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Crystal structure of 2-(4-(dimethylamino)phenyl)-10-methylacridin-9(10*H*)-one, C₂₂H₂₀N₂O

Table 1: Data collection and handling.

Crystal:	Rod, yellow
Size:	0.27 × 0.27 × 0.16 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.08 mm ⁻¹
Diffractometer, scan mode:	Saturn724+, ω -scans at fixed $\chi = 45^\circ$
$\theta_{\max}$, completeness:	25°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	9902, 2816, 0.043
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2624
$N(\text{param})_{\text{refined}}$:	229
Programs:	Rigaku program [1], SHELX [2, 3]

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Abstract

C₂₂H₂₀N₂O, monoclinic, $P2_1/n$ (no. 14), $a = 8.316(2)$ Å, $b = 9.247(2)$ Å, $c = 20.908(5)$ Å, $\beta = 93.538(5)^\circ$, $V = 1604.7(7)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0618$, $wR_{\text{ref}}(F^2) = 0.1527$, $T = 173(2)$ K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of materials

The title compound was obtained by C–C bond formation of 2-bromo-10-methylacridin-9(10*H*)-one and (4-(dimethylamino)phenyl)boronic acid via a Suzuki coupling reaction with equal ratio in toluene under the catalysis of Pd(PPh₃)₄. The compound was further purified through flash column chromatography with dichloromethane as eluent. Single crystals were obtained by crystallization from methanol and dichloromethane.

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.27602(19)	0.18905(18)	0.05131(8)	0.0458(5)
N1	0.6039(2)	0.51239(18)	0.09521(8)	0.0289(4)
N2	−0.3893(2)	0.4571(2)	0.33768(9)	0.0368(5)
C1	0.5296(2)	0.2943(2)	0.03534(10)	0.0284(5)
C2	0.5679(3)	0.1896(2)	−0.00961(10)	0.0331(5)
H2	0.491642	0.116170	−0.021111	0.040*
C3	0.7129(3)	0.1905(2)	−0.03744(12)	0.0397(6)
H3	0.737020	0.119072	−0.068082	0.048*
C4	0.8239(3)	0.2981(3)	−0.01990(12)	0.0433(6)
H4	0.925641	0.297997	−0.038193	0.052*
C5	0.7903(3)	0.4045(2)	0.02316(11)	0.0369(5)
H5	0.867842	0.477560	0.033671	0.044*
C6	0.6408(2)	0.4056(2)	0.05188(10)	0.0284(5)
C7	0.4642(2)	0.5036(2)	0.12823(9)	0.0266(5)
C8	0.3517(2)	0.3921(2)	0.11535(10)	0.0264(5)
C9	0.3768(2)	0.2843(2)	0.06611(10)	0.0300(5)
C10	0.4302(2)	0.6051(2)	0.17607(10)	0.0307(5)
H10	0.503118	0.682343	0.185610	0.037*
C11	0.2930(2)	0.5932(2)	0.20888(10)	0.0306(5)
H11	0.273100	0.663691	0.240507	0.037*
C12	0.1803(2)	0.4810(2)	0.19766(10)	0.0271(5)
C13	0.2131(2)	0.3831(2)	0.15025(10)	0.0279(5)
H13	0.139008	0.306737	0.140898	0.033*
C14	0.0358(2)	0.4683(2)	0.23560(10)	0.0272(5)
C15	0.0275(2)	0.5330(2)	0.29572(10)	0.0314(5)
H15	0.119273	0.583131	0.313630	0.038*
C16	−0.1090(3)	0.5271(2)	0.33017(10)	0.0318(5)
H16	−0.108455	0.571924	0.371058	0.038*
C17	−0.2490(2)	0.4553(2)	0.30546(10)	0.0295(5)

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Table 2 (continued)

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C18	−0.2384(2)	0.3827(2)	0.24710(11)	0.0319(5)
H18	−0.327528	0.327341	0.230334	0.038*
C19	−0.1005(2)	0.3901(2)	0.21332(10)	0.0299(5)
H19	−0.098377	0.340266	0.173642	0.036*
C20	0.7136(3)	0.6347(2)	0.10633(12)	0.0378(6)
H20B	0.653322	0.718228	0.121003	0.057*
H20A	0.762915	0.659288	0.066367	0.057*
H20C	0.797997	0.608639	0.139081	0.057*
C21	−0.5216(3)	0.3618(3)	0.31858(11)	0.0382(6)
H21A	−0.539146	0.362829	0.271797	0.057*
H21C	−0.619501	0.394767	0.337953	0.057*
H21B	−0.495837	0.263207	0.333040	0.057*
C22	−0.3912(3)	0.5206(3)	0.40119(11)	0.0406(6)
H22A	−0.330894	0.458493	0.432166	0.061*
H22C	−0.502764	0.529550	0.413253	0.061*
H22B	−0.341168	0.616538	0.400992	0.061*

Experimental details

The hydrogen atoms were placed with common isotropic displacement factors $U_{\text{iso}}(\text{H}) = 1.2$ times U_{eq} (C, aromatic ring), and $U_{\text{iso}}(\text{H}) = 1.5$ times U_{eq} (C, methyl). The final refinement succeeded using geometrical restraints, with C—H = 0.95 Å (aromatic ring), and C—H = 0.98 Å (methyl).

Comment

The organic small molecules with tuning optical nonlinear properties have attracted considerable academic and technological research attention [4–7]. Those molecules usually have a donor-acceptor (D–A) structure and the properties could be tuned through matching the suitable units. Acridone derivatives with electron-deficient properties are acceptor candidates in the constructing D–A molecules [8, 9]. Meanwhile, the *N,N*-dimethylaniline plays the role of donor units [10] and the two parts are connected by a C–C single bond of 1.485(3) Å, which is shorter than that in 2-bromo-7-(4-(dimethylamino)phenyl)-10-methylacridin-9(10*H*)-one, because of the electron-withdrawing property of bromine atom. This molecule was expected to be applied in the optical tuning field. The asymmetric unit contains one molecule of the title compound with a dihedral angle of $-21.6(3)^\circ$ between the two planes of the acridonyl [11] and the aryl moiety.

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