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2-(5-Chloropyridin-2-yl)-2,3-dihydro-1*H*-isoindole-1,3-dione

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.119
Data-to-parameter ratio = 14.3

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

The title compound, $C_{13}H_7ClN_2O_2$, crystallizes in the centrosymmetric group $P\overline{1}$ with one molecule in the asymmetric unit. The torsion angle between the phthalimidyl and chloropyridine moieties is about 45°.

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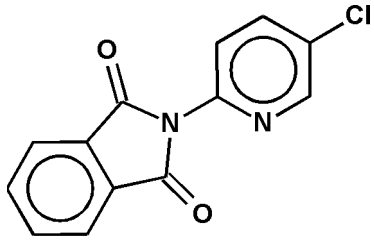
Comment

The title compound, (I), a potential substrate for the synthesis of biologically active compounds, forms centrosymmetric triclinic crystals with one molecule in the asymmetric unit. Two rigid groups, phthalimidyl and chloropyridine, are connected in the molecule by a single C—N bond with the interplanar angle equal to 43.87 (4)°.



(I)

Experimental

The title compound was obtained by melting 2-amino-5-chloropyridine with phthalic anhydride. After reaction and cooling, the solid mixture was dissolved in hot tetrahydrofuran and crystals were grown by slow cooling (m.p. 424–425 K).

Crystal data

$C_{13}H_7ClN_2O_2$
M_r = 258.66
Triclinic, $P\overline{1}$
a = 7.494 (1) Å
b = 7.974 (2) Å
c = 10.303 (2) Å
α = 100.58 (3)°
β = 98.38 (3)°
γ = 107.98 (3)°
V = 562.00 (19) Å^3
Z = 2
D_x = 1.528 Mg m^{-3}
D_m = 1.530 Mg m^{-3}
D_m measured by flotation
Mo $K\alpha$ radiation
Cell parameters from 1144 reflections
θ = 3.4–24.5°
μ = 0.33 mm^{-1}
T = 298 (2) K
Prism, colourless
0.38 × 0.38 × 0.15 mm

Data collection

Kuma Diffraction KM4CCD diffractometer
ω scans
3767 measured reflections
2342 independent reflections
2244 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 27.1°
$h = -9 \rightarrow 5$
$k = -10 \rightarrow 10$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0757P)^2 + 0.1249P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.040$	$(\Delta/\sigma)_{max} = 0.035$
$wR(F^2) = 0.120$	$\Delta\rho_{max} = 0.24$ e Å^{-3}
$S = 1.05$	$\Delta\rho_{min} = -0.27$ e Å^{-3}
2342 reflections	Extinction correction: *SHELXL*97
164 parameters	Extinction coefficient: 0.104 (13)
H atoms constrained	

Table 1
Selected geometric parameters (Å, °).

Cl1—C12	1.7297 (15)	N2—C8	1.4192 (18)
O1—C8	1.2023 (17)	N2—C9	1.4215 (17)
O2—C1	1.2038 (17)	C9—C10	1.385 (2)
N1—C9	1.3323 (19)	C10—C11	1.383 (2)
N1—C13	1.3382 (18)	C11—C12	1.383 (2)
N2—C1	1.4113 (16)	C12—C13	1.382 (2)
C9—N1—C13	117.28 (12)	N2—C8—C7	105.66 (11)
O2—C1—N2	125.01 (13)	N1—C9—N2	115.39 (12)
N2—C1—C2	105.81 (11)	C10—C9—N2	120.16 (12)
O1—C8—N2	125.38 (13)	C11—C12—C13	120.00 (13)
C9—N2—C1—O2	1.8 (2)	C8—N2—C9—N1	−45.09 (18)
C1—N2—C9—N1	136.68 (14)		

Data collection: *Kuma KM4CCD Software* (Kuma, 1999); cell refinement: *Kuma KM4CCD Software*; data reduction: *Kuma KM4CCD Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

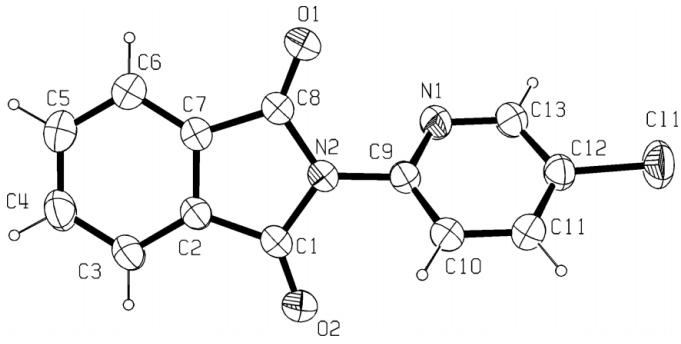


Figure 1
View of the title molecule. The displacement ellipsoids are drawn at the 50% probability level.

References

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Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
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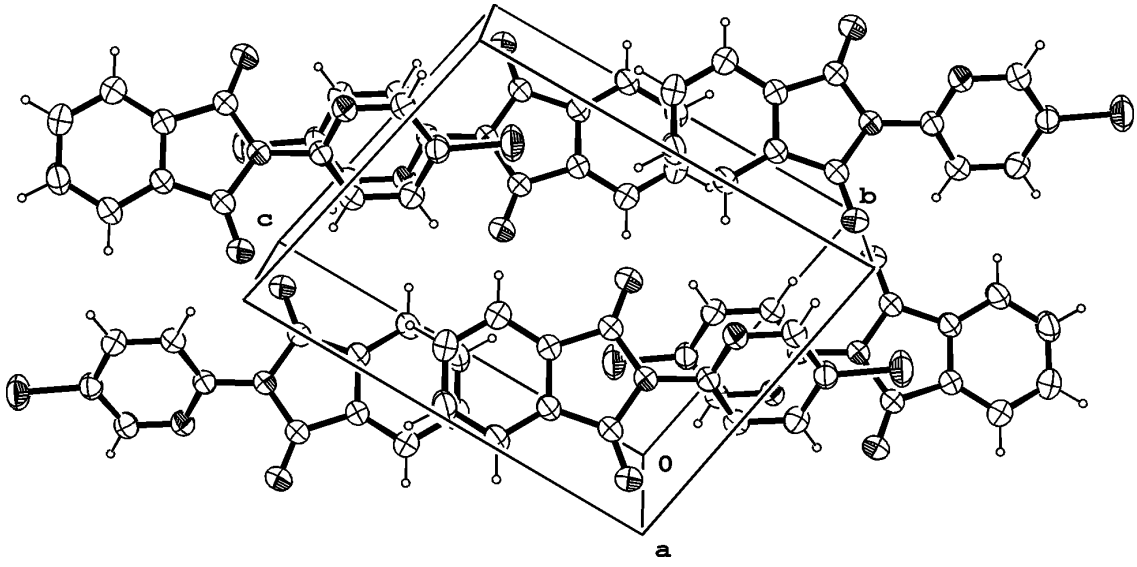

Figure 2
View of the packing of the molecules in the crystal structure of the title molecule.