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N-(3,5-Dimethylpyrazol-1-ylmethyl)-pyridin-2-ylamine

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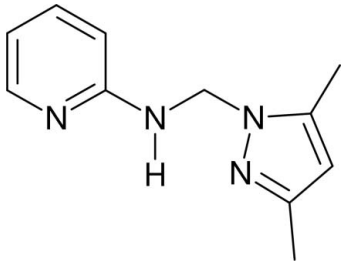
Key indicators: single-crystal X-ray study; T = 300 K; mean σ(C–C) = 0.002 Å; R factor = 0.045; wR factor = 0.136; data-to-parameter ratio = 18.4.

In the title compound, $C_{11}H_{14}N_4$, the dihedral angle between the ring planes is 74.76 (8)°. In the crystal structure, N—H···N hydrogen bonds result in centrosymmetric dimers.

Related literature

For related literature, see: Baldy *et al.* (1985); Sorrell *et al.* (1987); Touzani *et al.* (2003).



Experimental

Crystal data

$C_{11}H_{14}N_4$
M_r = 202.26
Triclinic, $P\overline{1}$
a = 8.4299 (13) Å
b = 8.5720 (14) Å
c = 9.1803 (15) Å
α = 70.283 (3)°
β = 89.506 (3)°
γ = 61.056 (2)°
V = 536.77 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 300 (2) K
0.50 × 0.30 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
8403 measured reflections
2614 independent reflections
2265 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.136
S = 1.06
2614 reflections
142 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···N2^{i}	0.886 (17)	2.177 (17)	3.0524 (17)	169.8 (15)

Symmetry code: (i) $-x, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2504).

References

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Sorrell, T. N., Shen, C. C. & O'Connor, C. J. (1987). *Inorg. Chem.* **26**, 1755–1758.
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supplementary materials

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N-(3,5-Dimethylpyrazol-1-ylmethyl)pyridin-2-ylamine

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Comment

Polypyrazolyl-containing ligands are used in models for copper proteins to mimic active sites (Sorrell *et al.*, 1987). As part of our studies in this area, we prepared the title compound, (I), which contains amine, pyrazolyl and pyridyl functionalities.

The molecule of (I) is not planar (Fig. 1), the dihedral angle between the aromatic ring planes being 74.76 (8)°. Slight differences between (I) and the known 3,5-dimethylpyrazole, (II), (Baldy *et al.*, 1985) are reflected in the C3—N1 bond length, the angle C3—N1—N2 and the torsion angle C2—C1—N2—N1. These have the values 1.3557 (14) Å, 112.17 (8)° and −0.35 (2)° in (I) and 1.3442 (16) Å, 108.64 (9)° and 0.45 (16)° in (II), respectively.

The packing in (I) is consolidated by N—H···N hydrogen bonds (Table 1) resulting in centrosymmetric dimers (Fig. 2).

Experimental

Compound (I) was made by the method of Touzani *et al.* (2003) from a mixture of 0.941 g (10 mmol) of 2-aminopyridine and 2.522 g (20 mmol) of (3,5-Dimethyl-pyrazol-1-yl)-methanol.

Refinement

The N-bound H atom was located in a differnce map and freely refined. The C-bound H atoms were geometrically placed and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

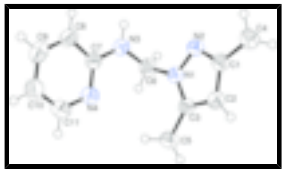

Fig. 1. View of the molecular structure of (I) showing 50% displacement ellispoids and arbitrary spheres for the H atoms.

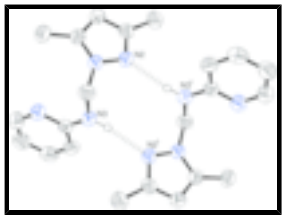

Fig. 2. A centrosymmetric dimer of (I) linked by N—H···N hydrogen bonds (double dashed lines). All H atoms except H3a omitted for clarity. Symmetry code as in Table 1.

N-(3,5-Dimethylpyrazol-1-ylmethyl)pyridin-2-ylamine

Crystal data

$C_{11}H_{14}N_4$	$V = 536.77\ (15)$ Å^3
$M_r = 202.26$	$Z = 2$
Triclinic, $P\overline{1}$	$F_{000} = 216$
Hall symbol: -P 1	$D_x = 1.251$ Mg m^{-3}
$a = 8.4299\ (13)$ Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 8.5720\ (14)$ Å	$\mu = 0.08$ mm^{-1}
$c = 9.1803\ (15)$ Å	$T = 300\ (2)$ K
$\alpha = 70.283\ (3)^o$	Prism, colourless
$\beta = 89.506\ (3)^o$	0.50 × 0.30 × 0.30 mm
$\gamma = 61.056\ (2)^o$	

Data collection

Bruker SMART CCD area-detector diffractometer	2265 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.042$
Monochromator: graphite	$\theta_{max} = 28.3^o$
$T = 300(2)$ K	$\theta_{min} = 2.4^o$
ω scans	$h = -11 \rightarrow 11$
Absorption correction: none	$k = -11 \rightarrow 11$
8403 measured reflections	$l = -12 \rightarrow 12$
2614 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difmap and geom
$R[F^2 > 2\sigma(F^2)] = 0.045$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.136$	$w = 1/[\sigma^2(F_o^2) + (0.0764P)^2 + 0.0625P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
2614 reflections	$\Delta\rho_{max} = 0.18$ e Å^{-3}
142 parameters	$\Delta\rho_{min} = -0.21$ 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	0.10021 (13)	0.48900 (13)	0.77976 (10)	0.0416 (2)
C1	0.18977 (15)	0.18891 (16)	0.87738 (13)	0.0438 (3)
N2	0.08931 (13)	0.34849 (14)	0.75052 (11)	0.0445 (2)
C2	0.26401 (16)	0.22673 (17)	0.98808 (13)	0.0461 (3)
H2A	0.3382	0.1389	1.0861	0.055*
N3	0.06940 (16)	0.70247 (16)	0.51613 (12)	0.0521 (3)
H3A	0.030 (2)	0.672 (2)	0.4467 (19)	0.060 (4)*
C3	0.20498 (15)	0.42005 (17)	0.92246 (12)	0.0419 (3)
N4	0.28260 (16)	0.76674 (16)	0.59911 (12)	0.0522 (3)
C4	0.2099 (2)	0.00185 (19)	0.88881 (17)	0.0576 (3)
H4A	0.1581	0.0163	0.7891	0.086*
H4B	0.1462	−0.0351	0.9682	0.086*
H4C	0.3383	−0.0958	0.9164	0.086*
C5	0.24125 (19)	0.5422 (2)	0.98353 (16)	0.0543 (3)
H5A	0.2914	0.6065	0.9084	0.082*
H5B	0.3279	0.4626	1.0814	0.082*
H5C	0.1279	0.6363	1.0002	0.082*
C6	0.00114 (16)	0.68493 (17)	0.65997 (14)	0.0486 (3)
H6A	−0.1283	0.7257	0.6382	0.058*
H6B	0.0100	0.7711	0.7016	0.058*
C7	0.21626 (16)	0.72951 (15)	0.49199 (12)	0.0440 (3)
C8	0.29132 (19)	0.71889 (18)	0.35594 (14)	0.0526 (3)
H8A	0.2427	0.6925	0.2829	0.063*
C9	0.4366 (2)	0.74785 (19)	0.33276 (16)	0.0594 (3)
H9A	0.4893	0.7396	0.2442	0.071*
C10	0.5052 (2)	0.7897 (2)	0.44195 (18)	0.0627 (4)
H10A	0.6030	0.8118	0.4281	0.075*
C11	0.4238 (2)	0.7973 (2)	0.57054 (17)	0.0607 (3)
H11A	0.4695	0.8258	0.6437	0.073*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0475 (5)	0.0452 (5)	0.0381 (5)	−0.0274 (4)	0.0095 (4)	−0.0170 (4)
C1	0.0472 (5)	0.0465 (6)	0.0436 (5)	−0.0269 (5)	0.0140 (4)	−0.0193 (5)
N2	0.0526 (5)	0.0507 (5)	0.0412 (5)	−0.0321 (4)	0.0111 (4)	−0.0208 (4)
C2	0.0489 (6)	0.0489 (6)	0.0400 (5)	−0.0261 (5)	0.0066 (4)	−0.0145 (5)

N3	0.0675 (6)	0.0596 (6)	0.0377 (5)	−0.0414 (5)	0.0050 (4)	−0.0141 (5)
C3	0.0431 (5)	0.0514 (6)	0.0385 (5)	−0.0276 (5)	0.0118 (4)	−0.0202 (5)
N4	0.0662 (6)	0.0564 (6)	0.0467 (5)	−0.0383 (5)	0.0119 (5)	−0.0227 (5)
C4	0.0681 (8)	0.0502 (7)	0.0617 (8)	−0.0341 (6)	0.0133 (6)	−0.0233 (6)
C5	0.0630 (7)	0.0629 (7)	0.0522 (7)	−0.0390 (6)	0.0108 (5)	−0.0282 (6)
C6	0.0477 (6)	0.0457 (6)	0.0485 (6)	−0.0235 (5)	0.0066 (5)	−0.0141 (5)
C7	0.0559 (6)	0.0361 (5)	0.0367 (5)	−0.0243 (5)	0.0041 (4)	−0.0089 (4)
C8	0.0685 (7)	0.0492 (6)	0.0384 (6)	−0.0302 (6)	0.0076 (5)	−0.0146 (5)
C9	0.0670 (8)	0.0547 (7)	0.0481 (7)	−0.0290 (6)	0.0171 (6)	−0.0138 (6)
C10	0.0623 (8)	0.0638 (8)	0.0636 (8)	−0.0387 (7)	0.0131 (6)	−0.0159 (7)
C11	0.0717 (8)	0.0675 (8)	0.0585 (8)	−0.0459 (7)	0.0094 (6)	−0.0252 (7)

Geometric parameters (Å, °)

N1—C3	1.3557 (14)	C4—H4B	0.9600
N1—N2	1.3626 (13)	C4—H4C	0.9600
N1—C6	1.4627 (15)	C5—H5A	0.9600
C1—N2	1.3287 (15)	C5—H5B	0.9600
C1—C2	1.3998 (16)	C5—H5C	0.9600
C1—C4	1.4948 (17)	C6—H6A	0.9700
C2—C3	1.3747 (16)	C6—H6B	0.9700
C2—H2A	0.9300	C7—C8	1.4057 (17)
N3—C7	1.3689 (16)	C8—C9	1.364 (2)
N3—C6	1.4263 (16)	C8—H8A	0.9300
N3—H3A	0.885 (17)	C9—C10	1.386 (2)
C3—C5	1.4876 (16)	C9—H9A	0.9300
N4—C7	1.3325 (15)	C10—C11	1.365 (2)
N4—C11	1.3435 (17)	C10—H10A	0.9300
C4—H4A	0.9600	C11—H11A	0.9300
C3—N1—N2	111.98 (9)	H5A—C5—H5B	109.5
C3—N1—C6	129.84 (10)	C3—C5—H5C	109.5
N2—N1—C6	118.18 (9)	H5A—C5—H5C	109.5
N2—C1—C2	110.81 (10)	H5B—C5—H5C	109.5
N2—C1—C4	120.70 (11)	N3—C6—N1	113.48 (10)
C2—C1—C4	128.49 (11)	N3—C6—H6A	108.9
C1—N2—N1	105.12 (9)	N1—C6—H6A	108.9
C3—C2—C1	106.05 (10)	N3—C6—H6B	108.9
C3—C2—H2A	127.0	N1—C6—H6B	108.9
C1—C2—H2A	127.0	H6A—C6—H6B	107.7
C7—N3—C6	123.05 (10)	N4—C7—N3	118.30 (10)
C7—N3—H3A	117.4 (10)	N4—C7—C8	122.12 (11)
C6—N3—H3A	118.4 (10)	N3—C7—C8	119.58 (10)
N1—C3—C2	106.05 (10)	C9—C8—C7	118.93 (12)
N1—C3—C5	123.20 (11)	C9—C8—H8A	120.5
C2—C3—C5	130.74 (11)	C7—C8—H8A	120.5
C7—N4—C11	117.04 (11)	C8—C9—C10	119.59 (12)
C1—C4—H4A	109.5	C8—C9—H9A	120.2
C1—C4—H4B	109.5	C10—C9—H9A	120.2
H4A—C4—H4B	109.5	C11—C10—C9	117.53 (13)

C1—C4—H4C	109.5	C11—C10—H10A	121.2
H4A—C4—H4C	109.5	C9—C10—H10A	121.2
H4B—C4—H4C	109.5	N4—C11—C10	124.77 (13)
C3—C5—H5A	109.5	N4—C11—H11A	117.6
C3—C5—H5B	109.5	C10—C11—H11A	117.6
C2—C1—N2—N1	0.36 (12)	C3—N1—C6—N3	115.73 (13)
C4—C1—N2—N1	179.74 (10)	N2—N1—C6—N3	−64.89 (13)
C3—N1—N2—C1	−0.19 (12)	C11—N4—C7—N3	−178.41 (11)
C6—N1—N2—C1	−179.67 (9)	C11—N4—C7—C8	1.09 (18)
N2—C1—C2—C3	−0.40 (12)	C6—N3—C7—N4	−9.23 (17)
C4—C1—C2—C3	−179.72 (11)	C6—N3—C7—C8	171.26 (11)
N2—N1—C3—C2	−0.06 (12)	N4—C7—C8—C9	−0.08 (19)
C6—N1—C3—C2	179.35 (10)	N3—C7—C8—C9	179.42 (11)
N2—N1—C3—C5	179.43 (9)	C7—C8—C9—C10	−0.9 (2)
C6—N1—C3—C5	−1.17 (17)	C8—C9—C10—C11	0.9 (2)
C1—C2—C3—N1	0.27 (12)	C7—N4—C11—C10	−1.2 (2)
C1—C2—C3—C5	−179.16 (11)	C9—C10—C11—N4	0.2 (2)
C7—N3—C6—N1	−84.59 (14)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···N2^{i}	0.886 (17)	2.177 (17)	3.0524 (17)	169.8 (15)

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

Fig. 1

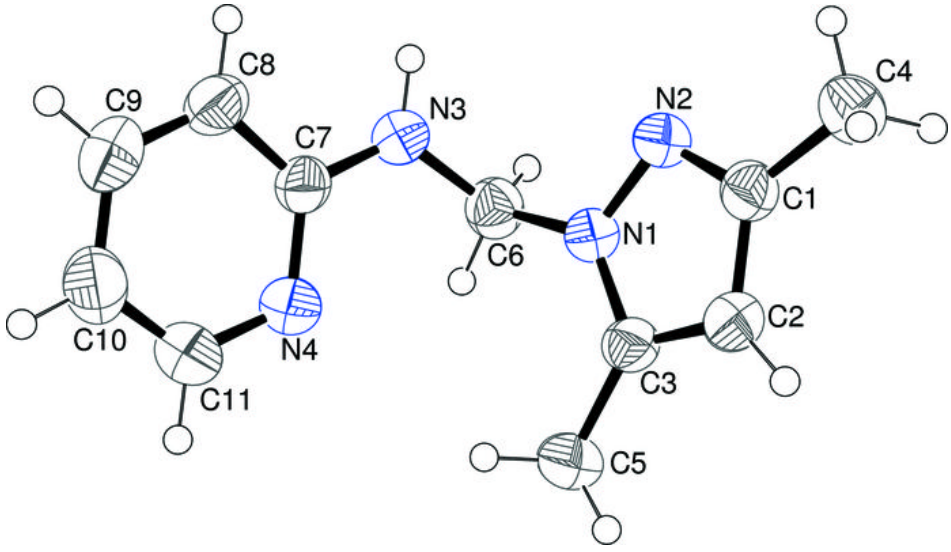

Fig. 2