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Crystal structure of 2-bromo-7-(4-(dimethylamino)phenyl)-10-methylacridin-9 (10*H*)-one, $C_{22}H_{19}BrN_2O$

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Abstract

$C_{22}H_{19}BrN_2O$, monoclinic, $P2_1/n$ (no. 14), $a = 8.0338(16)$ Å, $b = 9.0803(18)$ Å, $c = 24.281(5)$ Å, $\beta = 95.78(3)^\circ$, $V = 1762.28(60)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0871$, $wR_{ref}(F^2) = 0.1595$, $T = 173(2)$ K.

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The 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 Suzuki coupling reaction of 2,7-dibromo-10-methylacridin-9(10*H*)-one and 4-(dimethylamino)phenylboronic acid with 1/1 ratio. The compound was purified through flash column chromatography. Single crystals were obtained by crystallization of the title compound from methanol.

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Table 1: Data collection and handling.

Crystal:	Yellow needle
Size:	$0.28 \times 0.27 \times 0.16$ mm
Wavelength:	Cu $K\alpha$ radiation (1.54178 Å)
μ :	3.28 mm^{-1}
Diffractometer, scan mode:	Raxis Rapid IP, ω -scans
$\theta_{\max}$, completeness:	68.2° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	10538, 3191, 0.072
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2473
$N(\text{param})_{\text{refined}}$:	238
Programs:	Rigaku programs [1], SHELX [2, 3]

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	1.23583(11)	0.90232(9)	0.45257(3)	0.0455(3)
O1	0.7414(6)	0.7378(5)	0.57442(19)	0.0400(13)
N1	1.0834(6)	0.4050(6)	0.6071(2)	0.0263(12)
N2	0.1123(7)	0.4600(6)	0.8303(2)	0.0289(13)
C1	1.1854(9)	0.7441(8)	0.4991(3)	0.0309(16)
C2	1.3011(9)	0.6334(8)	0.5112(3)	0.0393(19)
H2	1.4036(13)	0.6346(69)	0.4947(68)	0.047*
C3	1.2694(9)	0.5212(8)	0.5468(3)	0.0383(18)
H3	1.3505(9)	0.4460(89)	0.5548(88)	0.046*
C4	1.1172(8)	0.5167(7)	0.5713(2)	0.0240(14)
C5	1.0035(8)	0.6337(7)	0.5594(2)	0.0226(14)
C6	1.0382(8)	0.7449(7)	0.5229(2)	0.0260(15)
H6	0.9593(89)	0.8216(89)	0.5145(27)	0.031*
C7	0.8461(8)	0.6418(7)	0.5857(3)	0.0242(14)
C8	0.8286(8)	0.5293(6)	0.6287(2)	0.0195(13)
C9	0.9469(7)	0.4158(7)	0.6377(2)	0.0215(13)
C10	1.1916(9)	0.2771(8)	0.6129(3)	0.0371(18)
H10A	1.2412(3)	0.2600(60)	0.5782(34)	0.056*
H10B	1.1260(91)	0.1906(18)	0.6216(61)	0.056*
H10C	1.2807(15)	0.2939(82)	0.6429(66)	0.056*
C11	0.9252(8)	0.3134(7)	0.6805(2)	0.0252(15)
H11	1.0022(37)	0.2347(62)	0.6878(45)	0.030*
C12	0.7915(8)	0.3287(7)	0.7115(3)	0.0255(15)
H12	0.7805(7)	0.2602(40)	0.7404(45)	0.031*
C13	0.6706(7)	0.4403(6)	0.7024(2)	0.0195(13)
C14	0.6948(7)	0.5401(7)	0.6606(2)	0.0192(13)
H14	0.6171(65)	0.6183(94)	0.6535(30)	0.023*
C15	0.5289(7)	0.4515(6)	0.7366(2)	0.0182(13)
C16	0.3813(7)	0.5261(7)	0.7184(2)	0.0223(14)
H16	0.3733(90)	0.5740(37)	0.6834(17)	0.027*
C17	0.2474(8)	0.5324(7)	0.7492(3)	0.0260(14)

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
H17	0.150504	0.585659	0.735289	0.031*
C18	0.2496(8)	0.4630(7)	0.8004(2)	0.0219(14)
C19	0.3999(8)	0.3930(7)	0.8201(3)	0.0270(15)
H19	0.409255	0.348762	0.855766	0.032*
C20	0.5339(8)	0.3872(7)	0.7890(2)	0.0236(14)
H20	0.632944	0.337879	0.803613	0.028*
C21	0.1252(9)	0.3969(8)	0.8852(3)	0.0350(17)
H21A	0.177047	0.299327	0.884544	0.053*
H21B	0.013237	0.387777	0.897583	0.053*
H21C	0.194074	0.460933	0.910805	0.053*
C22	−0.0270(8)	0.5581(8)	0.8158(3)	0.0336(17)
H22B	0.008547	0.660076	0.823194	0.050*
H22C	−0.118609	0.533811	0.837990	0.050*
H22A	−0.065424	0.547033	0.776414	0.050*

Experimental details

The hydrogen atoms were placed with common isotropic displacement factors $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C, aromatic ring})$, and $U_{\text{iso}}(\text{H}) = 1.5$ times $U_{\text{eq}}(\text{C, methyl})$. 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 donor-acceptor (D-A) molecular materials with tuning optical nonlinear properties have attracted considerable academic and technological research attention [4–7]. Acridone derivatives with electron-deficient properties are acceptor candidates in the constructing D-A molecules [8, 9]. *N,N*-dimethylaniline is the donor. The two parts are connected by a formal C–C single bond of 1.479(8) Å.

A view on the structure of the title molecule is shown in the figure. The asymmetric unit contains one molecule of the title compound. Bond lengths and angles are all in the expected ranges [11].

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