N4	0.0968 (3)	0.8138 (2)	1.28772 (16)	0.0564 (4)
N5	-0.0695 (2)	0.7314 (2)	1.26282 (16)	0.0543 (4)
C1	0.3340 (2)	0.74312 (19)	0.89977 (17)	0.0349 (3)
C2	0.3638 (3)	0.6558 (2)	0.6765 (2)	0.0526 (4)
H2	0.3095	0.6009	0.6157	0.063*
C3	0.5620 (3)	0.7281 (2)	0.61289 (19)	0.0525 (4)
H3	0.6422	0.7236	0.5109	0.063*
C4	0.6357 (3)	0.8070 (2)	0.7069 (2)	0.0511 (4)
H4	0.7702	0.8562	0.6671	0.061*
C5	0.2575 (3)	0.8247 (2)	1.16196 (19)	0.0483 (4)
H5	0.3898	0.8746	1.1478	0.058*
C6	0.0005 (3)	0.6975 (2)	1.12413 (19)	0.0464 (4)
H6	-0.0795	0.6422	1.0787	0.056*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0397 (6)	0.0550 (8)	0.0439 (7)	-0.0210 (6)	0.0051 (5)	-0.0192 (6)
N2	0.0507 (7)	0.0556 (8)	0.0394 (7)	-0.0242 (6)	0.0061 (5)	-0.0245 (6)
N3	0.0385 (6)	0.0415 (7)	0.0347 (7)	-0.0148 (5)	0.0037 (5)	-0.0172 (5)
N4	0.0665 (9)	0.0667 (9)	0.0457 (8)	-0.0241 (7)	0.0086 (6)	-0.0314 (7)
N5	0.0534 (8)	0.0674 (10)	0.0471 (8)	-0.0232 (7)	0.0136 (6)	-0.0278 (7)
C1	0.0347 (7)	0.0347 (8)	0.0336 (7)	-0.0089 (6)	0.0000 (5)	-0.0126 (6)
C2	0.0641 (10)	0.0598 (10)	0.0415 (9)	-0.0213 (8)	0.0045 (7)	-0.0266 (8)
C3	0.0561 (10)	0.0581 (10)	0.0371 (9)	-0.0134 (8)	0.0107 (7)	-0.0190 (8)
C4	0.0415 (8)	0.0609 (10)	0.0456 (9)	-0.0190 (8)	0.0097 (7)	-0.0151 (8)
C5	0.0556 (9)	0.0580 (10)	0.0448 (9)	-0.0256 (8)	0.0040 (7)	-0.0278 (8)
C6	0.0430 (8)	0.0593 (10)	0.0449 (9)	-0.0233 (7)	0.0090 (6)	-0.0245 (7)

Geometric parameters (\AA , $^\circ$)

N1—C1	1.3199 (18)	N5—C6	1.2927 (19)
N1—C4	1.3407 (19)	C2—C3	1.373 (2)
N2—C1	1.3185 (18)	C2—H2	0.9300
N2—C2	1.3386 (18)	C3—C4	1.368 (2)
N3—C6	1.3624 (18)	C3—H3	0.9300
N3—C5	1.3629 (18)	C4—H4	0.9300
N3—C1	1.4184 (17)	C5—H5	0.9300
N4—C5	1.2965 (19)	C6—H6	0.9300
N4—N5	1.3915 (19)		
C1—N1—C4	114.10 (13)	C4—C3—C2	116.74 (14)
C1—N2—C2	114.64 (13)	C4—C3—H3	121.6
C6—N3—C5	103.94 (12)	C2—C3—H3	121.6
C6—N3—C1	127.43 (12)	N1—C4—C3	122.95 (14)
C5—N3—C1	128.61 (12)	N1—C4—H4	118.5

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C5—N4—N5	106.86 (12)	C3—C4—H4	118.5
C6—N5—N4	107.05 (12)	N4—C5—N3	111.03 (13)
N2—C1—N1	129.15 (13)	N4—C5—H5	124.5
N2—C1—N3	115.06 (12)	N3—C5—H5	124.5
N1—C1—N3	115.79 (12)	N5—C6—N3	111.12 (13)
N2—C2—C3	122.41 (14)	N5—C6—H6	124.4
N2—C2—H2	118.8	N3—C6—H6	124.4
C3—C2—H2	118.8		
C5—N4—N5—C6	0.04 (17)	N2—C2—C3—C4	0.2 (2)
C2—N2—C1—N1	-1.0 (2)	C1—N1—C4—C3	0.0 (2)
C2—N2—C1—N3	178.77 (12)	C2—C3—C4—N1	-0.4 (2)
C4—N1—C1—N2	0.8 (2)	N5—N4—C5—N3	0.04 (18)
C4—N1—C1—N3	-179.02 (12)	C6—N3—C5—N4	-0.10 (17)
C6—N3—C1—N2	-3.3 (2)	C1—N3—C5—N4	178.59 (13)
C5—N3—C1—N2	178.33 (13)	N4—N5—C6—N3	-0.11 (17)
C6—N3—C1—N1	176.55 (13)	C5—N3—C6—N5	0.13 (17)
C5—N3—C1—N1	-1.8 (2)	C1—N3—C6—N5	-178.59 (13)
C1—N2—C2—C3	0.5 (2)		

Fig. 1

