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Crystal structure of (*E*)-2-(2-(4-(diethylamino) styryl)-1-ethyl-1,4-dihydroquinolin-4-yl) malononitrile, $C_{26}H_{26}N_4$

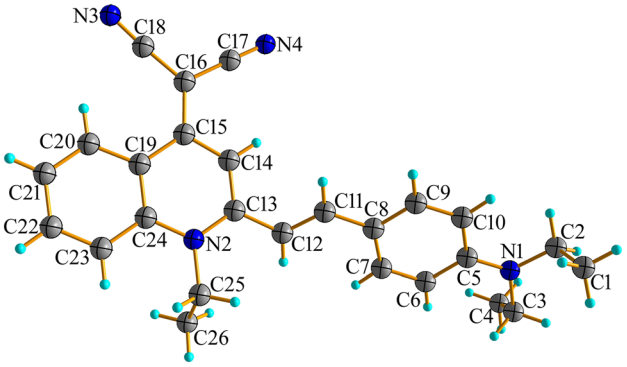

Table 1: Data collection and handling.

Crystal:	Red block
Size:	0.23 × 0.21 × 0.19 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.07 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.0°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	20,345, 3840, 0.073
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2035
$N(param)_{refined}$:	275
Programs:	Olex2 [1], Bruker [2], SHELX [3], Diamond [4]

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Abstract

$C_{26}H_{26}N_4$, monoclinic, $P2_1/c$ (no. 14), a = 16.565(2) Å, b = 17.468(2) Å, c = 7.5778(10) Å, β = 94.551(4)°, V = 2185.8(5) $Å^3$, Z = 4, $R_{gt}(F)$ = 0.0591, $wR_{ref}(F^2)$ = 0.1830, T = 300(2) 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.

1 Source of materials

Quinolinemalononitrile was synthesized according to the method described in reference [8]. Weigh quinolinemalononitrile (0.48 g, 2 mmol) and 4-(diethylamino)benzaldehyde (0.36 g, 2 mmol) into a 100 mL round-bottom flask. Add 60 mL of absolute ethanol solution, and five drops of piperidine were added, heat and reflux for 9 h, cool to room temperature, separate out solids, filter, wash with ethanol four times, vacuum dry, and obtain 0.6 g of a red solid. The yield is 75 %. Take a small amount of the target compound and heat it to dissolve in 10 mL of chloroform. Cool it and let it evaporate naturally for nine days before precipitation of crystals.

2 Experimental details

Using Olex2 [1], the structure was solved using Charge Flipping and refined with the ShelXL [3] refinement. All hydrogen atoms were positioned geometrically, with the d(C—H) = 0.97–0.99 Å, U_{iso}(H) = 1.2 times U_{eq}(C) and U_{iso}(H) = 1.5 times U_{eq}(O).

3 Comment

Dicyanomethylene (DCM) derivatives are important luminescent materials with a long wavelength, typically intramolecular charge transfer luminescence, and are mainly used in organically modified light-emitting devices [5]. However, as a classical donor–π–acceptor (D–π–A) feature and quasi-planar configuration, DCM systems suffer from quenching due to π–π aggregation in solid state or aggregated state (aggregation-caused quenching, ACQ) [6], which greatly limits their applications in high-efficiency solid-state

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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	0.9899 (2)	0.3511 (3)	0.1997 (5)	0.1165 (14)
H1A	0.9476	0.3525	0.1056	0.175*
H1B	1.0333	0.3194	0.1656	0.175*
H1C	1.0097	0.4020	0.2235	0.175*
C2	0.95735 (17)	0.31912 (17)	0.3621 (4)	0.0767 (9)
H2A	0.9382	0.2675	0.3372	0.092*
H2B	1.0010	0.3161	0.4550	0.092*
C3	0.91565 (17)	0.42710 (16)	0.5444 (4)	0.0710 (8)
H3A	0.8858	0.4725	0.5045	0.085*
H3B	0.9728	0.4374	0.5365	0.085*
C4	0.9011 (2)	0.41241 (19)	0.7349 (4)	0.0930 (11)
H4A	0.8448	0.4017	0.7441	0.139*
H4B	0.9164	0.4568	0.8044	0.139*
H4C	0.9329	0.3694	0.7778	0.139*
C5	0.81308 (15)	0.35581 (14)	0.3561(3)	0.0550 (7)
C6	0.75108 (16)	0.40285 (14)	0.4109 (3)	0.0564 (7)
H6	0.7639	0.4414	0.4930	0.068*
C7	0.67235 (16)	0.39335 (14)	0.3465 (3)	0.0548 (7)
H7	0.6331	0.4255	0.3871	0.066*
C8	0.64860 (15)	0.33725 (14)	0.2224 (3)	0.0515 (6)
C9	0.71031 (17)	0.29158 (15)	0.1649 (4)	0.0645 (8)
H9	0.6973	0.2541	0.0802	0.077*
C10	0.78986 (18)	0.29999 (16)	0.2290 (4)	0.0692 (8)
H10	0.8290	0.2680	0.1873	0.083*
C11	0.56549 (16)	0.32549 (14)	0.1529 (3)	0.0553 (7)
H11	0.5564	0.2845	0.0756	0.066*
C12	0.50024 (15)	0.36647 (14)	0.1865 (3)	0.0531 (7)
H12	0.5068	0.4095	0.2585	0.064*
C13	0.41904 (14)	0.34561 (14)	0.1134 (3)	0.0495 (6)
C14	0.39694 (15)	0.26976 (13)	0.1004 (3)	0.0509 (6)
H14	0.4345	0.2333	0.1430	0.061*
C15	0.32193 (15)	0.24411 (14)	0.0275 (3)	0.0486 (6)
C16	0.30862 (16)	0.16380 (15)	0.0181 (3)	0.0561 (7)
C17	0.37110 (19)	0.11388 (16)	0.0866 (4)	0.0615 (7)
C18	0.2389 (2)	0.12571 (16)	−0.0555 (4)	0.0691 (8)
C19	0.26396 (15)	0.30286 (14)	−0.0293 (3)	0.0503 (6)
C20	0.18540 (17)	0.28774 (17)	−0.1030 (4)	0.0677 (8)
H20	0.1688	0.2370	−0.1152	0.081*
C21	0.13238 (19)	0.3439 (2)	−0.1574 (4)	0.0805 (9)
H21	0.0809	0.3314	−0.2068	0.097*
C22	0.15557 (18)	0.41939 (19)	−0.1388 (4)	0.0746 (9)
H22	0.1193	0.4580	−0.1747	0.090*
C23	0.23133 (17)	0.43793 (16)	−0.0680 (4)	0.0659 (8)
H23	0.2461	0.4892	−0.0569	0.079*
C24	0.28741 (15)	0.38090 (14)	−0.0117 (3)	0.0502 (6)
C25	0.38956 (15)	0.48224 (13)	0.0573 (4)	0.0601 (7)
H25A	0.3667	0.5060	−0.0510	0.072*
H25B	0.4481	0.4847	0.0571	0.072*
C26	0.36390 (19)	0.52769 (16)	0.2130 (4)	0.0788 (9)
H26A	0.3064	0.5234	0.2184	0.118*
H26B	0.3781	0.5805	0.1993	0.118*
H26C	0.3909	0.5081	0.3204	0.118*
N1	0.89166 (13)	0.36367 (13)	0.4262 (3)	0.0690 (7)
N2	0.36467 (12)	0.40092 (11)	0.0574 (3)	0.0506 (5)
N3	0.42228 (17)	0.07447 (15)	0.1425 (4)	0.0837 (8)
N4	0.18428 (19)	0.09114 (16)	−0.1143 (4)	0.1006 (10)

light-emitting devices. To prevent the intermolecular aggregation of DCM luminescent materials, researchers have constructed a new aggregation-induced fluorescence-enhancing parent quinolinemalonitrile (QM) by substituting N-ethyl for the oxygen atoms in benzopyranonitrile, which can realize the fluorescence extension to the red light and the near-infrared [7].

The crystal structure shows that the methyl group of the quinolinemalononitrile has reacted with the aldehyde group of the 4-(diethylamino)benzaldehyde. The double bond links the benzene ring and quinoline to form a compound with a D–π–A structure. The benzene ring and quinoline ring are not parallel, with a dihedral angle of 137.37° [9, 10].

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