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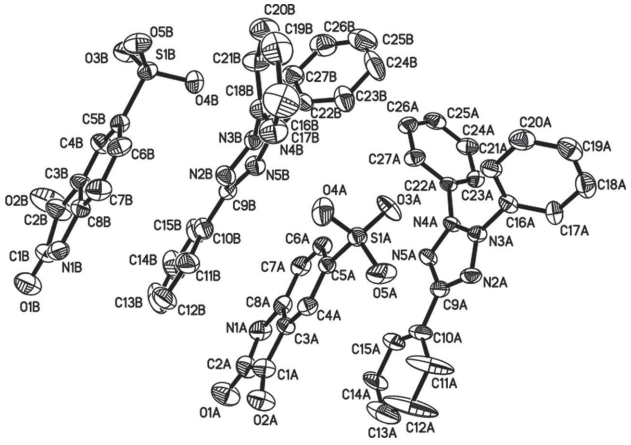
The crystal structure of 2,3,5-triphenyl-2,3-dihydro-1*H*-tetrazol-1-ium 2,3-dioxoindoline-5-sulfonate, $C_{27}H_{19}N_5O_5S$



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Abstract

$C_{27}H_{19}N_5O_5S$, monoclinic, $P2_1/c$ (no. 14), $a = 14.2789(4)$ Å, $b = 27.3722(9)$ Å, $c = 13.0126(4)$ Å, $\beta = 101.805(2)°$, $V = 4978.3(3)$ Å^3, $Z = 8$, $R_{gt}(F) = 0.0809$, $wR_{ref}(F^2) = 0.1705$.

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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.

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Table 1: Data collection and handling.

Crystal:	Yellow plate
Size:	$0.42 \times 0.27 \times 0.05$ mm
Wavelength:	Cu $K\alpha$ radiation (1.54178 Å)
μ:	15.7 cm^{-1}
Diffractometer, scan mode:	Bruker APEX II, φ and ω-scans
$2\theta_{max}$, completeness:	130°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	34603, 8430, 0.150
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4123
$N(param)_{refined}$:	694
Programs:	Bruker programs [1], SHELX [2]

Source of material

To a solution of sodium 2,3-dioxoindoline-5-sulfonate dihydrat (0.28521 g, 1 mmol) in water (10 ml) a solution of 2,3,5-triphenyl-2,3-dihydro-1*H*-tetrazol-1-ium chloride (0.3348 g, 1 mmol) in water (10 ml) was added. A yellow precipitate was formed and filtered off, washed with cold water. The precipitate was dried under vacuum to give the title compound. After recrystallization from acetonitrile the title compound was obtained in 80% yield.

Experimental details

Hydrogen atoms were placed in calculated positions and were included in the refinement using the riding model approximation, with U_{iso}(H) set to $1.2U_{eq}$(C).

The ellipsoids of C11A and C12A are obviously too large (*cf.* the figure). This seems to be a consequence of the non-optimal data. Nevertheless, we are pretty sure that the C10A-C15A moiety is a phenyl group.

Discussion

Isatins (1*H*-indole-2,3-dione) are synthetically versatile substrates. They can be used for the synthesis of a large variety of heterocyclic compounds, such as indoles and quinolines [3–5]. Triphenyl tetrazolium chloride is often used as complexing agents and as electro-active pairing reagent for formation of many sensing materials [6, 7].

The asymmetric unit of the title structure contains two cations and two anions (*cf.* the figure). The molecules

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
S1A	0.72403(10)	0.63979(5)	0.10174(10)	0.0400(4)
O1A	0.7423(3)	0.91167(15)	0.2142(3)	0.0820(15)
O2A	0.7212(3)	0.84905(14)	0.0247(3)	0.0680(13)
O3A	0.7808(3)	0.60616(12)	0.1744(3)	0.0637(12)
O4A	0.6236(2)	0.62950(13)	0.0814(3)	0.0709(13)
O5A	0.7628(3)	0.64615(13)	0.0077(3)	0.0709(13)
N1A	0.7634(4)	0.8367(2)	0.2956(4)	0.0548(15)
C1A	0.7459(4)	0.8674(2)	0.2126(5)	0.0569(17)
C2A	0.7306(4)	0.8340(2)	0.1140(5)	0.0519(16)
C3A	0.7358(3)	0.78436(18)	0.1547(4)	0.0360(13)
C4A	0.7250(3)	0.73977(19)	0.1049(4)	0.0386(13)
H4AA	0.7093	0.7378	0.0305	0.046*
C5A	0.7377(3)	0.69776(18)	0.1655(4)	0.0338(12)
C6A	0.7587(3)	0.7017(2)	0.2754(4)	0.0434(14)
H6AA	0.7662	0.6727	0.3165	0.052*
C7A	0.7688(4)	0.7461(2)	0.3251(4)	0.0477(15)
H7AA	0.7834	0.7481	0.3996	0.057*
C8A	0.7571(4)	0.7877(2)	0.2643(4)	0.0421(14)
S1B	0.26535(9)	0.63303(5)	0.36060(10)	0.0408(4)
O1B	0.2461(3)	0.90384(16)	0.2446(3)	0.0789(14)
O2B	0.2513(4)	0.84304(16)	0.4317(3)	0.111(2)
O3B	0.2403(3)	0.64122(13)	0.4616(3)	0.0686(13)
O4B	0.3645(2)	0.61948(13)	0.3691(3)	0.0655(12)
O5B	0.1982(3)	0.60057(12)	0.2952(3)	0.0582(12)
N1B	0.2376(4)	0.82885(19)	0.1643(4)	0.0524(14)
C1B	0.2457(4)	0.8596(2)	0.2464(5)	0.0584(18)
C2B	0.2524(5)	0.8270(2)	0.3443(5)	0.071(2)
C3B	0.2513(4)	0.7770(2)	0.3058(4)	0.0469(15)
C4B	0.2602(4)	0.73298(19)	0.3560(4)	0.0475(15)
H4BA	0.2714	0.7315	0.4304	0.057*
C5B	0.2529(3)	0.69047(18)	0.2971(4)	0.0368(13)
C6B	0.2407(4)	0.6935(2)	0.1884(4)	0.0482(15)
H6BA	0.2369	0.6644	0.1482	0.058*
C7B	0.2340(4)	0.7380(2)	0.1381(4)	0.0543(16)
H7BA	0.2242	0.7396	0.0638	0.065*
C8B	0.2417(4)	0.7800(2)	0.1963(4)	0.0443(15)
N2A	0.9981(3)	0.62280(16)	0.1345(3)	0.0427(12)
N3A	0.9912(3)	0.58792(15)	0.2021(3)	0.0360(11)
N4A	0.9817(3)	0.60685(14)	0.2931(3)	0.0342(11)
N5A	0.9798(3)	0.65473(15)	0.2870(3)	0.0420(12)
C9A	0.9909(4)	0.6639(2)	0.1885(4)	0.0412(14)
C10A	0.9915(4)	0.7134(2)	0.1471(5)	0.0529(17)
C11A	0.9918(6)	0.7212(3)	0.0435(6)	0.122(4)
H11A	0.9922	0.6946	−0.0033	0.146*
C12A	0.9917(7)	0.7698(3)	0.0080(7)	0.161(6)
H12A	0.9908	0.7762	−0.0640	0.193*
C13A	0.9928(6)	0.8073(3)	0.0748(9)	0.112(4)
H13A	0.9942	0.8398	0.0496	0.134*
C14A	0.9920(5)	0.7998(3)	0.1754(8)	0.111(4)
H14A	0.9917	0.8267	0.2216	0.134*
C15A	0.9915(4)	0.7524(2)	0.2119(6)	0.079(2)
H15A	0.9911	0.7470	0.2839	0.094*
C16A	0.9920(4)	0.53615(18)	0.1769(4)	0.0366(13)
C17A	1.0743(4)	0.51647(19)	0.1558(4)	0.0482(15)
H17A	1.1310	0.5355	0.1634	0.058*
C18A	1.0729(5)	0.4683(2)	0.1234(4)	0.0616(18)
H18A	1.1290	0.4535	0.1088	0.074*
C19A	0.9900(5)	0.4422(2)	0.1124(4)	0.0596(18)
H19A	0.9890	0.4093	0.0885	0.072*
C20A	0.9075(4)	0.4619(2)	0.1351(4)	0.0596(17)
H20A	0.8512	0.4427	0.1288	0.072*
C21A	0.9083(4)	0.51019(19)	0.1671(4)	0.0476(15)
H21A	0.8523	0.5250	0.1818	0.057*
C22A	0.9725(4)	0.58201(17)	0.3896(4)	0.0315(12)
C23A	1.0552(4)	0.57081(17)	0.4595(4)	0.0416(14)
H23A	1.1160	0.5739	0.4412	0.050*
C24A	1.0463(4)	0.55472(19)	0.5589(4)	0.0500(16)
H24A	1.1020	0.5465	0.6095	0.060*
C25A	0.9582(4)	0.55075(18)	0.5841(4)	0.0506(16)
H25A	0.9536	0.5404	0.6525	0.061*
C26A	0.8756(4)	0.56163(18)	0.5113(4)	0.0502(16)
H26A	0.8146	0.5581	0.5291	0.060*
C27A	0.8830(4)	0.57781(18)	0.4123(4)	0.0447(15)
H27A	0.8274	0.5858	0.3613	0.054*
N2B	0.4456(3)	0.65989(16)	0.1571(3)	0.0447(12)
N3B	0.4672(3)	0.61525(16)	0.1903(4)	0.0396(11)
N4B	0.5299(3)	0.61596(16)	0.2819(3)	0.0410(12)
N5B	0.5500(3)	0.66137(16)	0.3116(3)	0.0453(12)
C9B	0.4977(4)	0.68799(19)	0.2329(5)	0.0403(13)
C10B	0.4979(4)	0.7407(2)	0.2295(5)	0.0492(15)
C11B	0.4706(4)	0.7656(2)	0.1350(5)	0.0647(19)
H11B	0.4523	0.7478	0.0715	0.078*
C12B	0.4699(5)	0.8161(3)	0.1324(7)	0.086(3)
H12B	0.4508	0.8327	0.0675	0.103*
C13B	0.4969(5)	0.8420(3)	0.2240(8)	0.101(3)
H13B	0.4962	0.8767	0.2222	0.121*
C14B	0.5249(5)	0.8180(3)	0.3187(7)	0.092(3)
H14B	0.5445	0.8362	0.3816	0.110*
C15B	0.5246(4)	0.7674(2)	0.3220(5)	0.0639(18)
H15B	0.5425	0.7509	0.3874	0.077*
C16B	0.4240(4)	0.5723(2)	0.1359(5)	0.0479(16)
C17B	0.4251(4)	0.5693(2)	0.0307(5)	0.0647(19)
H17B	0.4535	0.5941	−0.0040	0.078*
C18B	0.3830(5)	0.5286(3)	−0.0224(6)	0.094(3)
H18B	0.3816	0.5253	−0.0954	0.112*
C19B	0.3432(5)	0.4930(3)	0.0295(7)	0.093(3)
H19B	0.3152	0.4651	−0.0081	0.112*
C20B	0.3430(4)	0.4970(2)	0.1347(6)	0.076(2)
H20B	0.3154	0.4721	0.1697	0.091*
C21B	0.3837(4)	0.5380(2)	0.1891(5)	0.0591(18)
H21B	0.3835	0.5420	0.2616	0.071*
C22B	0.5726(4)	0.57337(19)	0.3386(5)	0.0435(15)
C23B	0.6196(4)	0.5408(2)	0.2879(5)	0.0625(18)
H23B	0.6253	0.5459	0.2172	0.075*
C24B	0.6594(5)	0.4993(2)	0.3441(7)	0.088(3)
H24B	0.6919	0.4754	0.3118	0.106*
C25B	0.6504(5)	0.4939(3)	0.4463(7)	0.091(3)
H25B	0.6769	0.4657	0.4841	0.109*
C26B	0.6049(5)	0.5275(3)	0.4954(6)	0.079(2)
H26B	0.6010	0.5228	0.5667	0.094*
C27B	0.5641(4)	0.5686(2)	0.4419(5)	0.0581(17)
H27B	0.5318	0.5924	0.4749	0.070*
H1NA	0.761(3)	0.8442(17)	0.357(4)	0.033(16)*
H1NB	0.231(4)	0.837(2)	0.092(5)	0.10(3)*

are packed *via* intermolecular hydrogen bonds, N1A—H1NA...O5A[i], N1B—H1NB...O3B[ii]. The H...A distances are 2.01(5), 1.81(9) Å, respectively and the angles are 168(6), and 160(7), respectively. Symmetry codes: (i) x, $-y+3/2$, $z+1/2$; (ii) x, $-y+3/2$, $z-1/2$. Bond lengths and angels are all in the expected ranges. The phenyl moieties and the sulfonate groups are oriented to fill the needs of hydrogen bonding and sterical aspects.

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