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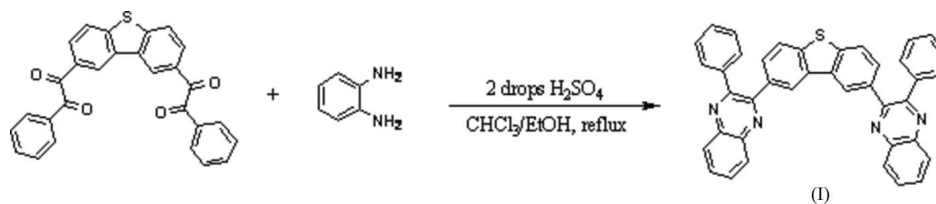
Key indicators

Single-crystal X-ray study
 $T = 100$ K
Mean $\sigma(C-C) = 0.005$ Å
 R factor = 0.059
 wR factor = 0.178
Data-to-parameter ratio = 12.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.2-Phenyl-3-[6-(3-phenylquinoxalin-2-yl)-dibenzo[*b,d*]thiophen-3-yl]quinoxaline

In the molecule of the title compound, $C_{40}H_{24}N_4S$, the two benzene rings fused to the thiophene ring form a dihedral angle of $2.3 (2)^\circ$. In the crystal structure, there are no significant hydrogen-bonding interactions, but there are π - π stacking interactions between molecules.

Comment

Electroluminescent (EL) devices based on small organic molecules or polymers have attracted considerable interest after the reports by Tang *et al.* (1987) and Burroughes *et al.* (1990). Thermally stable quinoxaline compounds are useful in organic light-emitting devices (OLEDs) (Thomas *et al.*, 2005). The quinoxaline group has been introduced into small molecules and successfully applied in *n*-type OLEDs (Bettenhausen *et al.*, 1997).



The title compound, (I), was synthesized by condensation of a (bis)dione with a diamine (see scheme) and it was shown that it could be used as an electron-transport material (Huang *et al.*, 2005). The molecular structure of (I) is shown in Fig. 1. The dihedral angles between the central thiophene ring (*P1*) and the quinoxaline rings (*P2* and *P3*) are $54.4 (1)$ and $24.5 (1)^\circ$, respectively, while the dihedral angles between *P2/*

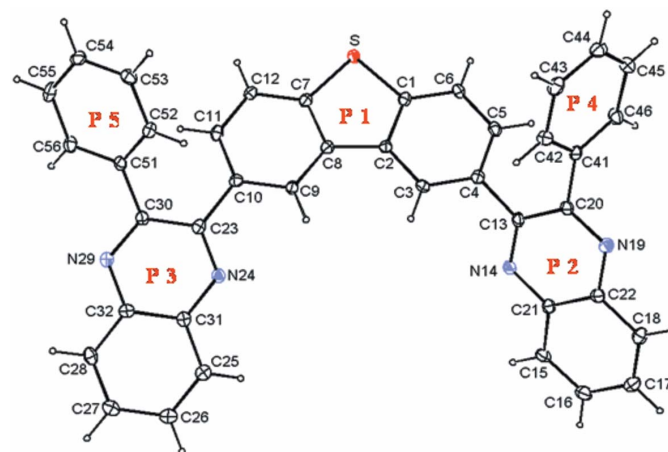


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii.

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P4 and *P3/P5* are 70.8 (1) and 35.2 (1)°, respectively. In the absence of significant hydrogen-bonding interactions, the crystal structure is stabilized by π - π stacking interactions between the dibenzothiophene groups of molecules related by centers of inversion. The closest ring centroid-centroid distance is 3.594 (2) Å with a perpendicular distance of 3.471 Å between rings S1/C1/C2/C7/C8 and C1-C6 related by the symmetry code $(-x, 1 - y, 2 - z)$ (see Fig. 2).

Experimental

To a two-necked round-bottomed flask charged with 1,2-phenylenediamine (216 mg, 2.2 mmol), 1-[8-(2-oxo-2-phenylacetyl)-dibenzothiophen-2-yl]-2-phenyl-ethane-1,2-dione (500 mg, 1.1 mmol) and CHCl_3 /ethanol (80 ml; ratio=1:2), two drops of sulfuric acid were added to initiate the reaction. The mixture was refluxed for 16 h. After cooling, the solvent was removed by Dean-Stark distillation. The resulting suspension was filtered, washed with methanol and dried. The residue was dissolved in CH_2Cl_2 and passed through 2 cm celite. The solution was pumped dry, and 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 white solid in 54% yield. FAB MS: *m/e* 592 ($M+H$)⁺; ¹H NMR (CDCl_3): 7.31–7.36 (*m*, 6H, *meta*-, *para*- C_6H_5), 7.44 (*d*, $J = 8.3$ Hz, 2H, C_6H_3), 7.55 (*d*, $J = 8.0$ Hz, 4H, *ortho*- C_6H_5); Anal. Calcd for $\text{C}_{40}\text{H}_{24}\text{N}_4\text{S}$: C, 81.06; H, 4.08; N, 9.45; Found: C, 81.15; H, 4.10; N, 9.42.

Crystal data

$\text{C}_{40}\text{H}_{24}\text{N}_4\text{S}$	$Z = 2$
$M_r = 592.69$	$D_x = 1.401 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 9.9452$ (7) Å	Cell parameters from 3810 reflections
$b = 11.6962$ (9) Å	$\theta = 2.4$ – 25.1°
$c = 12.7037$ (9) Å	$\mu = 0.15 \text{ mm}^{-1}$
$\alpha = 90.480$ (3)°	$T = 100.0$ (1) K
$\beta = 102.645$ (3)°	Prism, colourless
$\gamma = 102.501$ (2)°	$0.12 \times 0.10 \times 0.04 \text{ mm}$
$V = 1405.27$ (18) Å ³	

Data collection

Bruker SMART CCD area-detector diffractometer	4945 independent reflections
φ and ω scans	3300 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$R_{\text{int}} = 0.072$
$T_{\text{min}} = 0.982$, $T_{\text{max}} = 0.994$	$\theta_{\text{max}} = 25.0^\circ$
21681 measured reflections	$h = -11 \rightarrow 11$
	$k = -13 \rightarrow 13$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0656P)^2 + 1.9659P]$
$R[F^2 > 2\sigma(F^2)] = 0.059$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.179$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.09$	$\Delta\rho_{\text{max}} = 0.46 \text{ e } \text{Å}^{-3}$
4945 reflections	$\Delta\rho_{\text{min}} = -0.36 \text{ e } \text{Å}^{-3}$
407 parameters	Extinction correction: SHELXL97
H-atom parameters constrained	Extinction coefficient: 0.010 (2)

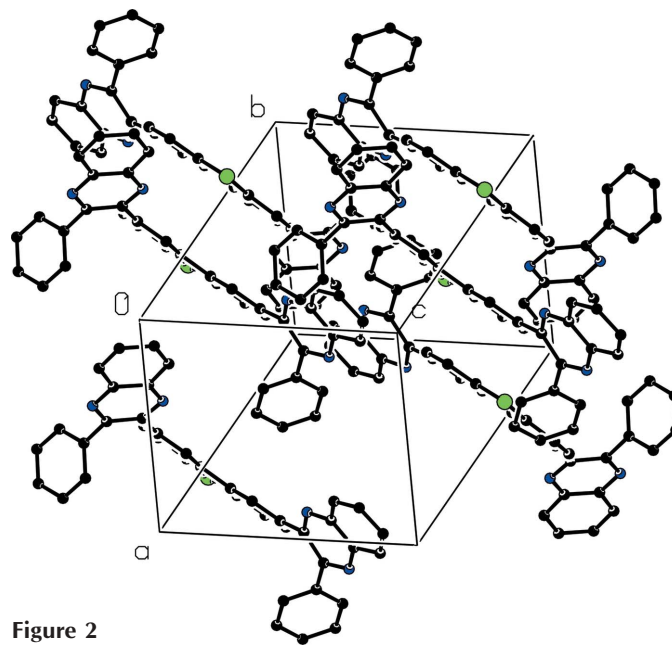


Figure 2 Packing diagram (Spek, 2003), showing π - π stacking interactions. H atoms have been omitted.

H atoms were positioned geometrically and treated as riding atoms, with $\text{C}-\text{H} = 0.95$ Å, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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: ORTEP3 for Windows (Farrugia, 1997) and PLATON (Spek, 2003); software used to prepare material for publication: WinGX (Farrugia, 1999).

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