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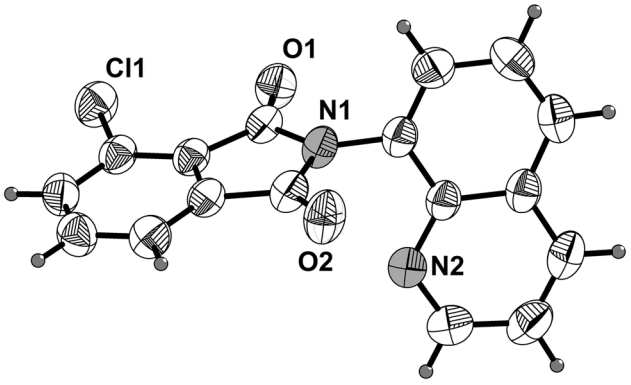
The crystal structure of 4-chloro-2-(quinolin-8-yl) isoindoline-1,3-dione, $C_{17}H_9ClN_2O_2$



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Abstract

$C_{17}H_9ClN_2O_2$, monoclinic, $P2_1/c$ (no. 14), a = 13.6888(4) Å, b = 8.3775(2) Å, c = 12.9180(3) Å, β = 110.515(3)°, V = 1387.46(7) Å^3, Z = 4, $R_{gt}(F)$ = 0.0420, $wR_{ref}(F^2)$ = 0.1224, T = 293(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.32 × 0.25 × 0.17 mm
Wavelength:	Cu $K\alpha$ radiation (1.54184 Å)
μ:	2.52 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	70.1°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8658, 2619, 0.026
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 2344
$N(param)_{refined}$:	199
Programs:	CrysAlis^{PRO} [1], Olex2 [2], SHELX [3, 4]

Source of material

All starting materials were used as received. The title compound was synthesized solvent-freely according to a reference [5]: 1.44 g 8-aminoquinoline (10 mmol), 1.82 g 4-chlorophthalic anhydride (10 mmol) were mixed well in a test tube. The mixture was heated moderately until the water vapour was no longer obviously observed, then extracted with about 100 mL ethanol, cooled to room temperature, and filtered. The crystals suitable for X-ray single analysis were harvested by evaporating the ethanolic solution, yield 42% (based on 8-aminoquinoline).

Experimental details

The structure was solved by direct methods with the SHELXS-2018 program. All H atoms were positioned with idealized geometry and refined isotropically (U_{iso}(H) = 1.2U_{eq}(C)) using a riding model with C–H = 0.93 Å. A disorder of the chloro substituent is seen in the difference Fourier map (difference peak at C10), which was not included because of the large ratio between the higher and the lower occupied site.

Comment

Known to own a potent biological activity such as cytotoxicity to various cell lines, phthalimide and its derivatives, especially *N*-pyridyl and *N*-quinolyl substituted phthalimides aroused more and more interest [5, 6]. In addition, *N*-quinolyl substituted phthalimides have also been studied in coordination chemistry [7]. Some crystal structures of *N*-quinolyl substituted amides containing the group of 1,3-dione have been reported elsewhere [8–12]. We

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.64581 (13)	0.55654 (19)	0.27861 (14)	0.0444 (4)
C2	0.62941 (13)	0.6014 (2)	0.38295 (14)	0.0454 (4)
C3	0.81617 (13)	0.6443 (2)	0.64089 (13)	0.0451 (4)
C4	0.84035 (14)	0.6650 (2)	0.75619 (14)	0.0492 (4)
C5	0.73132 (13)	0.4564 (2)	0.30417 (14)	0.0472 (4)
C6	0.72986 (13)	0.5459 (2)	0.58256 (14)	0.0469 (4)
C7	0.59386 (14)	0.6020 (2)	0.16999 (14)	0.0474 (4)
C8	0.77210 (14)	0.4303 (2)	0.42573 (15)	0.0513 (4)
C9	0.63071 (16)	0.5461 (2)	0.08896 (15)	0.0544 (4)
H9	0.597455	0.576464	0.015740	0.065*
C10	0.76824 (16)	0.3986 (2)	0.22452 (16)	0.0561 (4)
H10	0.825615	0.330859	0.242755	0.067*
C11	0.67046 (15)	0.4761 (2)	0.63512 (17)	0.0563 (5)
H11	0.614226	0.412014	0.595716	0.068*
C12	0.92798 (17)	0.7600 (2)	0.81295 (17)	0.0607 (5)
H12	0.946958	0.776446	0.888658	0.073*
C13	0.77685 (17)	0.5906 (2)	0.80822 (15)	0.0582 (5)
H13	0.792248	0.603691	0.883777	0.070*
C14	0.71602 (17)	0.4461 (2)	0.11624 (17)	0.0589 (5)
H14	0.739093	0.409690	0.060773	0.071*
C15	0.69405 (18)	0.5007 (3)	0.74909 (18)	0.0623 (5)
H15	0.652174	0.454646	0.784153	0.075*
C16	0.98421 (17)	0.8269 (3)	0.7565 (2)	0.0703 (6)
H16	1.042580	0.888810	0.792759	0.084*
C17	0.95267 (18)	0.8009 (3)	0.6419 (2)	0.0685 (6)
H17	0.991704	0.848683	0.604189	0.082*
Cl1	0.48669 (4)	0.72652 (6)	0.13399 (4)	0.06075 (19)
N1	0.70774 (11)	0.52013 (19)	0.46719 (12)	0.0499 (4)
N2	0.87224 (13)	0.7144 (2)	0.58437 (13)	0.0561 (4)
O1	0.56500 (11)	0.68757 (17)	0.39680 (11)	0.0590 (4)
O2	0.84377 (12)	0.3479 (2)	0.48067 (12)	0.0713 (4)

here reported the crystal structure of the title compound, 4-chloro-2-(quinolin-8-yl)isoindoline-1,3-dione (CQDO). All atoms of the 8-hydroxyquinolinyl group and the phthalimide moiety are nearly co-planar, respectively. There are weak non-classical hydrogen bonds, C–H···Cl and C–H···O, together with intermolecular C–H···π interactions. All the bond lenths of CQDO are comparable with its analogues [5, 7, 12].

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