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Pyrimidine-2-carboxamide

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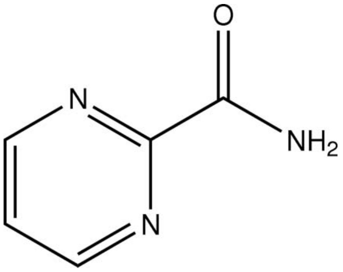
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.107; data-to-parameter ratio = 16.6.

In the crystal strucuture of the title compound, $C_5H_5N_3O$, which was obtained upon recrystallization of 2-cyanopyrimidine from aqueous sodium hydroxide, the amide group is twisted with respect to the aromatic ring by 24.9 (1)°. π–π stacking is observed between partially overlapped rings at a face-to-face separation of 3.439 (6) Å. The structure features a centrosymmetric pair of intermolecular N—H⋯O hydrogen bonds. Another N—H⋯O hydrogen bond between adjacent molecules links them into a helical chain motif.

Related literature

For general background, see: Cheng *et al.* (2000); Xu & Xu (2004); Zhang *et al.* (2008). For a similar structure, see: Zhang *et al.* (2007).



Experimental

Crystal data

$C_5H_5N_3O$
M_r = 123.12
Monoclinic, $P2_1/c$
a = 7.9241 (7) Å
b = 7.3059 (7) Å
c = 9.8223 (9) Å
β = 103.512 (6)°
V = 552.90 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 291 (2) K
0.34 × 0.26 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: none
7501 measured reflections
1365 independent reflections
1202 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.107
S = 1.01
1365 reflections
82 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max}$ = 0.25 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.19 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N3—H1A⋯O1$^{\rm i}$	0.94	2.06	2.994 (1)	172
N3—H1B⋯O1$^{\rm ii}$	0.96	2.04	2.986 (2)	167

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2399).

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supplementary materials

Acta Cryst. (2008). E**64**, o105 [**doi:10.1107/S1600536807062770**]

Pyrimidine-2-carboxamide

B.-Y. Zhang, **Q. Yang** and **J.-J. Nie**

Comment

In order to study the nature of π–π stacking, a series of metal complexes incorporating substituted benzoate ligand have been prepared in our laboratory (Cheng *et al.*, 2000; Xu & Xu, 2004). As a continuing work, metal complexes with pyrimidine-2-carboxylate ligand have recently been prepared (Zhang *et al.*, 2007). In the process of preparing pyrimidine-2-carboxylic acid from cyanopyrimidine, the title compound has been obtained.

The molecular structure of the title complex is shown in Fig. 1. The bond distances and angles are normal. The amide group is twisted with respect to the benzene ring by a dihedral angel of 24.92 (12)°. The amino group links with carbonyl groups of adjacent molecules *via* O—H···O hydrogen bonding (Table 1). π–π stacking is observed between parallel, partially overlapped N1-pyrimidine and N^{i}-pyrimidine rings (Fig. 1) [symmetry code: (i) $1 - x$, $1 - y$, $1 - z$], face-to-face separation being 3.439 (6) Å; similar to the situation found in the pyrimidine-2-carboxylate complex of copper(II) (Zhang *et al.*, 2007).

Experimental

2-Cyanopyrimidine (1.0 g, 9.5 mmol) was dissolved in 10 ml water, then a NaOH solution (0.1 *M*) was dropped to the solution until to pH = 12. Single crystals of the title compound were obtained from the solution after one week.

Refinement

Amino H atoms were located in a difference Fourier map and refined as riding in as-found relative positions with $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(N). Other H atoms were placed in calculated positions with C—H = 0.93 Å and refined in riding mode with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

Figures

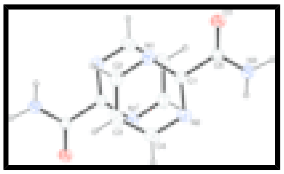

Fig. 1. The molecular structure of the title compound with 30% probability displacement (arbitrary spheres for H atoms) [symmetry codes: (i) $1 - x$, $1 - y$, $1 - z$].

pyrimidine-2-carboxamide

Crystal data

$C_5H_5N_3O$	F_{000} = 256
M_r = 123.12	D_x = 1.479 Mg m^{-3}

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

a = 7.9241 (7) Å

b = 7.3059 (7) Å

c = 9.8223 (9) Å

β = 103.512 (6)°

V = 552.90 (9) Å^3

Z = 4

Mo $K\alpha$ radiation
λ = 0.71073 Å

Cell parameters from 2086 reflections

θ = 3.0–25.5°

μ = 0.11 mm^{-1}

T = 291 (2) K

Prism, yellow

0.34 × 0.26 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 293(2) K

ω scans

Absorption correction: none

7501 measured reflections

1365 independent reflections

1202 reflections with $I > 2\sigma(I)$

$R_{\rm int}$ = 0.020

$\theta_{\rm max}$ = 28.3°

$\theta_{\rm min}$ = 2.6°

$h = -10\rightarrow10$

$k = -9\rightarrow9$

$l = -12\rightarrow13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.107$

S = 1.02

1365 reflections

82 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0584P)^2 + 0.1258P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\rm max} < 0.001$

$\Delta\rho_{\rm max}$ = 0.25 e Å^{-3}

$\Delta\rho_{\rm min}$ = −0.19 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 > 2sigma(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	$U_{\rm iso}$*/$U_{\rm eq}$
N1	0.35320 (14)	0.45375 (15)	0.64547 (11)	0.0431 (3)
N2	0.18202 (13)	0.54314 (14)	0.42171 (10)	0.0383 (3)
O1	0.13605 (12)	0.15236 (12)	0.61860 (8)	0.0431 (3)
N3	0.07527 (15)	0.18634 (15)	0.38330 (10)	0.0435 (3)
H1A	0.0949	0.2477	0.3043	0.065*
H1B	0.0039	0.0783	0.3675	0.065*
C1	0.23238 (14)	0.42647 (15)	0.52761 (11)	0.0315 (2)
C2	0.43153 (18)	0.6167 (2)	0.65658 (14)	0.0495 (3)
H2	0.5193	0.6412	0.7355	0.059*
C3	0.38709 (19)	0.74967 (19)	0.55555 (15)	0.0502 (3)
H3	0.4405	0.8638	0.5659	0.060*
C4	0.26039 (18)	0.70681 (18)	0.43855 (14)	0.0462 (3)
H4	0.2279	0.7944	0.3686	0.055*
C5	0.14304 (14)	0.24129 (15)	0.51331 (11)	0.0325 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0446 (6)	0.0418 (6)	0.0383 (5)	−0.0037 (4)	0.0002 (4)	−0.0014 (4)
N2	0.0417 (5)	0.0350 (5)	0.0375 (5)	0.0003 (4)	0.0080 (4)	0.0046 (4)
O1	0.0602 (6)	0.0366 (5)	0.0316 (4)	−0.0065 (4)	0.0087 (4)	0.0025 (3)
N3	0.0593 (7)	0.0389 (6)	0.0304 (5)	−0.0120 (5)	0.0065 (4)	−0.0018 (4)
C1	0.0325 (5)	0.0315 (5)	0.0311 (5)	0.0019 (4)	0.0085 (4)	−0.0016 (4)
C2	0.0478 (7)	0.0501 (8)	0.0473 (7)	−0.0108 (6)	0.0046 (5)	−0.0103 (6)
C3	0.0530 (8)	0.0377 (7)	0.0628 (9)	−0.0123 (5)	0.0194 (6)	−0.0072 (6)
C4	0.0506 (7)	0.0367 (6)	0.0538 (7)	0.0001 (5)	0.0175 (6)	0.0084 (5)
C5	0.0362 (5)	0.0304 (5)	0.0302 (5)	0.0018 (4)	0.0067 (4)	−0.0001 (4)

Geometric parameters (Å, °)

N1—C1	1.3336 (14)	N3—H1B	0.9622
N1—C2	1.3355 (18)	C1—C5	1.5182 (15)
N2—C1	1.3319 (14)	C2—C3	1.374 (2)
N2—C4	1.3397 (17)	C2—H2	0.9300
O1—C5	1.2335 (13)	C3—C4	1.374 (2)
N3—C5	1.3265 (14)	C3—H3	0.9300
N3—H1A	0.9406	C4—H4	0.9300
C1—N1—C2	115.46 (11)	C3—C2—H2	118.8
C1—N2—C4	115.41 (10)	C2—C3—C4	117.18 (12)
C5—N3—H1A	122.9	C2—C3—H3	121.4
C5—N3—H1B	119.6	C4—C3—H3	121.4
H1A—N3—H1B	117.5	N2—C4—C3	122.26 (12)
N2—C1—N1	127.28 (11)	N2—C4—H4	118.9
N2—C1—C5	116.74 (9)	C3—C4—H4	118.9

N1—C1—C5	115.99 (10)	O1—C5—N3	124.08 (11)
N1—C2—C3	122.37 (12)	O1—C5—C1	120.20 (9)
N1—C2—H2	118.8	N3—C5—C1	115.72 (9)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H1A···O1^{i}	0.94	2.06	2.994 (1)	172
N3—H1B···O1^{ii}	0.96	2.04	2.986 (2)	167

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

Fig. 1