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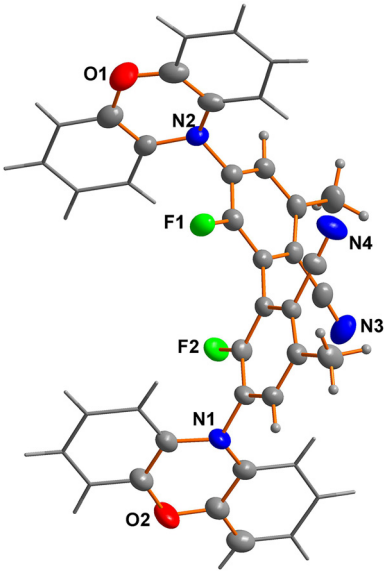
The crystal structure of 6,6′-difluoro-3,3′-dimethyl-5,5′-di(10*H*-phenoxazin-10-yl)-[1,1′-biphenyl]-2,2′-dicarbonitrile, $C_{40}H_{24}F_2N_4O_2$



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Abstract

$C_{40}H_{24}F_2N_4O_2$, monoclinic, $P2_1/c$ (no. 14), a = 11.6521(4) Å, b = 11.6491(4) Å, c = 23.0401(7) Å, β = 102.824(1)°, V = 3,049.37 (18) Å^3, Z = 4, R_{gt}(F) = 0.0431, wR_{ref}(F^2) = 0.1122, T = 190 K.

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

1 Source of materials

According to previous literature reports,[5] the title compond can be synthesized from 5,5′,6,6′-tetrafluoro-3,3′-dimethyl-[1,1′-biphenyl]-2, 2′-dicarbonitrile (3.04 g, 10.0 mmol) and caesium carbonate (3.26 g, 10.0 mmol) and 10*H*-phenoxazine (3.66 g, 20.0 mmol) in *N*,*N*- dimethylformamide (DMF, 50 mL). The mixture was stirred and refluxed for 24 h. Cooling to room temperature, the mixture was extracted with water and ethyl acetate three times. The combined organic layer was concentrated and further purified by silica gel column chromatography to a red solid (4.48 g, 7.10 mmol, 71.0 % yield) and recrystallized from dichloromethane and methanol diffusion to obtain the title compound as red block crystals.

Table 1: Data collection and handling.

Crystal:	Block
Size:	0.16 × 0.07 × 0.06 mm
Wavelength:	Ga *K*α radiation (1.34139 Å)
μ:	0.50 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω scans
θ_{max}, completeness:	53.9°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	21,409, 5,533, 0.046
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3,827
$N(param)_{refined}$:	529
Programs:	Bruker [1] Olex2 [2] SHELX[3,4]

2 Experimental details

The structure was solved with the SHELXS[3] in OLEX2,[2] structure solution program using Direct Methods and refined with the SHELXL[4] refinement package. The U_{iso} values of hydrogen atoms (C–H) were set to 1.2 U_{eq} of the parent atoms. Their U_{iso} values of hydrogen atoms (C–H,H,H) were set to 2.5 U_{eq}. All hydrogen atoms were included via riding models implemented in the SHELXL software.[3,4]

3 Comment

Thermally activated delayed fluorescence (TADF) materials have emerged as the third generation of organic

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light-emitting diodes emitters, garnering significant attention due to their theoretical achievement of 100 % internal quantum efficiency and cost-effectiveness without the reliance on precious metal elements.[6]

The efficacy of TADF materials in harnessing triplet exciton emission stems from a substantial twist angle between their electron donor and acceptor moieties, thereby reducing the overlap integral of highest occupied molecular orbital and lowest unoccupied molecular orbital. This reduction facilitates a decrease in energy difference between singlet and triplet excited states. Through thermal activation, reverse intersystem crossing enables the transformation of triplet into singlet excitons, ultimately leading to delayed fluorescence emission. The title compound exhibits phenoxazines as electron donors and a benzonitrile derivative as an acceptor. The dihedral angles between them approach 90° (see the figure), indicating the potential for achieving TADF properties. Bond lengths and angles are all in the expected ranges.[7]

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

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Author contribution: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

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