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2-Pyridone: monoclinic polymorph

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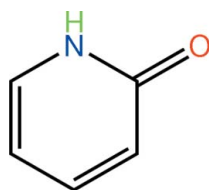
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Key indicators: single-crystal X-ray study; $T = 98$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.044; wR factor = 0.117; data-to-parameter ratio = 15.0.

The asymmetric unit in the title compound, $\text{C}_5\text{H}_5\text{NO}$, comprises two independent but virtually identical molecules of 2-pyridone, and represents a monoclinic polymorph of the previously reported orthorhombic ($P2_12_12_1$) form [Penfold (1953). *Acta Cryst.* **6**, 591–600; Ohms *et al.* (1984). *Z. Kristallogr.* **169**, 185–200; Yang & Craven (1998). *Acta Cryst.* **B54**, 912–920]. The independent molecules are linked into supramolecular dimers *via* eight-membered $\{\cdots\text{HNC}(\text{O})\}_2$ amide synthons in contrast to the helical supramolecular chains, mediated by $\{\cdots\text{HNC}(\text{O})\}$ links, found in the orthorhombic form.

Related literature

For the structure of the orthorhombic form of 2-pyridone, see: Penfold (1953); Ohms *et al.* (1984); Yang & Craven (1998). For related studies of co-crystal formation, see: Broker & Tiekink (2007); Ellis *et al.* (2009). For analysis of the geometric structures, see: Spek (2009).



Experimental

Crystal data

 $\text{C}_5\text{H}_5\text{NO}$ $M_r = 95.10$

Monoclinic, $P2_1/n$
 $a = 6.2027$ (13) Å
 $b = 16.327$ (4) Å
 $c = 9.1046$ (18) Å
 $\beta = 92.242$ (7)°
 $V = 921.3$ (3) Å³

$Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 98$ K
 $0.44 \times 0.39 \times 0.15$ mm

Data collection

Rigaku AFC12K/SATURN724 diffractometer
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.840$, $T_{\max} = 1$

6582 measured reflections
 1903 independent reflections
 1724 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.037$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.117$
 $S = 1.10$
 1903 reflections

127 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.21$ e Å⁻³
 $\Delta\rho_{\min} = -0.22$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1n}\cdots\text{O2}$	0.88	1.86	2.7450 (16)	177
$\text{N2}-\text{H2n}\cdots\text{O1}$	0.88	1.92	2.7915 (16)	171
$\text{C2}-\text{H2}\cdots\text{O1}^{\text{i}}$	0.95	2.53	3.3943 (18)	150
$\text{C4}-\text{H4}\cdots\text{O2}^{\text{ii}}$	0.95	2.54	3.2989 (18)	137

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

Data collection: *CrystalClear* (Rigaku/MS, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *pubCIF* (Westrip, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2602).

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supplementary materials

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2-Pyridone: monoclinic polymorph

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Comment

Crystals of the monoclinic polymorph of 2-pyridone, (I), were isolated during an on-going study into the phenomenon of co-crystal formation (Broker & Tiekink, 2007; Ellis *et al.*, 2009). The orthorhombic form of (I) has been characterized previously (Penfold, 1953; Ohms *et al.*, 1984; Yang & Craven, 1998).

In (I), two independent molecules comprise the asymmetric unit, Fig. 1, and these are virtually identical as seen in the r.m.s. values for bond distances and angles of 0.0025 Å and 0.184 °, respectively (Spek, 2009). Each molecule is essentially planar with the maximum deviation of 0.0102 (14) Å found for the C2 atom in the N1-molecule and 0.0029 (14) Å for the C6 atom in the N2-molecule. The pattern of bond distances matches those in the previously determined orthorhombic form.

The crystal packing in (I) is sustained by eight-membered $\{\cdots\text{HNC(O)}\}_2$ amide synthons whereby the two independent molecules are linked, Table 1 and Fig. 1. The dimeric aggregate is effectively planar with the dihedral between the two 2-pyridone rings being 7.88 (6) °, The dimers are connected into zigzag layers in the *ac* plane *via* C—H \cdots O interactions, Table 1 and Fig. 2. The major difference between the two polymeric forms of 2-pyridone rests in the mode of association between the 2-pyridone molecules. In the orthorhombic form, the molecules are lined into supramolecular helical chains through a continuing sequence of $\{\cdots\text{HNC(O)}\}$ links.

Experimental

2-Hydroxypyridine (Fluka) was dissolved in chloroform and layered with hexanes. Large rod-like colourless crystals formed within a week.

Refinement

The N- and C-bound H-atoms were placed in calculated positions (N—H = 0.88 Å and C—H 0.95 Å) and were included in the refinement in the riding model approximation with $U_{\text{iso}}(\text{H})$ set to $1.2U_{\text{eq}}(\text{N}, \text{C})$.

Figures

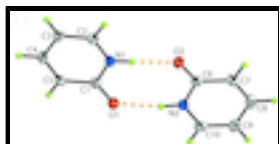


Fig. 1. Molecular structures of the two independent molecules comprising the asymmetric unit in (I), showing atom-labelling scheme and displacement ellipsoids at the 50% probability level. The molecules are connected by N—H \cdots O hydrogen bonds (orange dashed lines).

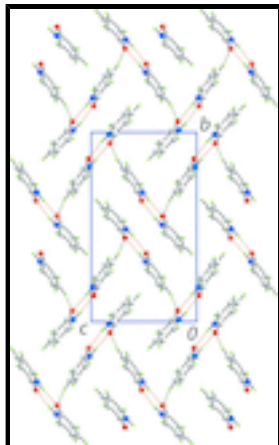


Fig. 2. View of the stacking of layers along the *b* axis in crystal structure of (I). Colour code: O, red; N, blue; C, grey; and H, green. The N–H···O hydrogen bonds (orange) and C–H···O contacts (green) are shown as dashed lines.

2-pyridone

Crystal data

C_5H_5NO

$M_r = 95.10$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2yn$

$a = 6.2027(13)\ \text{\AA}$

$b = 16.327(4)\ \text{\AA}$

$c = 9.1046(18)\ \text{\AA}$

$\beta = 92.242(7)^\circ$

$V = 921.3(3)\ \text{\AA}^3$

$Z = 8$

$F(000) = 400$

$D_x = 1.371\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71069\ \text{\AA}$

Cell parameters from 3046 reflections

$\theta = 3.3\text{--}40.2^\circ$

$\mu = 0.10\ \text{mm}^{-1}$

$T = 98\ \text{K}$

Prism, colourless

$0.44 \times 0.39 \times 0.15\ \text{mm}$

Data collection

Rigaku AFC12K/SATURN724
diffractometer

Radiation source: fine-focus sealed tube
graphite

ω scans

Absorption correction: multi-scan
(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.840$, $T_{\max} = 1$

6582 measured reflections

1903 independent reflections

1724 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.037$

$\theta_{\max} = 26.5^\circ$, $\theta_{\min} = 2.5^\circ$

$h = -7 \rightarrow 5$

$k = -20 \rightarrow 20$

$l = -11 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

Primary atom site location: structure-invariant direct
methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring
sites

$$wR(F^2) = 0.117$$

$$S = 1.10$$

1903 reflections

127 parameters

0 restraints

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 0.275P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\max} = 0.21 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$$

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 $F^2 > 2\sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.27541 (14)	0.36020 (6)	0.47704 (10)	0.0239 (2)
N1	-0.07408 (17)	0.31779 (7)	0.48531 (12)	0.0201 (3)
H1N	-0.1007	0.3587	0.5450	0.024*
C1	0.1321 (2)	0.30993 (8)	0.43716 (14)	0.0195 (3)
C2	-0.2397 (2)	0.26660 (8)	0.44686 (15)	0.0232 (3)
H2	-0.3795	0.2769	0.4819	0.028*
C3	-0.2074 (2)	0.20065 (8)	0.35857 (15)	0.0236 (3)
H3	-0.3219	0.1641	0.3330	0.028*
C4	0.0019 (2)	0.18832 (8)	0.30615 (14)	0.0224 (3)
H4	0.0289	0.1426	0.2450	0.027*
C5	0.1649 (2)	0.24113 (8)	0.34226 (14)	0.0209 (3)
H5	0.3033	0.2324	0.3039	0.025*
O2	-0.14759 (15)	0.44304 (6)	0.67815 (11)	0.0263 (3)
N2	0.19925 (17)	0.48837 (7)	0.67120 (12)	0.0204 (3)
H2N	0.2238	0.4519	0.6027	0.024*
C6	-0.0049 (2)	0.49182 (8)	0.72495 (14)	0.0199 (3)
C7	-0.0344 (2)	0.55309 (8)	0.83511 (15)	0.0236 (3)
H7	-0.1717	0.5592	0.8765	0.028*
C8	0.1311 (2)	0.60263 (9)	0.88132 (16)	0.0267 (3)
H8	0.1078	0.6427	0.9547	0.032*
C9	0.3370 (2)	0.59536 (9)	0.82168 (17)	0.0276 (3)
H9	0.4526	0.6299	0.8539	0.033*
C10	0.3652 (2)	0.53746 (9)	0.71679 (15)	0.0243 (3)
H10	0.5022	0.5313	0.6751	0.029*

supplementary materials

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0186 (5)	0.0256 (5)	0.0277 (5)	-0.0021 (4)	0.0025 (4)	-0.0048 (4)
N1	0.0186 (6)	0.0198 (5)	0.0219 (5)	0.0010 (4)	0.0027 (4)	-0.0035 (4)
C1	0.0180 (6)	0.0210 (6)	0.0195 (6)	0.0012 (5)	0.0000 (5)	0.0018 (5)
C2	0.0178 (6)	0.0248 (7)	0.0272 (7)	-0.0013 (5)	0.0026 (5)	-0.0022 (5)
C3	0.0208 (7)	0.0220 (7)	0.0281 (7)	-0.0021 (5)	0.0013 (5)	-0.0036 (5)
C4	0.0244 (7)	0.0202 (6)	0.0227 (6)	0.0036 (5)	-0.0004 (5)	-0.0025 (5)
C5	0.0179 (6)	0.0239 (7)	0.0211 (6)	0.0031 (5)	0.0031 (5)	-0.0010 (5)
O2	0.0206 (5)	0.0245 (5)	0.0342 (5)	-0.0041 (4)	0.0062 (4)	-0.0078 (4)
N2	0.0209 (6)	0.0183 (5)	0.0221 (5)	-0.0003 (4)	0.0029 (4)	-0.0014 (4)
C6	0.0191 (6)	0.0183 (6)	0.0222 (6)	0.0011 (5)	0.0009 (5)	0.0029 (5)
C7	0.0212 (6)	0.0252 (7)	0.0245 (7)	0.0031 (5)	0.0025 (5)	-0.0007 (5)
C8	0.0268 (7)	0.0262 (7)	0.0270 (7)	0.0035 (5)	-0.0010 (6)	-0.0063 (5)
C9	0.0227 (7)	0.0256 (7)	0.0342 (8)	-0.0026 (5)	-0.0024 (6)	-0.0043 (6)
C10	0.0176 (6)	0.0251 (7)	0.0304 (7)	-0.0016 (5)	0.0015 (5)	0.0016 (6)

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

O1—C1	1.2529 (16)	O2—C6	1.2530 (16)
N1—C2	1.3597 (17)	N2—C10	1.3567 (17)
N1—C1	1.3743 (17)	N2—C6	1.3762 (17)
N1—H1N	0.8800	N2—H2N	0.8800
C1—C5	1.4365 (18)	C6—C7	1.4335 (18)
C2—C3	1.3633 (19)	C7—C8	1.3607 (19)
C2—H2	0.9500	C7—H7	0.9500
C3—C4	1.4151 (18)	C8—C9	1.412 (2)
C3—H3	0.9500	C8—H8	0.9500
C4—C5	1.3590 (19)	C9—C10	1.360 (2)
C4—H4	0.9500	C9—H9	0.9500
C5—H5	0.9500	C10—H10	0.9500
C2—N1—C1	124.33 (11)	C10—N2—C6	124.37 (11)
C2—N1—H1N	117.8	C10—N2—H2N	117.8
C1—N1—H1N	117.8	C6—N2—H2N	117.8
O1—C1—N1	120.32 (11)	O2—C6—N2	120.04 (12)
O1—C1—C5	124.83 (12)	O2—C6—C7	124.99 (12)
N1—C1—C5	114.84 (11)	N2—C6—C7	114.96 (11)
N1—C2—C3	120.67 (12)	C8—C7—C6	121.03 (12)
N1—C2—H2	119.7	C8—C7—H7	119.5
C3—C2—H2	119.7	C6—C7—H7	119.5
C2—C3—C4	118.00 (12)	C7—C8—C9	120.93 (13)
C2—C3—H3	121.0	C7—C8—H8	119.5
C4—C3—H3	121.0	C9—C8—H8	119.5
C5—C4—C3	120.77 (12)	C10—C9—C8	118.12 (13)
C5—C4—H4	119.6	C10—C9—H9	120.9
C3—C4—H4	119.6	C8—C9—H9	120.9

C4—C5—C1	121.36 (12)	N2—C10—C9	120.59 (12)
C4—C5—H5	119.3	N2—C10—H10	119.7
C1—C5—H5	119.3	C9—C10—H10	119.7
C2—N1—C1—O1	179.47 (12)	C10—N2—C6—O2	-178.77 (12)
C2—N1—C1—C5	-1.04 (18)	C10—N2—C6—C7	0.61 (18)
C1—N1—C2—C3	2.1 (2)	O2—C6—C7—C8	178.83 (13)
N1—C2—C3—C4	-1.3 (2)	N2—C6—C7—C8	-0.51 (19)
C2—C3—C4—C5	-0.4 (2)	C6—C7—C8—C9	0.2 (2)
C3—C4—C5—C1	1.5 (2)	C7—C8—C9—C10	0.0 (2)
O1—C1—C5—C4	178.72 (12)	C6—N2—C10—C9	-0.4 (2)
N1—C1—C5—C4	-0.74 (18)	C8—C9—C10—N2	0.1 (2)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1n \cdots O2	0.88	1.86	2.7450 (16)	177
N2—H2n \cdots O1	0.88	1.92	2.7915 (16)	171
C2—H2 \cdots O1 ⁱ	0.95	2.53	3.3943 (18)	150
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Symmetry codes: (i) $x-1, y, z$; (ii) $x+1/2, -y+1/2, z-1/2$.

Fig. 1

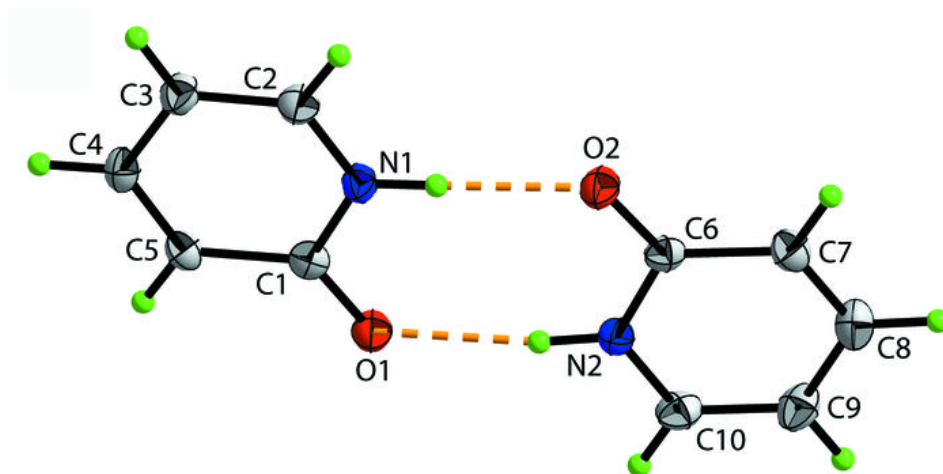


Fig. 2

