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3-(*N*-Phthalimidomethyl)pyridine

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Key indicators

Single-crystal X-ray study
T = 130 K
Mean σ(C–C) = 0.010 Å
R factor = 0.062
wR factor = 0.160
Data-to-parameter ratio = 15.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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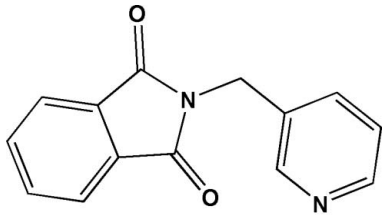
In the crystal structure of the title compound, $C_{14}H_{10}N_2O_2$, there are strong π–π interactions between molecules, resulting in a one-dimensional chain structure.

Comment

Interest in imine derivatives has increased greatly during recent years due to their different applications in various areas. In this paper, we report a new imine derivative, 3-(*N*-phthalimidomethyl)pyridine, (I).



(I)

Compound (I) is a primary amine of the form RNH_2, protected with phthalimide. The phthalimide group is planar, with a maximum deviation of 0.013 (1) Å for atom C6. The pyridine ring is essentially planar [maximum deviation of 0.007 (1) Å for atom C12]. The dihedral angle between the planes of these above-mentioned groups is 67.46 (2)° (Fig. 1). Selected bond lengths and angles are listed in Table 1. The twist in the molecule occurs at atom C14, the C10—C14—N2—C7 torsion angle being 80.07 (3)°.

There are two types of strong π–π interactions between molecules (Fig. 2). The shortest distance between adjacent pyridyl rings is only 3.267 (3) Å and the shortest distance between phthalimide groups is 2.923 (4) Å. Molecules of (I) extend into a one-dimensional chain structure through these

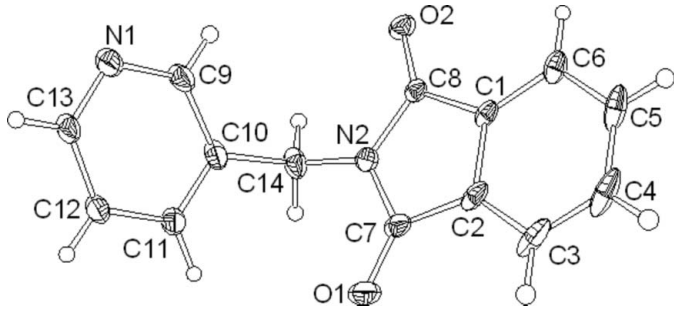


Figure 1
A view of (I), with 30% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii.

strong π–π interactions. There are no significant interactions between the chains.

Experimental

A mixture of phthalic anhydride (0.074 g, 0.5 mmol) and 3-(aminomethyl)pyridine (0.054 g, 0.5 mmol) in CH_3CN (15 ml) was heated to 333 K for 1 h with vigorous stirring. After cooling, the reaction mixture was filtered and well shaped crystals of (I) were obtained from the mother liquor by slow evaporation at room temperature for several days.

Crystal data

$C_{14}H_{10}N_2O_2$
M_r = 238.24
Triclinic, $P\overline{1}$
a = 7.13 (4) Å
b = 8.05 (4) Å
c = 10.57 (7) Å
α = 91.84 (8)°
β = 100.53 (9)°
γ = 109.15 (10)°
V = 561 (6) Å^3
Z = 2
D_x = 1.413 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 62 reflections
θ = 2.7–27.5°
μ = 0.10 mm^{-1}
T = 130.2 K
Prism, white
0.55 × 0.20 × 0.10 mm

Data collection

Siemeeens SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.977, T_{max} = 0.990
4353 measured reflections
2526 independent reflections
1950 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°
$h = -9 \rightarrow 7$
$k = -9 \rightarrow 10$
$l = -13 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.160
S = 1.08
2526 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0723P)^2 + 0.2262P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

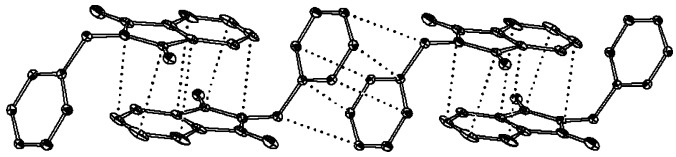


Figure 2
View of the one-dimensional chain structure, showing two types of π–π interactions (dashed lines).

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.218 (7)	N2—C8	1.396 (9)
O2—C8	1.214 (6)	N2—C7	1.399 (7)
N1—C13	1.341 (6)	N2—C14	1.462 (7)
N1—C9	1.345 (7)		
C13—N1—C9	116.3 (3)	C8—N2—C14	123.90 (19)
C8—N2—C7	111.6 (2)	C7—N2—C14	124.5 (3)

The H atoms were positioned geometrically and refined using a riding model, with C—H 0.93 − 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART* and *SAINT* (Siemens, 1994); data reduction: *SAINT* and *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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