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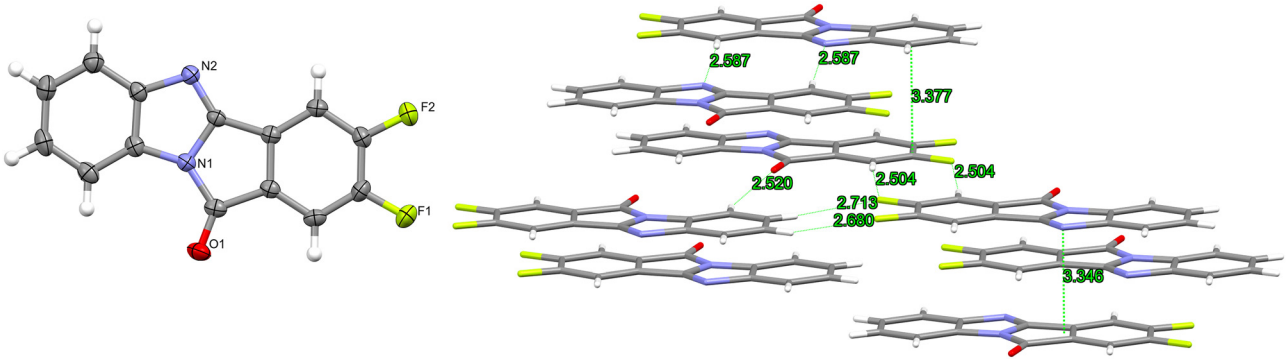
The crystal structure of 2,3-difluoro-11*H*-benzo-[4,5]imidazo[2,1-*a*]isoindol-11-one, $C_{14}H_6F_2N_2O$



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Abstract

$C_{14}H_6F_2N_2O$, triclinic, $P\bar{1}$ (no. 2), a = 5.9169(4) Å, b = 8.1225(7) Å, c = 11.6546(8) Å, α = 101.826(6)°, β = 104.661(6)°, γ = 93.190(6)°, V = 526.95(7) Å^3, Z = 2, $R_{gt}(F)$ = 0.0389, w$R_{ref}(F^2)$ = 0.0950, T = 170 K.

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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:	Yellow block
Size:	0.15 × 0.11 × 0.09 mm
Wavelength:	MoKα radiation (0.71073 Å)
μ:	0.13 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	25.0°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	3335, 1847, 0.016
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 $\sigma(I_{obs})$, 1574
$N(param)_{refined}$:	172
Programs:	Bruker [1], Olex2 [2], Shelx [3, 4]

1 Source of materials

The compound was prepared according to previous literature reports [5]. To a solution of 1,3-dione-5,6-difluoroisobenzofuran (1.84 g, 10.0 mmol) in acetic acid (AcOH, 40 mL) was added 1,2-phenylenediamine (1.08 g, 10.0 mmol), then the mixture was stirred and refluxed for 4 h. After cooling to room temperature, the precipitate was filtered and washed with ethanol to afford the crude product, which was further purified by silica gel column chromatography using dichloromethane and petroleum ether (1:10) as the mobile phase to obtain 2,3-difluoro-11*H*-benzo-[4,5]imidazo[2,1-*a*]isoindol-11-one (2.02 g, 7.90 mmol, 78.9 % yield) as a yellow solid and recrystallized from dichloromethane to obtain the title compound as yellow block crystals.

2 Experimental details

Hydrogen atoms were included using riding models implemented in the Shelxl software [3, 4]. Their U_{iso} values were set to 1.2U_{eq} of the parent atoms. Using Olex2 [2], the structure was solved with the ShelXS [3] program using Direct Methods and refined with the ShelXL [4] package.

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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}
F1	0.72741 (18)	0.64042 (14)	1.00453 (8)	0.0430 (3)
F2	0.30150 (18)	0.70198 (13)	0.89717 (9)	0.0397 (3)
O1	0.9242 (2)	0.20254 (15)	0.63280 (11)	0.0352 (3)
N1	0.5630 (2)	0.23595 (17)	0.50833 (12)	0.0252 (3)
N2	0.1998 (2)	0.29549 (17)	0.42129 (12)	0.0262 (3)
C1	0.6509 (3)	0.3873 (2)	0.70381 (14)	0.0245 (4)
C2	0.7589 (3)	0.4584 (2)	0.82472 (14)	0.0286 (4)
H2	0.908044	0.435560	0.862934	0.034*
C3	0.6338 (3)	0.5652 (2)	0.88575 (14)	0.0298 (4)
C4	0.4129 (3)	0.5992 (2)	0.82910 (15)	0.0281 (4)
C5	0.3041(3)	0.5308 (2)	0.70788 (14)	0.0263 (4)
H5	0.156091	0.556099	0.670050	0.032*
C6	0.4277 (3)	0.4222 (2)	0.64554 (14)	0.0240 (4)
C7	0.3716 (3)	0.3233 (2)	0.51956 (14)	0.0237 (4)
C8	0.7426 (3)	0.2651 (2)	0.61715 (15)	0.0263 (4)
C9	0.5064 (3)	0.1406 (2)	0.38861 (14)	0.0254 (4)
C10	0.6282 (3)	0.0315 (2)	0.32568 (16)	0.0323 (4)
H10	0.777985	0.007746	0.362126	0.039*
C11	0.5129 (3)	−0.0401 (2)	0.20499 (16)	0.0365 (5)
H11	0.587724	−0.113724	0.158561	0.044*
C12	0.2878 (3)	−0.0048 (2)	0.15110 (16)	0.0373 (5)
H12	0.215935	−0.055759	0.069835	0.045*
C13	0.1691 (3)	0.1042 (2)	0.21589 (16)	0.0334 (4)
H13	0.018467	0.126511	0.179615	0.040*
C14	0.2810 (3)	0.1788 (2)	0.33610 (14)	0.0260 (4)

3 Comment

Benzimidazole derivatives have garnered significant attention because of their widespread applications in organic electronics, such as organic light-emitting devices, organic thin-film transistors and organic photovoltaics [6]. The title compound features a planar and rigid molecular structure, ensuring both good stability and photoelectric performance. By employing arylamine and phenol derivatives, the fluorine atoms on the benzene ring can be modified, offering opportunities to further tailor the compound's photoelectric properties.

The crystal structure of the title compound is similar with the reported structure [5] of 11*H*-benzo[4,5]imidazo-[2,1-*a*]isoindol-11-one. All the atoms of the compound lie almost entirely within a single plane, encompassing carbon, nitrogen, oxygen, fluorine and hydrogen atoms, forming two five-membered and two six-membered rings (see left part of the figure). Adjacent to this core aromatic structure are the additional oxygen, fluorine, and hydrogen atoms. All the bond lengths and angles of this molecule are in the expected ranges [7].

The molecular packing diagram illustrates distinct intermolecular interactions. Notably, evident hydrogen bonding is observed between oxygen and adjacent hydrogen atoms, with a distance of 2.520 Å. Similar situations occur with fluorine and nitrogen atoms, demonstrating distances ranging from 2.504 to 2.713 Å between fluorine and hydrogen atoms, and a length of 2.587 Å for C–H···N interactions. Additionally, interlayer distances between adjacent layers approximate 3.350 Å, indicating π–π interactions between the molecular layers (see right part of the figure).

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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