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2-Amino-4,6-dimethylpyrimidine–benzoic acid (1/1)

A-Lan Meng, Jun-E Huang, Bin Zheng and Zhen-Jiang Li*

Qingdao University of Science and Technology, Qingdao 266061, People's Republic of China
Correspondence e-mail: zjli126@126.com

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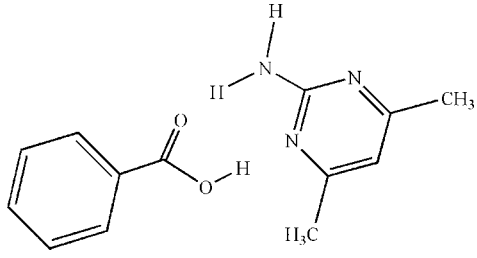
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.053; wR factor = 0.137; data-to-parameter ratio = 13.6.

The crystal of the title compound, $C_6H_9N_3{\cdot}C_7H_6O_2$, contains tetrameric hydrogen-bonded units comprising a central pair of 2-aminopyrimidine molecules linked across a centre of inversion by N—H···N hydrogen bonds and two pendant benzoic acid molecules attached through N—H···O and O—H···N hydrogen bonds. These hydrogen-bonded units are arranged into layers in (002).

Related literature

For the biological activity of pyrimidine and aminopyrimidine derivatives, see: Hunt *et al.* (1980); Baker & Santi (1965). For related structures, see: Skovsgaard & Bond (2009); Fun *et al.* (2006); Wang *et al.* (2007); Schwalbe & Williams (1982); Hu *et al.* (2002); Chinnakali *et al.* (1999).



Experimental

Crystal data

$C_6H_9N_3{\cdot}C_7H_6O_2$
M_r = 245.28
Monoclinic, $P2_1/c$
a = 6.7019 (9) Å
b = 7.6466 (10) Å
c = 25.285 (3) Å
β = 91.360 (2)°
V = 1295.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 K
0.18 × 0.15 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.985, T_{max} = 0.991
6594 measured reflections
2273 independent reflections
1228 reflections with $I > 2\sigma(I)$
R_{int} = 0.104

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.137
S = 1.01
2273 reflections
167 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.82	2.606 (2)	160
N3—H3A···O2	0.86	2.16	3.003 (3)	168
N3—H3B···N2^{i}	0.86	2.25	3.098 (3)	169

Symmetry code: (i) $-x, -y+2, -z+1$.

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: BI2374).

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supporting information

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2-Amino-4,6-dimethylpyrimidine–benzoic acid (1/1)

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S1. Comment

Pyrimidine and aminopyrimidine derivatives are biologically important compounds as they occur in nature as components of nucleic acids. Some aminopyrimidine derivatives are used as antifolate drugs (Hunt *et al.*, 1980; Baker & Santi, 1965). The crystal structures of aminopyrimidine derivatives (Schwalbe & Williams, 1982), aminopyrimidine carboxylates (Hu *et al.*, 2002) and co-crystal structures (Chinnakali *et al.*, 1999; Skovsgaard & Bond, 2009) have been reported.

The title compound (Fig. 1) was obtained as the product of an attempted synthesis of benzoic acid and 2-amino-4,6-dimethylpyrimidine in acetone. The bond lengths and angles in the pyrimidine ring and phenyl ring are generally normal (Fun *et al.*, 2006). The molecules associate through O—H···N, N—H···O and N—H···N hydrogen bonds into centrosymmetic tetrameric units. These units pack into stacked layers in the (002) planes (Fig. 2).

S2. Experimental

Single crystals of the title compound were obtained by reaction of benzoic acid (0.2 mmol) and 2-amino-4,6-dimethylpyrimidine (0.2 mmol) in refluxing acetone (50 ml). Single crystals suitable for X-ray analysis were obtained by recrystallization from ethanol solution at room temperature.

S3. Refinement

H atoms were fixed geometrically and allowed to ride on their attached atoms, with N—H = 0.86 Å, C—H = 0.93 or 0.96 Å, and with U_{iso}(H) = 1.5 U_{eq}(C) (for CH_3) or 1.2 U_{eq}(C) (for CH_2, aromatic CH and NH_2).

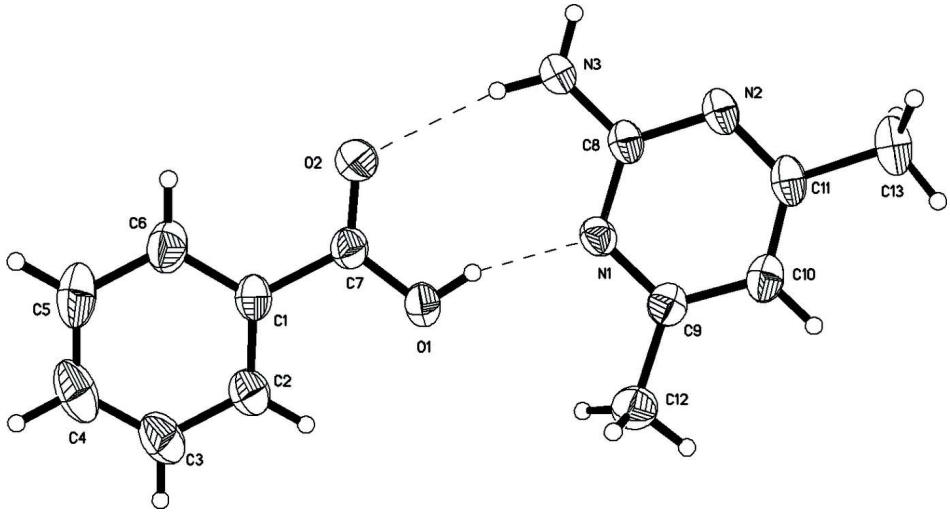

Figure 1

Molecular structure with displacement ellipsoids drawn at the 30% probability level for non-H atoms. Dashed lines denote hydrogen bonds.

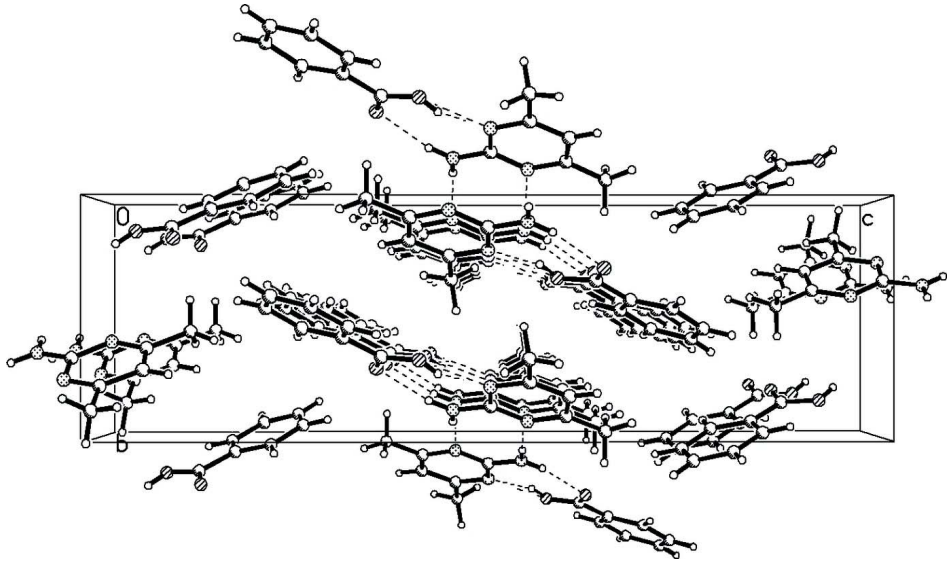

Figure 2

Packing diagram showing one layer of molecules connected by N—H···O and O—H···N hydrogen bonds (dashed lines).

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V = 1295.4 (3) Å^3
Z = 4
F(000) = 520
D_x = 1.258 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 167 reflections
θ = 1.6–25.0°
μ = 0.09 mm^{-1}

T = 295 K
Block, colourless

0.18 × 0.15 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.985, T_{max} = 0.991

6594 measured reflections
2273 independent reflections
1228 reflections with $I > 2\sigma(I)$
R_{int} = 0.104
θ_{max} = 25.0°, θ_{min} = 1.6°
$h = -7 \rightarrow 7$
$k = -9 \rightarrow 9$
$l = -22 \rightarrow 30$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.137
S = 1.01
2273 reflections
167 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
$w = 1/[\sigma^2(F_o^2) + (0.0352P)^2 + 0.012P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0077 (16)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.6583 (2)	0.6591 (2)	0.41923 (6)	0.0678 (5)
H1	0.5870	0.7100	0.4402	0.102*
O2	0.3940 (3)	0.6933 (3)	0.36625 (7)	0.0787 (6)
N1	0.4633 (3)	0.7645 (2)	0.50129 (7)	0.0482 (5)
N2	0.1976 (3)	0.9074 (2)	0.54612 (8)	0.0560 (6)
N3	0.1836 (3)	0.8632 (2)	0.45633 (8)	0.0646 (6)
H3A	0.2332	0.8250	0.4275	0.078*
H3B	0.0689	0.9137	0.4557	0.078*
C1	0.6891 (4)	0.5714 (3)	0.33125 (9)	0.0540 (6)
C2	0.8886 (4)	0.5334 (3)	0.34037 (10)	0.0662 (7)
H2	0.9484	0.5593	0.3730	0.079*
C3	0.9993 (5)	0.4573 (4)	0.30126 (13)	0.0813 (9)

H3	1.1337	0.4326	0.3075	0.098*
C4	0.9124 (6)	0.4184 (4)	0.25352 (13)	0.0892 (10)
H4	0.9866	0.3641	0.2276	0.107*
C5	0.7167 (6)	0.4587 (4)	0.24346 (11)	0.0931 (10)
H5	0.6586	0.4332	0.2106	0.112*
C6	0.6032 (4)	0.5382 (4)	0.28248 (10)	0.0754 (8)
H6	0.4708	0.5683	0.2754	0.090*
C7	0.5664 (4)	0.6473 (3)	0.37388 (10)	0.0542 (7)
C8	0.2837 (4)	0.8443 (3)	0.50166 (10)	0.0497 (6)
C9	0.5618 (3)	0.7431 (3)	0.54739 (9)	0.0522 (6)
C10	0.4805 (4)	0.8019 (3)	0.59401 (10)	0.0620 (7)
H10	0.5481	0.7868	0.6262	0.074*
C11	0.2973 (4)	0.8831 (3)	0.59146 (10)	0.0579 (7)
C12	0.7598 (4)	0.6537 (3)	0.54573 (11)	0.0699 (8)
H12A	0.7401	0.5309	0.5397	0.105*
H12B	0.8303	0.6706	0.5788	0.105*
H12C	0.8361	0.7022	0.5176	0.105*
C13	0.1975 (4)	0.9484 (3)	0.64045 (10)	0.0793 (9)
H13A	0.1886	1.0737	0.6393	0.119*
H13B	0.2743	0.9136	0.6712	0.119*
H13C	0.0658	0.8996	0.6421	0.119*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0593 (11)	0.0969 (15)	0.0473 (11)	0.0084 (10)	0.0053 (9)	−0.0141 (10)
O2	0.0568 (12)	0.1232 (16)	0.0564 (12)	0.0167 (11)	0.0055 (9)	−0.0012 (10)
N1	0.0425 (11)	0.0546 (12)	0.0480 (12)	−0.0031 (9)	0.0092 (9)	−0.0005 (9)
N2	0.0584 (13)	0.0594 (13)	0.0510 (13)	−0.0063 (10)	0.0179 (10)	−0.0042 (11)
N3	0.0552 (13)	0.0919 (16)	0.0472 (13)	0.0168 (11)	0.0084 (10)	−0.0057 (11)
C1	0.0620 (17)	0.0566 (15)	0.0439 (15)	−0.0070 (13)	0.0109 (12)	0.0003 (12)
C2	0.0670 (19)	0.0707 (18)	0.0617 (17)	−0.0002 (14)	0.0157 (14)	−0.0015 (14)
C3	0.081 (2)	0.085 (2)	0.080 (2)	0.0071 (17)	0.0337 (18)	−0.0012 (18)
C4	0.119 (3)	0.073 (2)	0.078 (2)	−0.003 (2)	0.056 (2)	−0.0027 (18)
C5	0.119 (3)	0.113 (3)	0.0486 (19)	−0.020 (2)	0.0181 (18)	−0.0134 (17)
C6	0.0767 (19)	0.098 (2)	0.0513 (17)	−0.0100 (16)	0.0084 (14)	−0.0062 (16)
C7	0.0529 (16)	0.0653 (17)	0.0448 (16)	−0.0014 (13)	0.0080 (13)	0.0025 (12)
C8	0.0524 (15)	0.0516 (14)	0.0456 (15)	−0.0068 (12)	0.0121 (12)	−0.0030 (12)
C9	0.0502 (15)	0.0550 (16)	0.0516 (16)	−0.0112 (12)	0.0041 (12)	0.0032 (12)
C10	0.0705 (19)	0.0703 (17)	0.0454 (16)	−0.0090 (15)	0.0058 (13)	0.0030 (13)
C11	0.0694 (18)	0.0566 (16)	0.0486 (16)	−0.0128 (14)	0.0196 (13)	−0.0031 (12)
C12	0.0561 (17)	0.0836 (18)	0.0700 (18)	0.0001 (14)	0.0004 (13)	0.0025 (15)
C13	0.100 (2)	0.0828 (19)	0.0562 (17)	−0.0108 (17)	0.0289 (15)	−0.0094 (15)

Geometric parameters (Å, º)

O1—C7	1.292 (3)	C4—C5	1.365 (4)
O1—H1	0.820	C4—H4	0.930

O2—C7	1.218 (3)	C5—C6	1.399 (4)
N1—C9	1.336 (3)	C5—H5	0.930
N1—C8	1.350 (3)	C6—H6	0.930
N2—C11	1.326 (3)	C9—C10	1.385 (3)
N2—C8	1.364 (3)	C9—C12	1.494 (3)
N3—C8	1.322 (3)	C10—C11	1.376 (3)
N3—H3A	0.860	C10—H10	0.930
N3—H3B	0.860	C11—C13	1.507 (3)
C1—C6	1.372 (3)	C12—H12A	0.960
C1—C2	1.382 (3)	C12—H12B	0.960
C1—C7	1.489 (3)	C12—H12C	0.960
C2—C3	1.379 (4)	C13—H13A	0.960
C2—H2	0.930	C13—H13B	0.960
C3—C4	1.361 (4)	C13—H13C	0.960
C3—H3	0.930		

C7—O1—H1	109.5	O1—C7—C1	114.2 (2)
C9—N1—C8	118.13 (19)	N3—C8—N1	118.5 (2)
C11—N2—C8	116.7 (2)	N3—C8—N2	117.4 (2)
C8—N3—H3A	120.0	N1—C8—N2	124.1 (2)
C8—N3—H3B	120.0	N1—C9—C10	120.4 (2)
H3A—N3—H3B	120.0	N1—C9—C12	116.9 (2)
C6—C1—C2	119.6 (2)	C10—C9—C12	122.7 (2)
C6—C1—C7	119.7 (2)	C11—C10—C9	118.4 (2)
C2—C1—C7	120.7 (2)	C11—C10—H10	120.8
C3—C2—C1	120.3 (3)	C9—C10—H10	120.8
C3—C2—H2	119.9	N2—C11—C10	122.3 (2)
C1—C2—H2	119.9	N2—C11—C13	116.1 (3)
C4—C3—C2	120.1 (3)	C10—C11—C13	121.6 (3)
C4—C3—H3	119.9	C9—C12—H12A	109.5
C2—C3—H3	119.9	C9—C12—H12B	109.5
C3—C4—C5	120.3 (3)	H12A—C12—H12B	109.5
C3—C4—H4	119.8	C9—C12—H12C	109.5
C5—C4—H4	119.8	H12A—C12—H12C	109.5
C4—C5—C6	120.2 (3)	H12B—C12—H12C	109.5
C4—C5—H5	119.9	C11—C13—H13A	109.5
C6—C5—H5	119.9	C11—C13—H13B	109.5
C1—C6—C5	119.4 (3)	H13A—C13—H13B	109.5
C1—C6—H6	120.3	C11—C13—H13C	109.5
C5—C6—H6	120.3	H13A—C13—H13C	109.5
O2—C7—O1	123.4 (2)	H13B—C13—H13C	109.5
O2—C7—C1	122.4 (2)		

C6—C1—C2—C3	−2.1 (4)	C9—N1—C8—N3	−178.84 (19)
C7—C1—C2—C3	177.7 (2)	C9—N1—C8—N2	1.2 (3)
C1—C2—C3—C4	−0.3 (4)	C11—N2—C8—N3	178.20 (19)
C2—C3—C4—C5	1.8 (5)	C11—N2—C8—N1	−1.8 (3)
C3—C4—C5—C6	−0.9 (5)	C8—N1—C9—C10	−0.1 (3)

C2—C1—C6—C5	3.0 (4)	C8—N1—C9—C12	179.75 (19)
C7—C1—C6—C5	−176.8 (2)	N1—C9—C10—C11	−0.4 (3)
C4—C5—C6—C1	−1.5 (4)	C12—C9—C10—C11	179.9 (2)
C6—C1—C7—O2	−5.3 (4)	C8—N2—C11—C10	1.4 (3)
C2—C1—C7—O2	175.0 (2)	C8—N2—C11—C13	−178.11 (19)
C6—C1—C7—O1	174.4 (2)	C9—C10—C11—N2	−0.3 (4)
C2—C1—C7—O1	−5.3 (3)	C9—C10—C11—C13	179.1 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.82	2.606 (2)	160
N3—H3*A*···O2	0.86	2.16	3.003 (3)	168
N3—H3*B*···N2^{i}	0.86	2.25	3.098 (3)	169

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