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5-Amino-3-(4-pyridyl)isoxazole

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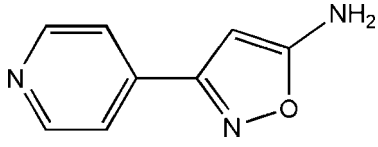
Key indicators: single-crystal X-ray study; T = 187 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.120; data-to-parameter ratio = 13.8.

In the title compound, $C_8H_7N_3O$, there are two independent molecules in the asymmetric unit, in which the angles between the pyridine ring and the isoxazole ring are 35.8 (6) and 10.6 (2)°. The crystal packing is stabilized by N—H···N hydrogen bonds, which result in the molecules forming a two-dimensional supramolecular layer.

Related literature

The title compound was prepared according to a known procedure (Schmidt *et al.*, 1966). For hydrogen-bond motif definitions, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_8H_7N_3O$
M_r = 161.17
Monoclinic, $P2_1/c$
a = 14.6411 (13) Å
b = 10.9272 (10) Å
c = 10.0060 (9) Å
β = 106.9870 (10)°
V = 1531.0 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 187 (2) K
0.42 × 0.18 × 0.10 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.960, T_{max} = 0.990
8396 measured reflections
3018 independent reflections
2509 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.120
S = 1.02
3018 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···N4	0.88	2.09	2.970 (2)	177
N3—H3B···N2^{i}	0.88	2.20	3.077 (2)	169
N6—H6A···N1^{ii}	0.88	2.12	2.976 (2)	164
N6—H6B···N5^{iii}	0.88	2.09	2.970 (2)	174

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); 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: BV2079).

References

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Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supporting information

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5-Amino-3-(4-pyridyl)isoxazole

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S1. Comment

The title compound, (I), is an intermediate for our drug development program. Its structure is shown in Fig. 1. The asymmetric unit was formed by two independent molecules, in which the angles between the pyridine ring and the isoxazole ring are 35.8 (6)° and 10.6 (2)° respectively. Four types of N—H···N hydrogen bonds in the structure are present, which generate two rings, $R_4^4(18)$ and $R_4^4(28)$ (Bernstein *et al.*, 1995). These hydrogen bonds extend the monomer into a two-dimensional supramolecular layer (Fig. 2 and Table 1).

S2. Experimental

The title compound was prepared according to a known procedure (Schmidt *et al.*, 1966). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a ethanol solution at room temperature.

S3. Refinement

H atoms were found on difference Fourier maps and refined as riding, with C—H distance of 0.95 Å and N—H distance of 0.88 Å, and with U_{iso}(H) = 1.2U_{eq}(C,*N*).

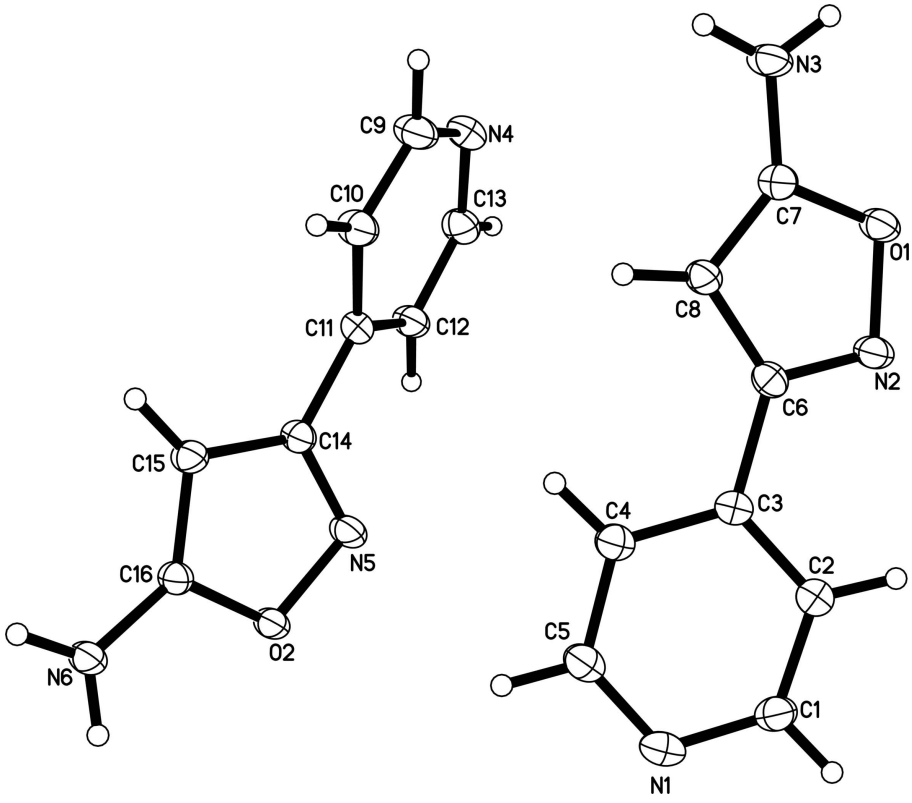

Figure 1

A view of (I), with the atom-labeling scheme and 30% probability displacement ellipsoids.

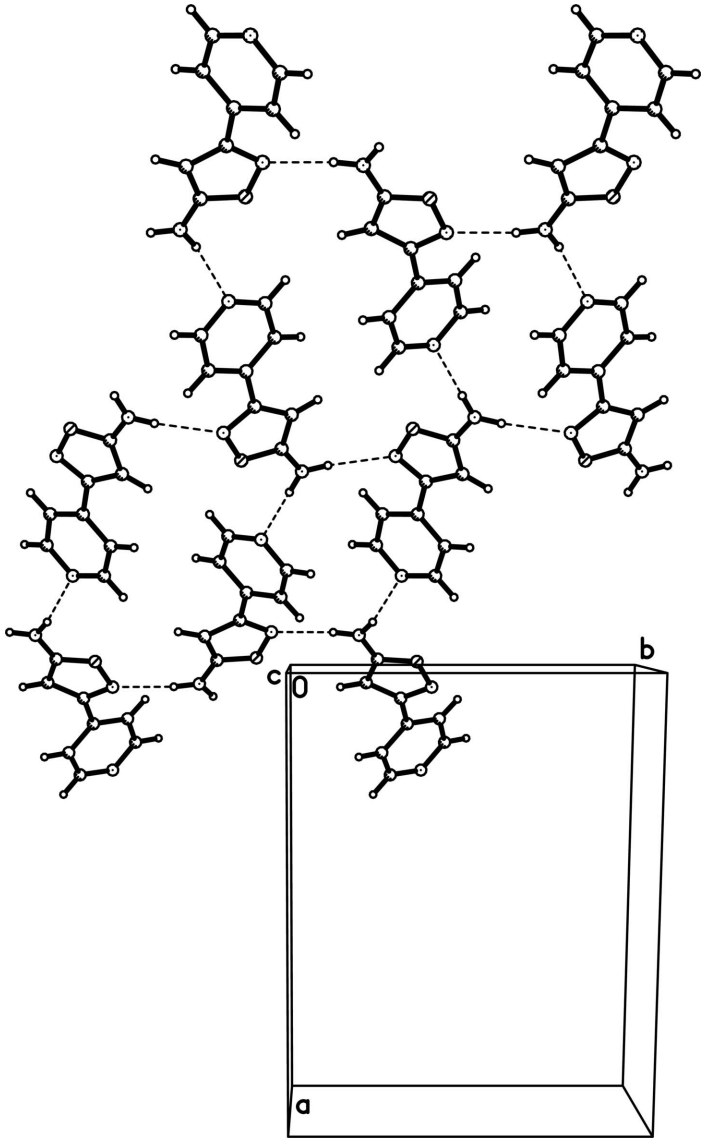

Figure 2

View of the three-dimensional supramolecular structure in (I). Dashed lines indicate hydrogen bonds.

5-amino-3-(4-pyridyl)isoxazole

Crystal data

$C_8H_7N_3O$
$M_r = 161.17$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 14.6411\ (13)$ Å
$b = 10.9272\ (10)$ Å
$c = 10.0060\ (9)$ Å
$\beta = 106.987\ (1)°$
$V = 1531.0\ (2)$ Å^3
$Z = 8$
$F(000) = 672$
$D_x = 1.398$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2830 reflections
$\theta = 2.4–25.9°$
$\mu = 0.10$ mm^{-1}
$T = 187$ K
Block, colourless
0.42 × 0.18 × 0.10 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.960, T_{max} = 0.990
8396 measured reflections
3018 independent reflections
2509 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.0°, θ_{min} = 1.5°
h = −18→14
k = −10→13
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.120
S = 1.02
3018 reflections
218 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 0.2315P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0047 (10)

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}
O1	0.46333 (7)	0.85688 (9)	0.20940 (11)	0.0346 (3)
O2	0.00420 (8)	0.88480 (9)	0.77638 (11)	0.0336 (3)
N1	0.79693 (9)	0.83254 (13)	−0.07659 (13)	0.0383 (3)
N2	0.52225 (9)	0.80823 (11)	0.13072 (13)	0.0337 (3)
N3	0.44141 (10)	1.03237 (12)	0.31848 (14)	0.0388 (3)
H3A	0.3946	0.9950	0.3407	0.047*
H3B	0.4558	1.1086	0.3447	0.047*
N4	0.28672 (10)	0.90935 (13)	0.40458 (14)	0.0398 (3)
N5	0.06798 (9)	0.93321 (11)	0.70626 (14)	0.0359 (3)
N6	−0.06051 (10)	0.70441 (11)	0.81376 (14)	0.0377 (3)
H6A	−0.0927	0.7458	0.8606	0.045*
H6B	−0.0675	0.6246	0.8048	0.045*
C1	0.72429 (11)	0.75481 (15)	−0.08875 (15)	0.0358 (4)
H1	0.7222	0.6830	−0.1430	0.043*
C2	0.65244 (11)	0.77244 (14)	−0.02749 (15)	0.0346 (4)

H2	0.6026	0.7141	−0.0398	0.042*
C3	0.65383 (10)	0.87660 (13)	0.05244 (14)	0.0271 (3)
C4	0.72841 (11)	0.95824 (14)	0.06540 (16)	0.0368 (4)
H4	0.7322	1.0310	0.1188	0.044*
C5	0.79718 (12)	0.93253 (15)	−0.00027 (18)	0.0419 (4)
H5	0.8477	0.9896	0.0096	0.050*
C6	0.58040 (10)	0.89855 (13)	0.12468 (13)	0.0270 (3)
C7	0.49043 (11)	0.97363 (13)	0.24510 (14)	0.0289 (3)
C8	0.56482 (10)	1.00383 (13)	0.19470 (14)	0.0292 (3)
H8	0.5984	1.0793	0.2049	0.035*
C9	0.29569 (12)	0.80896 (15)	0.48351 (17)	0.0399 (4)
H9	0.3461	0.7540	0.4845	0.048*
C10	0.23625 (11)	0.77991 (14)	0.56385 (16)	0.0351 (4)
H10	0.2452	0.7065	0.6170	0.042*
C11	0.16304 (10)	0.86076 (13)	0.56504 (14)	0.0286 (3)
C12	0.15291 (11)	0.96543 (14)	0.48390 (15)	0.0331 (4)
H12	0.1038	1.0227	0.4820	0.040*
C13	0.21520 (12)	0.98536 (15)	0.40568 (16)	0.0379 (4)
H13	0.2068	1.0570	0.3496	0.045*
C14	0.09696 (10)	0.83758 (13)	0.65003 (14)	0.0272 (3)
C15	0.05754 (11)	0.72799 (13)	0.67909 (15)	0.0310 (3)
H15	0.0689	0.6476	0.6514	0.037*
C16	−0.00128 (10)	0.76260 (13)	0.75652 (14)	0.0274 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0346 (6)	0.0288 (6)	0.0488 (6)	−0.0019 (4)	0.0251 (5)	−0.0016 (5)
O2	0.0403 (6)	0.0237 (5)	0.0474 (6)	−0.0025 (4)	0.0294 (5)	−0.0020 (4)
N1	0.0352 (7)	0.0459 (8)	0.0394 (7)	0.0043 (6)	0.0198 (6)	0.0003 (6)
N2	0.0330 (7)	0.0304 (7)	0.0443 (7)	0.0000 (5)	0.0216 (6)	−0.0034 (5)
N3	0.0443 (8)	0.0306 (7)	0.0545 (8)	−0.0018 (6)	0.0347 (7)	−0.0025 (6)
N4	0.0369 (8)	0.0452 (8)	0.0452 (7)	−0.0045 (6)	0.0242 (6)	−0.0018 (6)
N5	0.0415 (8)	0.0270 (7)	0.0502 (8)	−0.0038 (6)	0.0303 (6)	0.0000 (6)
N6	0.0488 (8)	0.0247 (7)	0.0527 (8)	−0.0031 (6)	0.0353 (7)	−0.0018 (6)
C1	0.0382 (9)	0.0391 (9)	0.0328 (8)	0.0022 (7)	0.0146 (7)	−0.0053 (7)
C2	0.0331 (8)	0.0370 (9)	0.0361 (8)	−0.0039 (7)	0.0138 (7)	−0.0038 (7)
C3	0.0270 (7)	0.0287 (8)	0.0268 (7)	0.0030 (6)	0.0098 (6)	0.0026 (6)
C4	0.0364 (9)	0.0340 (9)	0.0458 (9)	−0.0031 (7)	0.0209 (7)	−0.0060 (7)
C5	0.0382 (9)	0.0418 (9)	0.0538 (10)	−0.0065 (7)	0.0263 (8)	−0.0063 (8)
C6	0.0251 (7)	0.0283 (7)	0.0284 (7)	0.0005 (6)	0.0088 (6)	0.0043 (6)
C7	0.0321 (8)	0.0258 (8)	0.0313 (7)	0.0020 (6)	0.0129 (6)	0.0030 (6)
C8	0.0308 (8)	0.0269 (7)	0.0343 (7)	−0.0030 (6)	0.0164 (6)	−0.0006 (6)
C9	0.0351 (9)	0.0421 (10)	0.0491 (9)	0.0051 (7)	0.0225 (7)	0.0015 (8)
C10	0.0353 (8)	0.0328 (8)	0.0417 (8)	0.0037 (7)	0.0181 (7)	0.0040 (7)
C11	0.0270 (7)	0.0300 (8)	0.0312 (7)	−0.0035 (6)	0.0124 (6)	−0.0026 (6)
C12	0.0336 (8)	0.0314 (8)	0.0398 (8)	0.0011 (6)	0.0193 (7)	0.0023 (7)
C13	0.0431 (9)	0.0347 (9)	0.0423 (9)	−0.0030 (7)	0.0225 (7)	0.0038 (7)

C14	0.0266 (7)	0.0268 (7)	0.0301 (7)	0.0015 (6)	0.0113 (6)	0.0017 (6)
C15	0.0387 (8)	0.0223 (7)	0.0386 (8)	0.0016 (6)	0.0214 (7)	0.0006 (6)
C16	0.0309 (7)	0.0227 (7)	0.0322 (7)	0.0010 (6)	0.0150 (6)	0.0016 (6)

Geometric parameters (Å, º)

O1—C7	1.3527 (17)	C3—C4	1.386 (2)
O1—N2	1.4295 (14)	C3—C6	1.4798 (18)
O2—C16	1.3490 (17)	C4—C5	1.382 (2)
O2—N5	1.4237 (14)	C4—H4	0.9500
N1—C5	1.332 (2)	C5—H5	0.9500
N1—C1	1.339 (2)	C6—C8	1.3999 (19)
N2—C6	1.3164 (18)	C7—C8	1.3677 (19)
N3—C7	1.3319 (18)	C8—H8	0.9500
N3—H3A	0.8800	C9—C10	1.383 (2)
N3—H3B	0.8800	C9—H9	0.9500
N4—C9	1.336 (2)	C10—C11	1.392 (2)
N4—C13	1.339 (2)	C10—H10	0.9500
N5—C14	1.3145 (17)	C11—C12	1.385 (2)
N6—C16	1.3322 (18)	C11—C14	1.4847 (18)
N6—H6A	0.8800	C12—C13	1.3816 (19)
N6—H6B	0.8800	C12—H12	0.9500
C1—C2	1.377 (2)	C13—H13	0.9500
C1—H1	0.9500	C14—C15	1.3963 (19)
C2—C3	1.388 (2)	C15—C16	1.3692 (19)
C2—H2	0.9500	C15—H15	0.9500
C7—O1—N2	108.58 (10)	N3—C7—O1	115.87 (13)
C16—O2—N5	108.34 (10)	N3—C7—C8	134.62 (14)
C5—N1—C1	116.20 (13)	O1—C7—C8	109.51 (12)
C6—N2—O1	104.42 (11)	C7—C8—C6	104.48 (12)
C7—N3—H3A	120.0	C7—C8—H8	127.8
C7—N3—H3B	120.0	C6—C8—H8	127.8
H3A—N3—H3B	120.0	N4—C9—C10	124.22 (15)
C9—N4—C13	116.52 (13)	N4—C9—H9	117.9
C14—N5—O2	104.82 (10)	C10—C9—H9	117.9
C16—N6—H6A	120.0	C9—C10—C11	118.44 (14)
C16—N6—H6B	120.0	C9—C10—H10	120.8
H6A—N6—H6B	120.0	C11—C10—H10	120.8
N1—C1—C2	124.11 (14)	C12—C11—C10	118.03 (13)
N1—C1—H1	117.9	C12—C11—C14	120.03 (13)
C2—C1—H1	117.9	C10—C11—C14	121.94 (13)
C1—C2—C3	119.13 (14)	C13—C12—C11	119.13 (14)
C1—C2—H2	120.4	C13—C12—H12	120.4
C3—C2—H2	120.4	C11—C12—H12	120.4
C4—C3—C2	117.40 (13)	N4—C13—C12	123.65 (15)
C4—C3—C6	120.98 (13)	N4—C13—H13	118.2
C2—C3—C6	121.60 (13)	C12—C13—H13	118.2

C5—C4—C3	119.20 (14)	N5—C14—C15	112.83 (12)
C5—C4—H4	120.4	N5—C14—C11	117.08 (12)
C3—C4—H4	120.4	C15—C14—C11	130.08 (12)
N1—C5—C4	123.96 (15)	C16—C15—C14	104.33 (12)
N1—C5—H5	118.0	C16—C15—H15	127.8
C4—C5—H5	118.0	C14—C15—H15	127.8
N2—C6—C8	113.02 (12)	N6—C16—O2	115.30 (12)
N2—C6—C3	118.22 (13)	N6—C16—C15	135.03 (14)
C8—C6—C3	128.72 (13)	O2—C16—C15	109.67 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N4	0.88	2.09	2.970 (2)	177
N3—H3*B*···N2^{i}	0.88	2.20	3.077 (2)	169
N6—H6*A*···N1^{ii}	0.88	2.12	2.976 (2)	164
N6—H6*B*···N5^{iii}	0.88	2.09	2.970 (2)	174

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