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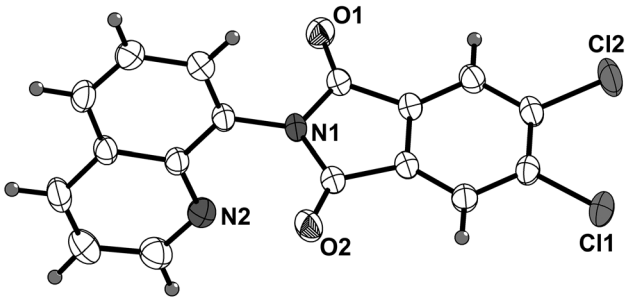
The crystal structure of 5,6-dichloro-2-(quinolin-8-yl)isoindoline-1,3-dione, $C_{17}H_8Cl_2N_2O_2$



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Abstract

$C_{17}H_8Cl_2N_2O_2$, triclinic, $P\bar{1}$ (no. 2), a = 7.9032(2) Å, b = 9.0843(3) Å, c = 10.8051(2) Å, α = 85.2310(10)°, β = 85.0270(10)°, γ = 71.013(2)°, V = 729.54(3) Å^3, Z = 2, R_{gt} (F) = 0.0417, wR_{ref} (F^2) = 0.1051, 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:	0.22 × 0.13 × 0.11 mm
Wavelength:	Cu$K\alpha$ radiation (1.54184 Å)
μ:	4.10 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	66.6°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	4172, 2584, 0.015
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2489
$N(param)_{refined}$:	208
Programs:	SuperNova [1], Olex2 [2], SHELX [3, 4]

Source of material

The title compound, 5,6-dichloro-2-(quinolin-8-yl)isoindoline- 1,3-dione, has been synthesized according to the literature [5]. A mixture of 1.175 g 4,5-dichlorophthalic acid (5 mmol) and 1.44 g 8-aminoquinoline (10 mmol) in 2 mL DMF was heated at 393 K for 30 min. Then 30 mL ethanol (95%) was added. Any insoluble matter was removed by filtration. Crystals of the title compound were harvested after slowly evaporation of the filtrate, yield 56% (based on 8-aminoquinoline).

Experimental details

The structure was solved by direct methods with the SHELXS-program. All hydrogen atoms were positioned with idealized geometry and refined isotropic (U_{iso}(H) = 1.2U_{eq}(C)) using a riding model with C—H = 0.93 Å.

Comment

Thalidomide, lenalidomide and phthalimides are famous for their biological activities [6]. Some 5,6–Di-chloride-substituted phthalimides, such as 5,6-di-chloro-2-(2-hydroxyphenyl)-isoindoline-1,3-dione [5], 5,6-dichloro-2-(3-methoxyphenyl) isoindoline-1,3-dione [7], 5,6-dichloro -2-(2-fluorophenyl)isoindoline-1,3-dione [8] and 2-(4-acetyl-2,6-dimethylphenyl)-5,6-dichloro-1*H*-iso-indole-1,3(2*H*)-dione [9] have been reported. There are also some crystal structures of *N*-quinolyl substituted phthalimides have been published, including 2-(quinolin-8-yl)-1*H*-isoindole-1,3(2*H*)-dione and its silver complex [10, 11], and 5-phenyl-2-(quinolin-8-yl)-1*H*-isoindole-1,3(2*H*)-dione [12]. Recently, two very similar structure, 4-chloro-2-(quinolin-8-yl)-isoindoline-1,3-dione [13] and 4-chloro-2-(quinolin-8-yl)-isoindoline-1,3-dione [14], have

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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}
Cl1	0.06929 (5)	1.20154 (5)	0.46903 (4)	0.04028 (16)
Cl2	0.16636 (7)	0.99251 (6)	0.71499 (4)	0.04909 (17)
O1	0.73179 (16)	0.49158 (14)	0.50049 (11)	0.0389 (3)
O2	0.58952 (18)	0.79890 (16)	0.14137 (11)	0.0444 (3)
N1	0.69874 (18)	0.61806 (16)	0.30415 (12)	0.0309 (3)
N2	0.66662 (19)	0.41383 (18)	0.13416 (14)	0.0359 (3)
C1	0.4576 (2)	0.83274 (18)	0.35330 (14)	0.0278 (3)
C2	0.8344 (2)	0.41590 (18)	0.15396 (14)	0.0279 (3)
C3	0.8544 (2)	0.51791 (19)	0.23960 (15)	0.0299 (3)
C4	0.5828 (2)	0.75504 (19)	0.24967 (15)	0.0308 (3)
C5	0.5012 (2)	0.74074 (17)	0.46204 (14)	0.0268 (3)
C6	0.9921 (2)	0.32078 (19)	0.09098 (14)	0.0301 (3)
C7	0.3241 (2)	0.97436 (19)	0.35238 (15)	0.0308 (3)
H7	0.294675	1.035203	0.278932	0.037*
C8	0.6557 (2)	0.59993 (18)	0.43202 (14)	0.0277 (3)
C9	0.2346 (2)	1.02311 (18)	0.46586 (15)	0.0296 (3)
C10	0.2783 (2)	0.92988 (19)	0.57536 (15)	0.0307 (3)
C11	0.4126 (2)	0.78582 (19)	0.57477 (15)	0.0311 (3)
H11	0.441158	0.722873	0.647340	0.037*
C12	1.1617 (2)	0.3293 (2)	0.11558 (16)	0.0362 (4)
H12	1.264843	0.266228	0.074564	0.043*
C13	1.0195 (2)	0.5247 (2)	0.26132 (16)	0.0358 (4)
H13	1.029106	0.593032	0.317801	0.043*
C14	1.1750 (2)	0.4291 (2)	0.19885 (17)	0.0384 (4)
H14	1.286909	0.434098	0.214366	0.046*
C15	0.9717 (3)	0.2223 (2)	0.00324 (17)	0.0396 (4)
H15	1.071413	0.157799	−0.040071	0.048*
C16	0.6562 (3)	0.3203 (2)	0.05023 (18)	0.0423 (4)
H16	0.542836	0.318805	0.034729	0.051*
C17	0.8036 (3)	0.2229 (2)	−0.01724 (18)	0.0449 (4)
H17	0.787143	0.159521	−0.075263	0.054*

been reported. 5,6–Dichloro-2-(quinolin-8-yl)isoindoline-1,3-dione crystalizes in $P\bar{1}$, with one molecule in the asymmetric unit (see the Figure). The *N*-quinolyl residue and the isoindoline-1,3-dione are co-planar, respectively and the two residues are rotatet about the C-N bond with an angle of nearly 90°. All the bond lengths are similar to the reported results [5, 7–14]. The molecules are linked by weak CH···N hydrogen bonds and van der Waals interactions.

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