

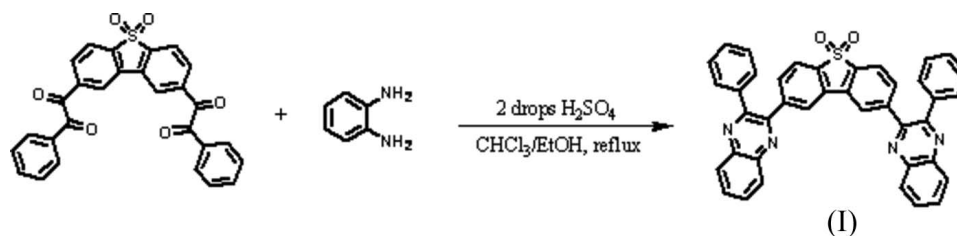
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Key indicators

Single-crystal X-ray study
 $T = 100\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.037
 wR factor = 0.066
Data-to-parameter ratio = 12.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.2,8-Bis(3-phenylquinoxalin-2-yl)-5 λ^6 -dibenzo[*b,d*]thiophene-5,5-dioneThe bond lengths and angles in the title compound, $\text{C}_{40}\text{H}_{24}\text{N}_4\text{O}_2\text{S}$, are normal. The dihedral angles between the dibenzothiophene-*S,S*-dioxide and two quinoxaline groups are $34.88(1)$ and $45.86(1)^\circ$.

Comment

The application of organic electroluminescent (OEL) in flat-panel displays using small organic molecules or organic polymers has been intensively pursued after the reports of Kodak's team (Tang & Van Slyke, 1987) and Cambridge's group (Burroughes *et al.*, 1990). Recently, the quinoxaline system has been introduced into small molecules (Thomas *et al.*, 2005) and successfully applied in organic light emitting devices (OLEDs) for electron-transport materials (Bettenhausen *et al.*, 1997).In our search for new compounds that could be used as *n*-type OLEDs (Huang *et al.*, 2005), the title compound, (I) (Fig. 1), has been synthesized by the condensation of a bis-dione with a diamine (see scheme). All bond lengths and angles in (I) are normal (Table 1). The mean planes of the dibenzothiophene-*S,S*-dioxide (*P1*), two quinoxaline (*P4* and *P5*) and two phenyl (*P6* and *P7*) groups (see Fig. 1) make dihedral angles *P1/P4*, *P1/P5*, *P1/P6*, *P1/P7*, *P4/P6* and *P5/P7* of $34.88(1)$, $45.86(1)$, $52.50(1)$, $56.68(1)$, $42.50(1)$ and $50.50(1)^\circ$, respectively. The crystal packing is stabilized by van der Waals forces.

Experimental

A two-necked round-bottomed flask was charged with 1,2-phenylenediamine (216 mg, 2.2 mmol), 1-[5,5-dioxo-8-(2-oxo-2-phenylacetyl)-5H-5 λ^6 -dibenzo[2,1-*b*]thiophen-2-yl]-2-phenylethane-1,2-dione (528 mg, 1.1 mmol) and CHCl_3 /ethanol (80 ml; ratio 1:2). Two drops of sulfuric acid were then added to initiate the reaction. The mixture was refluxed for 24 h. After cooling, the solvent was removed by Dean–Stark distillation. The resulting suspension was separated by filtration, washed with methanol and dried. The solid was sublimed to provide a powdery product. Crystals suitable for single-crystal X-ray diffraction were grown from a CH_2Cl_2 solution layered with *n*-hexane at room temperature. The compound was obtained as a colourless solid in 62% yield. FAB MS: m/e 624 ($\text{M}+\text{H}^+$); $^1\text{H NMR}$ (CDCl_3): δ 7.39–7.42 (*m*, 6H, *ortho*-, *para*- C_6H_5), 7.50–7.54 (*m*, 6H, C_6H_3 , *meta*-

C_6H_5), 7.69 (*d*, 2H, $J = 8.0$ Hz, C_6H_3), 7.83–7.86 (*m*, 4H, C_6H_4), 8.13 (*s*, 2H, C_6H_3), 8.19–8.25 (*m*, 4H, C_6H_4). Analysis calculated for $C_{40}H_{24}N_4O_2S$: C 76.90, H 3.87, N 8.97%; found: C 77.02, H 4.01, N 8.86%.

Crystal data

$C_{40}H_{24}N_4O_2S$

$M_r = 624.69$

Triclinic, $P\bar{1}$

$a = 10.7261$ (3) Å

$b = 12.0606$ (4) Å

$c = 13.4213$ (4) Å

$\alpha = 107.719$ (2)°

$\beta = 103.656$ (2)°

$\gamma = 108.751$ (2)°

$V = 1454.81$ (8) Å³

$Z = 2$

$D_x = 1.426$ Mg m⁻³

Mo $K\alpha$ radiation

Cell parameters from 2322

reflections

$\theta = 2.8$ – 27.8 °

$\mu = 0.16$ mm⁻¹

$T = 100.0$ (1) K

Prism, colourless

$0.16 \times 0.15 \times 0.14$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

φ and ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2001)

$T_{\min} = 0.873$, $T_{\max} = 0.980$

10660 measured reflections

5107 independent reflections

3245 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.042$

$\theta_{\text{max}} = 25.0$ °

$h = -12 \rightarrow 12$

$k = -14 \rightarrow 13$

$l = -15 \rightarrow 14$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.066$

$S = 0.82$

5107 reflections

425 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0197P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.31$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.38$ e Å⁻³

Extinction correction: SHELXL97

Extinction coefficient: 0.0012 (4)

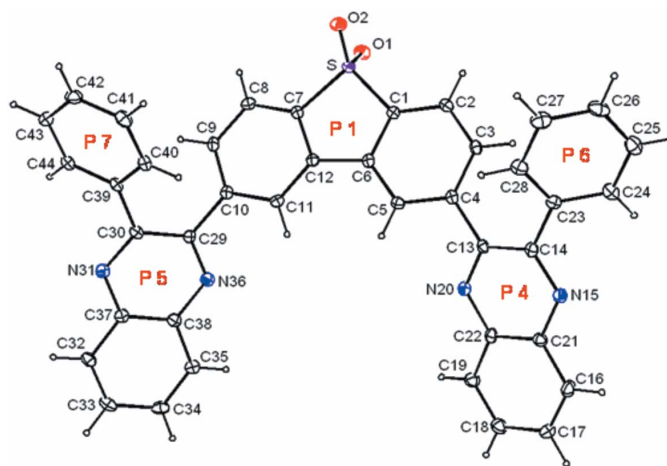


Figure 1

The molecular structure of (I), showing the atom-numbering scheme and 30% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

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Table 1

Selected geometric parameters (Å, °).

S—O1	1.4353 (13)	N31—C30	1.325 (2)
S—O2	1.4407 (13)	N31—C37	1.365 (2)
S—C1	1.7669 (19)	N36—C29	1.320 (2)
S—C7	1.7747 (19)	N36—C38	1.370 (2)
N15—C14	1.322 (2)	C4—C13	1.489 (2)
N15—C21	1.366 (2)	C10—C29	1.489 (2)
N20—C13	1.315 (2)	C14—C23	1.483 (3)
N20—C22	1.362 (2)	C30—C39	1.484 (3)
O1—S—O2	117.01 (8)	C1—C6—C12	112.79 (17)
O1—S—C7	110.72 (8)	C12—C7—S	110.89 (14)
C6—C1—S	110.78 (14)	C7—C12—C6	112.89 (16)

H atoms were located geometrically and treated as riding, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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