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3-(2-Oxo-2*H*-pyridin-1-yl)phthalonitrile

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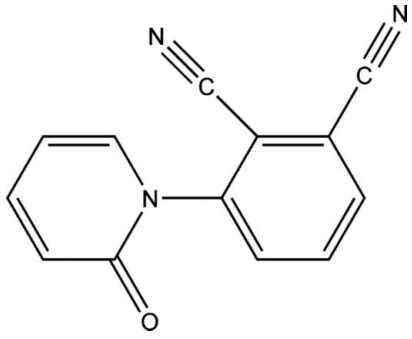
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.100; data-to-parameter ratio = 15.8.

In the title compound, $C_{13}H_7N_3O$, the dihedral angle between the pyridine and the benzene ring is 65.94 (7)°. In the crystal structure, molecules are linked by a pair of C—H···N hydrogen bonds into a centrosymmetric dimer.

Related literature

For related literature, see: Leznoff & Lever (1989–1996); Subbiah Pandi *et al.* (2002); Yu *et al.* (2006).



Experimental

Crystal data

$C_{13}H_7N_3O$
M_r = 221.22
Monoclinic, $P2_1/n$
a = 8.132 (6) Å
b = 11.739 (6) Å
c = 11.224 (6) Å
β = 97.21 (3)°
V = 1063.0 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 173 (2) K
0.50 × 0.10 × 0.05 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: none
10183 measured reflections
2438 independent reflections
1736 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.100
S = 1.09
2438 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···N2^{i}	0.95	2.60	3.530 (3)	165

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

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2004); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2353).

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Yu, H.-Y., Xue, J.-P., Chen, N.-S. & Huang, J.-L. (2006). *Acta Cryst.* E**62**, o480–o481.

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supplementary materials

Acta Cryst. (2007). E**63**, o2434 [**doi:10.1107/S1600536807017096**]

3-(2-Oxo-2*H*-pyridin-1-yl)phthalonitrile

J.-P. Xue, H.-L. Zhu, N.-S. Chen and J.-L. Huang

Comment

Substituted phthalonitriles have been used as starting materials for phthalocyanines. Phthalocyanines and metallophthalocyanines have been investigated for many years because of their wide range of applications, including use in chemical sensors, electrochromism, batteries, semiconductor materials,liquid crystals, Langmuir- Blodgett films and non-linear optics (Leznoff & Lever, 1989-1996; Huang *et al.*, 2005; Huang *et al.*, 2006). We report here the crystal structure of the title compound, (I).

The molecular structure of (I) is shown in Fig. 1. The benzene ring of the phthalonitrile group and the pyridinone ring make a dihedral angle of 65.94 (7)°. The C≡N bond distances [N2≡C12 = 1.1380 (12) Å and N3≡C13 = 1.1352 (19) Å] compare well with values reported in the literature (Subbiah Pandi *et al.*, 2002; Yu *et al.*, 2005, 2006). As expected, the N≡C—C angles [N2≡C12—C7 176.84 (16)° and N3≡C13—C8 179.40 (17)°] are linear.

In the crystal structure, the molecules are linked by a pair of C—H···N hydrogen bonds into a centrosymmetric dimer (Table 1).

Experimental

3-Nitrophthalonitrile (0.87 g, 5 mmol) and 2-pyridone (0.42 g, 5 mmol) were heated at 353 K in dry DMSO (10 ml) under argon atmosphere. After stirring for about 20 min, dry fine-powderd potassium carbonate (1.4 g, 10 mmol) was added portionwise over 2 h with vigorous stirring. The reaction was stirred for 6 h at 353 K, and ffter cooling, poured into ice-water (100 g). The reaction mixture was filtered off and washed with water until the filtrate was neutral. Recrystallization from ethanol gave a light yellow product (yield 10%). Single crystals of (I) were obtained from absolute ethanol at room temperature by slow evaporation (m.p.503-504 K).

Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

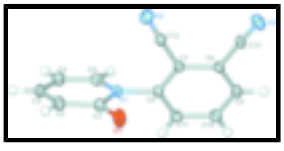
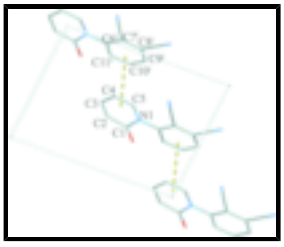


Figure 1 The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level



3-(2-Oxo-2*H*-pyridin-1-yl)phthalonitrile

Crystal data

$C_{13}H_7N_3O$
$M_r = 221.22$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 8.132$ (6) Å
$b = 11.739$ (6) Å
$c = 11.224$ (6) Å
$\beta = 97.21$ (3)º
$V = 1063.0$ (11) Å^3
$Z = 4$
$F_{000} = 456$
$D_x = 1.382$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 3144 reflections
$\theta = 12$–27.5º
$\mu = 0.09$ mm^{-1}
$T = 173$ (2) K
Plate, colourless
0.50 × 0.10 × 0.05 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: rotor target
Monochromator: graphite
$T = 173(2)$ K
ω scans
Absorption correction: none
10183 measured reflections
2438 independent reflections
1736 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 27.5$º
$\theta_{min} = 3.1$º
$h = -10 \rightarrow 10$
$k = -15 \rightarrow 15$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.100$
$S = 1.09$
2438 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 0.0958P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Extinction correction: none

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}
O1	0.31247 (16)	0.12379 (10)	0.34925 (9)	0.0625 (4)
N1	0.49154 (14)	0.27336 (9)	0.37337 (9)	0.0351 (3)
N2	0.71257 (19)	0.03731 (12)	0.26652 (12)	0.0597 (4)
N3	0.64943 (19)	0.07514 (12)	−0.08270 (12)	0.0636 (4)
C1	0.40276 (18)	0.18427 (11)	0.41863 (12)	0.0415 (3)
C2	0.4276 (2)	0.17428 (13)	0.54678 (12)	0.0494 (4)
H2A	0.3771	0.1130	0.5838	0.059*
C3	0.5210 (2)	0.24964 (15)	0.61644 (12)	0.0518 (4)
H3A	0.5337	0.2407	0.7012	0.062*
C4	0.5996 (2)	0.34088 (13)	0.56606 (13)	0.0495 (4)
H4A	0.6630	0.3946	0.6158	0.059*
C5	0.58317 (18)	0.35060 (12)	0.44602 (12)	0.0426 (3)
H5A	0.6358	0.4120	0.4106	0.051*
C6	0.47567 (16)	0.28870 (10)	0.24546 (11)	0.0340 (3)
C7	0.54359 (16)	0.20828 (10)	0.17489 (11)	0.0334 (3)
C8	0.52876 (16)	0.22445 (11)	0.05010 (11)	0.0363 (3)
C9	0.45006 (18)	0.32051 (12)	−0.00116 (12)	0.0437 (3)
H9A	0.4418	0.3321	−0.0855	0.052*
C10	0.38409 (19)	0.39884 (12)	0.07032 (13)	0.0459 (4)
H10A	0.3298	0.4645	0.0349	0.055*
C11	0.39565 (18)	0.38340 (11)	0.19317 (12)	0.0410 (3)
H11A	0.3486	0.4379	0.2416	0.049*
C12	0.63438 (18)	0.11190 (11)	0.22724 (11)	0.0396 (3)
C13	0.59691 (19)	0.14098 (12)	−0.02375 (12)	0.0426 (3)

Atomic displacement parameters (Å^2)

U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

O1	0.0785 (9)	0.0619 (7)	0.0466 (6)	−0.0349 (6)	0.0061 (6)	−0.0005 (5)
N1	0.0397 (7)	0.0339 (5)	0.0324 (5)	−0.0030 (5)	0.0072 (4)	−0.0011 (5)
N2	0.0674 (10)	0.0559 (8)	0.0550 (8)	0.0180 (7)	0.0040 (7)	0.0084 (7)
N3	0.0749 (11)	0.0649 (9)	0.0555 (8)	0.0055 (8)	0.0254 (7)	−0.0114 (7)
C1	0.0472 (9)	0.0402 (7)	0.0379 (7)	−0.0059 (6)	0.0087 (6)	0.0024 (6)
C2	0.0562 (10)	0.0537 (9)	0.0397 (7)	−0.0022 (7)	0.0110 (7)	0.0098 (7)
C3	0.0536 (10)	0.0686 (10)	0.0327 (6)	0.0110 (8)	0.0041 (6)	0.0010 (7)
C4	0.0503 (10)	0.0533 (9)	0.0433 (8)	0.0001 (7)	−0.0001 (6)	−0.0125 (7)
C5	0.0423 (8)	0.0381 (7)	0.0474 (8)	−0.0035 (6)	0.0058 (6)	−0.0064 (6)
C6	0.0360 (7)	0.0336 (7)	0.0331 (6)	−0.0043 (5)	0.0074 (5)	0.0013 (5)
C7	0.0330 (7)	0.0336 (6)	0.0340 (6)	−0.0019 (5)	0.0055 (5)	0.0026 (5)
C8	0.0346 (7)	0.0402 (7)	0.0353 (6)	−0.0014 (5)	0.0090 (5)	0.0005 (6)
C9	0.0473 (9)	0.0492 (8)	0.0354 (7)	0.0027 (7)	0.0086 (6)	0.0099 (6)
C10	0.0500 (9)	0.0405 (7)	0.0483 (8)	0.0078 (6)	0.0102 (6)	0.0127 (6)
C11	0.0451 (9)	0.0343 (7)	0.0458 (7)	0.0028 (6)	0.0137 (6)	0.0016 (6)
C12	0.0442 (9)	0.0402 (7)	0.0347 (7)	0.0033 (6)	0.0056 (6)	−0.0012 (6)
C13	0.0462 (9)	0.0494 (8)	0.0337 (7)	−0.0003 (7)	0.0108 (6)	0.0024 (6)

Geometric parameters (Å, °)

O1—C1	1.2272 (17)	C5—H5A	0.95
N1—C5	1.3747 (17)	C6—C11	1.3813 (19)
N1—C1	1.4019 (18)	C6—C7	1.3905 (18)
N1—C6	1.4366 (17)	C7—C8	1.4036 (18)
N2—C12	1.1380 (18)	C7—C12	1.4358 (19)
N3—C13	1.1352 (19)	C8—C9	1.386 (2)
C1—C2	1.432 (2)	C8—C13	1.439 (2)
C2—C3	1.350 (2)	C9—C10	1.373 (2)
C2—H2A	0.95	C9—H9A	0.95
C3—C4	1.402 (2)	C10—C11	1.382 (2)
C3—H3A	0.95	C10—H10A	0.95
C4—C5	1.342 (2)	C11—H11A	0.95
C4—H4A	0.95		
C5—N1—C1	122.86 (11)	C11—C6—N1	120.26 (11)
C5—N1—C6	118.96 (11)	C7—C6—N1	119.47 (11)
C1—N1—C6	118.03 (10)	C6—C7—C8	119.09 (12)
O1—C1—N1	119.74 (12)	C6—C7—C12	121.50 (11)
O1—C1—C2	126.01 (13)	C8—C7—C12	119.37 (11)
N1—C1—C2	114.25 (12)	C9—C8—C7	120.12 (12)
C3—C2—C1	121.78 (14)	C9—C8—C13	120.41 (12)
C3—C2—H2A	119.1	C7—C8—C13	119.46 (12)
C1—C2—H2A	119.1	C10—C9—C8	119.76 (13)
C2—C3—C4	121.25 (13)	C10—C9—H9A	120.1
C2—C3—H3A	119.4	C8—C9—H9A	120.1
C4—C3—H3A	119.4	C9—C10—C11	120.83 (13)
C5—C4—C3	118.48 (14)	C9—C10—H10A	119.6
C5—C4—H4A	120.8	C11—C10—H10A	119.6
C3—C4—H4A	120.8	C6—C11—C10	119.92 (13)
C4—C5—N1	121.18 (14)	C6—C11—H11A	120.0

C4—C5—H5A	119.4	C10—C11—H11A	120.0
N1—C5—H5A	119.4	N2—C12—C7	176.84 (16)
C11—C6—C7	120.26 (12)	N3—C13—C8	179.40 (17)
C5—N1—C1—O1	174.04 (14)	C11—C6—C7—C8	−0.36 (19)
C6—N1—C1—O1	−1.4 (2)	N1—C6—C7—C8	−179.45 (11)
C5—N1—C1—C2	−5.38 (19)	C11—C6—C7—C12	176.94 (13)
C6—N1—C1—C2	179.18 (12)	N1—C6—C7—C12	−2.14 (19)
O1—C1—C2—C3	−175.48 (16)	C6—C7—C8—C9	1.18 (19)
N1—C1—C2—C3	3.9 (2)	C12—C7—C8—C9	−176.18 (13)
C1—C2—C3—C4	−0.7 (2)	C6—C7—C8—C13	−179.26 (12)
C2—C3—C4—C5	−1.5 (2)	C12—C7—C8—C13	3.38 (19)
C3—C4—C5—N1	0.1 (2)	C7—C8—C9—C10	−1.1 (2)
C1—N1—C5—C4	3.6 (2)	C13—C8—C9—C10	179.32 (14)
C6—N1—C5—C4	179.00 (13)	C8—C9—C10—C11	0.2 (2)
C5—N1—C6—C11	−63.99 (18)	C7—C6—C11—C10	−0.5 (2)
C1—N1—C6—C11	111.63 (15)	N1—C6—C11—C10	178.57 (12)
C5—N1—C6—C7	115.10 (14)	C9—C10—C11—C6	0.6 (2)
C1—N1—C6—C7	−69.28 (17)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2A···N2^{i}	0.95	2.60	3.530 (3)	165

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

Fig. 1

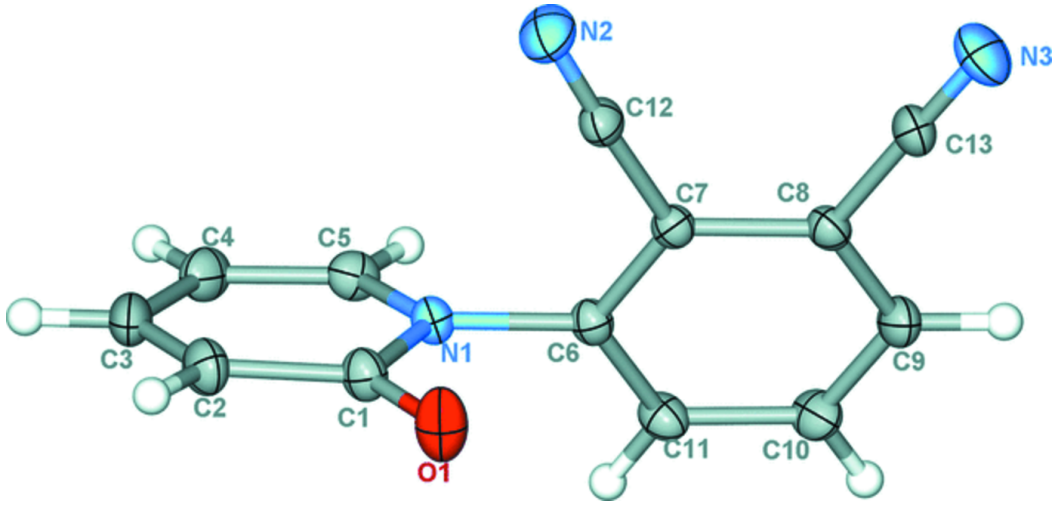


Fig. 2