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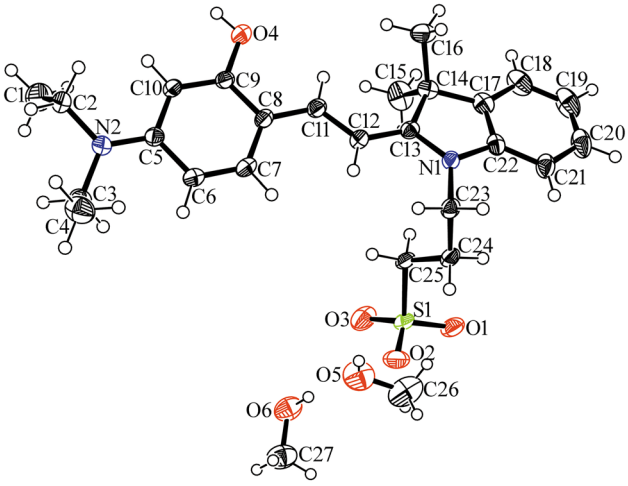
Crystal structure of (*E*)-3-(2-(4-(diethylamino)-2-hydroxystyryl)-3,3-dimethyl-3*H*-indol-1-ium-1-yl)propane-1-sulfonate – methanol (1/2), $C_{25}H_{32}N_2O_4S{\cdot}2CH_3OH$



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Abstract

$C_{27}H_{40}N_2O_6S$, monoclinic, $P2_1/c$ (no. 14), a = 11.2654(15) Å, b = 21.630(3) Å, c = 12.2868(17) Å, β = 111.422(3)°, V = 2787.1(7) Å^3, Z = 4, $R_{gt}(F)$ = 0.0493, w$R_{ref}(F^2)$ = 0.1313, T = 198(2) K.

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

Source of material

The 2,3,3-trimethyl-1-(3-sulfonatepropyl)- 3*H*-indolium (2.81 g, 10 mmol) and 4-(diethylamino)-2-hydroxybenzaldehyde (1.93 g, 10 mmol) were dissolved in 50 ml of ethanol for heating reflux of 12 h. The reaction mixture was cooled to room temperature and the orange solid was precipitated. The solid was washed three times with a little ethanol and ether. About 0.1 mmol of the orange solid was added to 20 ml of ethanol solution, heated and dissolved. Then, it was left stand for crystallization for five days at room temperature, precipitating crystals with suitable size.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.21 × 0.19 × 0.17 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	0.16 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	28.4°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	38842, 6940, 0.036
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 5872
$N(param)_{refined}$:	334
Programs:	OLEX2 [1], Bruker [2], SHELX [3], DIAMOND [4]

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).

Comment

The compounds with an electron donor-π-electron acceptor structure have entered into a focus of attention for researchers in recent years. These compounds are widely used in photodynamic anticancer and anti-bacteria, luminescent materials and photovoltaic materials [5, 6]. The electron donor in the molecule can raise the HOMO energy level of the molecule. However, the electron acceptor can reduce the LUMO energy level of the molecule. The push-pull

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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	0.5257 (3)	0.19299 (10)	0.8842 (2)	0.0585 (6)
H1A	0.4406	0.2076	0.8350	0.088*
H1B	0.5283	0.1858	0.9638	0.088*
H1C	0.5446	0.1543	0.8523	0.088*
C2	0.62389 (19)	0.24132 (8)	0.88679 (15)	0.0352 (4)
H2A	0.6017	0.2809	0.9152	0.042*
H2B	0.7084	0.2282	0.9426	0.042*
C3	0.72702 (17)	0.21352 (8)	0.74625 (15)	0.0326 (4)
H3A	0.6968	0.2056	0.6611	0.039*
H3B	0.7346	0.1731	0.7861	0.039*
C4	0.85622 (19)	0.24318 (10)	0.78445 (19)	0.0470 (5)
H4A	0.8499	0.2829	0.7443	0.071*
H4B	0.9151	0.2160	0.7649	0.071*
H4C	0.8880	0.2500	0.8691	0.071*
C5	0.56172 (15)	0.29443 (7)	0.69664 (13)	0.0249 (3)
C6	0.58518 (16)	0.30979 (8)	0.59298 (14)	0.0295 (3)
H6	0.6493	0.2884	0.5750	0.035*
C7	0.51605 (16)	0.35491 (8)	0.52012 (14)	0.0293 (3)
H7	0.5358	0.3652	0.4535	0.035*
C8	0.41597 (15)	0.38731 (7)	0.53905 (13)	0.0247 (3)
C9	0.39102 (15)	0.37039 (7)	0.64084 (13)	0.0240 (3)
C10	0.46240 (15)	0.32617 (7)	0.71718 (13)	0.0256 (3)
H10	0.4445	0.3168	0.7852	0.031*
C11	0.34276 (15)	0.43402 (7)	0.46399 (13)	0.0259 (3)
H11	0.2709	0.4491	0.4787	0.031*
C12	0.36657 (15)	0.45961 (7)	0.37116 (13)	0.0260 (3)
H12	0.4413	0.4465	0.3591	0.031*
C13	0.28935 (14)	0.50337 (7)	0.29342 (13)	0.0230 (3)
C14	0.15753 (15)	0.52682 (7)	0.28251 (14)	0.0272 (3)
C15	0.1600 (2)	0.56442 (9)	0.38981 (17)	0.0411 (4)
H15A	0.2239	0.5973	0.4054	0.062*
H15B	0.1820	0.5371	0.4580	0.062*
H15C	0.0759	0.5827	0.3743	0.062*
C16	0.06173 (18)	0.47333 (10)	0.2578 (2)	0.0468 (5)
H16A	−0.0245	0.4900	0.2384	0.070*
H16B	0.0832	0.4470	0.3274	0.070*
H16C	0.0653	0.4488	0.1921	0.070*
C17	0.12508 (16)	0.56838 (7)	0.17681 (14)	0.0299 (3)
C18	0.01696 (18)	0.60293 (9)	0.11984 (18)	0.0423 (4)
H18	−0.0532	0.6028	0.1452	0.051*
C19	0.0144 (2)	0.63775 (10)	0.02444 (19)	0.0514 (6)
H19	−0.0593	0.6616	−0.0163	0.062*
C20	0.1161 (2)	0.63884 (9)	−0.01332 (17)	0.0462 (5)
H20	0.1110	0.6635	−0.0788	0.055*
C21	0.22552 (19)	0.60433 (8)	0.04320 (14)	0.0347 (4)
H21	0.2964	0.60	0.0187	0.042*
C22	0.22506 (15)	0.56905 (7)	0.13766 (13)	0.0263 (3)
C23	0.43574 (15)	0.51662 (7)	0.18261 (14)	0.0260 (3)
H23A	0.5015	0.4979	0.2522	0.031*
H23B	0.4701	0.5561	0.1656	0.031*
C24	0.40901 (17)	0.47322 (7)	0.07889 (14)	0.0290 (3)
H24A	0.3492	0.4940	0.0083	0.035*
H24B	0.4897	0.4662	0.0660	0.035*
C25	0.35327 (16)	0.41090 (7)	0.09134 (13)	0.0264 (3)
H25A	0.2650	0.4165	0.0887	0.032*
H25B	0.4045	0.3924	0.1678	0.032*
C26	0.1441 (3)	0.25081 (15)	−0.2880 (2)	0.0715 (8)
H26A	0.0929	0.2232	−0.3509	0.107*
H26B	0.2206	0.2636	−0.3022	0.107*
H26C	0.0937	0.2874	−0.2859	0.107*
C27	0.2409 (3)	0.06949 (13)	−0.2219 (2)	0.0613 (6)
H27A	0.2277	0.0849	−0.3004	0.092*
H27B	0.2338	0.0243	−0.2239	0.092*
H27C	0.3259	0.0816	−0.1680	0.092*
N1	0.32159 (12)	0.52935 (6)	0.20886 (11)	0.0227 (3)
N2	0.63219 (14)	0.25129 (6)	0.77153 (12)	0.0301 (3)
O1	0.27643 (12)	0.39111 (7)	−0.13207 (10)	0.0379 (3)
O2	0.48420 (13)	0.35368 (7)	−0.01110 (11)	0.0427 (3)
O3	0.29415 (17)	0.30363 (6)	−0.00425 (12)	0.0505 (4)
O4	0.29517 (13)	0.40069 (6)	0.65956 (11)	0.0365 (3)
H4	0.2949	0.3913	0.7258	0.055*
O5	0.18036 (19)	0.21919 (8)	−0.17912 (17)	0.0671 (5)
H5	0.2218	0.2433	−0.1249	0.101*
O6	0.14789 (15)	0.09481 (8)	−0.18360 (15)	0.0538 (4)
H6A	0.1575	0.1333	−0.1769	0.081*
S1	0.35262 (4)	0.36044 (2)	−0.02290 (3)	0.02971 (11)

electronic structure formed by introducing the electron donor and the electron acceptor in the conjugated molecular system can effectively reduce the molecular energy band gap. Specifically, the narrower the energy band gap of the molecule is, the longer the luminescent wavelength of the molecule is. As a result, the construction of compounds with an electron donor-π-electron acceptor structure is an effective strategy to construct near-infrared luminescent materials and photodynamic therapy materials [7, 8]. It can be seen from the crystal structure of the target compound that the asymmetric structural unit of the target compound contains one target compound molecule and two methanol molecules. The diethylamino-hydroxy-phenyl moiety and the indole ring are connected by a double bond. All bond lengths and bond angles are within the normal range [9]. The dihedral angle between the aryl ring and the indole ring is 162.31°. The O3 of the compound molecule and the O5 of the methanol molecule form an intermolecular O5—H5···O3 hydrogen bond. The O5 of the methanol molecule and the O6 of another methanol molecule form an intermolecular O6—H6A···O5 hydrogen bond. The molecules and molecules expand through the O4—H4···O1 hydrogen bond to form a chain structure.

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

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