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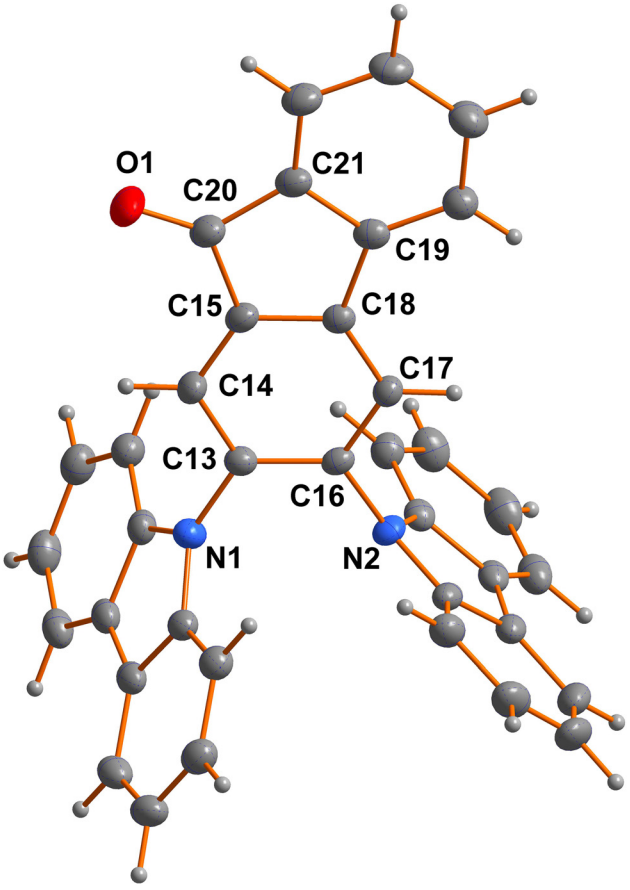
The crystal structure of 2,3-di(9*H*-carbazol-9-yl)-9*H*-fluoren-9-one, $C_{37}H_{22}N_2O$



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Abstract

$C_{37}H_{22}N_2O$, monoclinic, $P2/n$ (no. 13), a = 8.9663(3) Å, b = 9.1812(3) Å, c = 30.8083(9) Å, β = 93.714(3)°, Z = 4, V = 2530.86(14) Å^3, $R_{gt}(F)$ = 0.0445, w$R_{ref}(F^2)$ = 0.1192, T = 150 K.

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Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.15 × 0.12 × 0.10 mm
Wavelength:	CuKα radiation (1.54184 Å)
μ:	0.63 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	74.0°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9905, 4986, 0.039
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3982
$N(param)_{refined}$:	361
Programs:	Bruker [1], Olex2 [2], Shelx [3, 4]

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

1 Source of materials

A mixture of 2,3-difluoro-9*H*-fluoren-9-one (216 mg, 1 mmol), 9*H*-carbazole (367 mg, 2.2 mmol) and potassium carbonate (414 mg, 3 mmol) in 50 mL hydrofuran under nitrogen was refluxed for 12 h. After cooling down to room temperature, the product was extracted with dichloromethane and washed with water. The combined organic phase was dried over anhydrous sodium sulfate and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel using dichloromethane/petroleum to afford a yellow solid. Crystals were obtained by slow evaporation within 5 days.

2 Experimental details

Hydrogen atoms were included using riding models implemented in the Shelxl software [3, 4]. Using Olex2 [2], the structure was solved with the ShelXS [3] structure solution program and refined with the ShelXL [4] package.

3 Comment

Thermally activated delayed fluorescence (TADF) materials offer a promising avenue for future commercial organic

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
O1	1.02951 (17)	0.52811 (16)	0.24738 (5)	0.0451 (4)
N1	0.65632 (16)	0.32558 (15)	0.36732 (5)	0.0258 (3)
N2	0.56823 (15)	0.59757 (15)	0.40313 (4)	0.0225 (3)
C1	0.51130 (19)	0.27029 (18)	0.36092 (5)	0.0245 (3)
C2	0.3913 (2)	0.32477 (19)	0.33515 (5)	0.0286 (4)
H2	0.399893	0.411425	0.318646	0.034*
C3	0.2584 (2)	0.2475 (2)	0.33450 (6)	0.0321 (4)
H3	0.173639	0.283081	0.317655	0.039*
C4	0.2461 (2)	0.1182 (2)	0.35811 (6)	0.0333 (4)
H4	0.153548	0.067583	0.357025	0.040*
C5	0.3669 (2)	0.06333 (19)	0.38292 (6)	0.0309 (4)
H5	0.358323	−0.024799	0.398725	0.037*
C6	0.50229 (19)	0.13976 (18)	0.38442 (5)	0.0252 (3)
C7	0.6477 (2)	0.11435 (18)	0.40589 (5)	0.0263 (4)
C8	0.7053 (2)	0.00699 (19)	0.43436 (6)	0.0309 (4)
H8	0.643498	−0.069954	0.443336	0.037*
C9	0.8540 (2)	0.0146 (2)	0.44928 (6)	0.0342 (4)
H9	0.894413	−0.057917	0.468638	0.041*
C10	0.9456 (2)	0.1275 (2)	0.43628 (6)	0.0340 (4)
H10	1.047918	0.128895	0.446430	0.041*
C11	0.8905 (2)	0.23787 (19)	0.40883 (6)	0.0298 (4)
H11	0.952608	0.315322	0.400378	0.036*
C12	0.74075 (19)	0.23022 (18)	0.39425 (5)	0.0250 (3)
C13	0.70628 (18)	0.46012 (18)	0.35058 (5)	0.0232 (3)
C14	0.80629 (19)	0.45846 (19)	0.31750 (6)	0.0279 (4)
H14	0.840770	0.368878	0.306403	0.034*
C15	0.85368 (18)	0.58925 (19)	0.30136 (5)	0.0252 (3)
C16	0.65867 (17)	0.59324 (18)	0.36672 (5)	0.0206 (3)
C17	0.70441 (18)	0.72516 (18)	0.34937 (5)	0.0220 (3)
H17	0.668566	0.815142	0.359803	0.026*
C18	0.80329 (17)	0.72205 (18)	0.31657 (5)	0.0210 (3)
C19	0.87574 (18)	0.84156 (19)	0.29338 (5)	0.0238 (3)
C20	0.9616 (2)	0.6177 (2)	0.26712 (6)	0.0293 (4)
C21	0.96905 (19)	0.77980 (19)	0.26369 (5)	0.0260 (4)
C22	1.0510 (2)	0.8647 (2)	0.23692 (6)	0.0321 (4)
H22	1.114640	0.821644	0.217042	0.038*
C23	1.0376 (2)	1.0150 (2)	0.23993 (6)	0.0344 (4)
H23	1.091364	1.076015	0.221543	0.041*
C24	0.9464 (2)	1.0764 (2)	0.26955 (6)	0.0355 (4)
H24	0.939505	1.179437	0.271264	0.043*
C25	0.8642 (2)	0.99113 (19)	0.29698 (6)	0.0290 (4)
H25	0.802608	1.034389	0.317373	0.035*
C26	0.42219 (18)	0.65095 (17)	0.40215 (5)	0.0239 (3)
C27	0.3186 (2)	0.66548 (19)	0.36691 (6)	0.0302 (4)
H27	0.343108	0.641435	0.338236	0.036*
C28	0.1778 (2)	0.7165 (2)	0.37531 (7)	0.0382 (4)
H28	0.104553	0.727686	0.351867	0.046*
C29	0.1411 (2)	0.7519 (2)	0.41739 (7)	0.0408 (5)
H29	0.043143	0.785207	0.422126	0.049*
C30	0.2454 (2)	0.7391 (2)	0.45223 (7)	0.0357 (4)
H30	0.220116	0.764018	0.480771	0.043*
C31	0.38859 (19)	0.68897 (18)	0.44478 (6)	0.0266 (4)
C32	0.5226 (2)	0.66515 (17)	0.47236 (5)	0.0253 (3)
C33	0.5605 (2)	0.6872 (2)	0.51655 (6)	0.0337 (4)
H33	0.487976	0.721648	0.535240	0.040*
C34	0.7039 (2)	0.6583 (2)	0.53267 (6)	0.0366 (4)
H34	0.730146	0.672477	0.562745	0.044*
C35	0.8119 (2)	0.6083 (2)	0.50544 (6)	0.0346 (4)
H35	0.910815	0.590812	0.517256	0.041*
C36	0.7773 (2)	0.58380 (19)	0.46150 (5)	0.0278 (4)
H36	0.850261	0.549206	0.442986	0.033*
C37	0.63189 (19)	0.61189 (17)	0.44574 (5)	0.0224 (3)

light-emitting diode (OLED) applications as they efficiently harness both singlet (S_1) and triplet (T_1) excitons without relying on noble metals [5]. A general strategy in designing TADF molecules involve connecting the donor (D) and acceptor (A) components by σ bond. This arrangement ensures a wide separation of electron distribution and enables the realization of emission at various wavelengths by modulating the intensity of D–A pairs [6].

Herein, a TADF molecule with 9*H*-fluoren-9-one for yellow OLEDs, namely DCM, is reported. In the molecular structure, the bond length of O1–C20 is 1.210(2) Å, which belongs to the typical C=O double bonds. The C–N bond lengths of the aromatic rings were between 1.395(2) and 1.403(2) Å, while the one that connects the two rings were slightly longer, at 1.422(2) and 1.4265(18) Å, respectively. The angles of C12–N1–C1 and O1–C20–C15 were measured at 108.65(14)° and 127.14(17)° respectively. Other bond lengths and bond angles are all in the normal ranges [7, 8]. The groups O1–C20–C21–C22 and O1–C20–C21–C19 exhibit torsion angles with the value of 1.7(3)° and –178.1(2)°, respectively, which indicate that the 9*H*-fluoren-9-one rings are almost coplanar. It can be observed that there is a significant angle between the donor (carbazole) and acceptor (9*H*-fluoren-9-one) with the torsion angles of 70.4(2)°. The twisted configuration of the carbazoles and acceptor skeleton allows for efficient separation of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), leading to an effective reverse intersystem crossing (RISC) process.

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

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