Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Phenyl-3-[6-(3-phenylquinoxalin-2-yl)-dibenzo[*b*,*d*]thiophen-3-yl]quinoxaline

Tai-Hsiang Huang,[a] Wha-Tzong Whang,[a]* Yuh-Sheng Wen[b] and Jiann T. Lin[b]

[a]Department of Materials Science and Enginnering, National Chiao Tung University, 1001 Ta Hsueh Rd, Hsin Chu, Taiwan, and [b]Institute of Chemistry, Academia Sinica, Nankang, Taipei, Taiwan

Correspondence e-mail: redman@chem.sinica.edu.tw

Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.005 Å
R factor = 0.059
wR factor = 0.178
Data-to-parameter ratio = 12.1

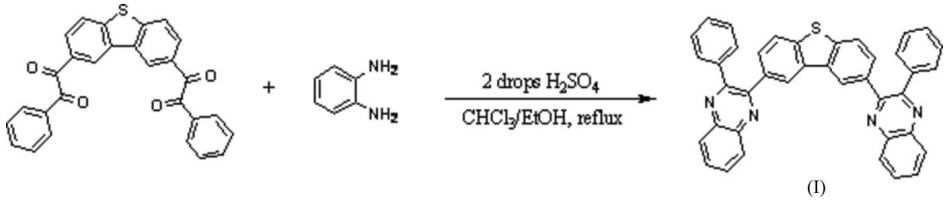
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 24 October 2005
Accepted 16 November 2005
Online 23 November 2005

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)°. 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).



(I)

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 (*P*1) and the quinoxaline rings (*P*2 and *P*3) are 54.4 (1) and 24.5 (1)°, respectively, while the dihedral angles between *P*2/

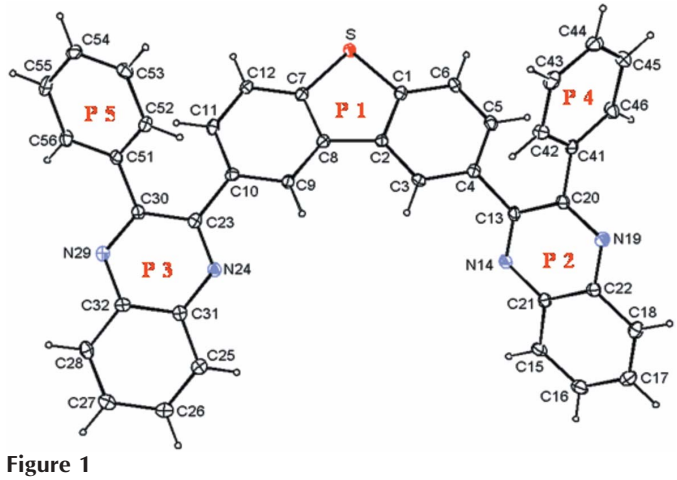


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii.

*P*4 and *P*3/*P*5 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).

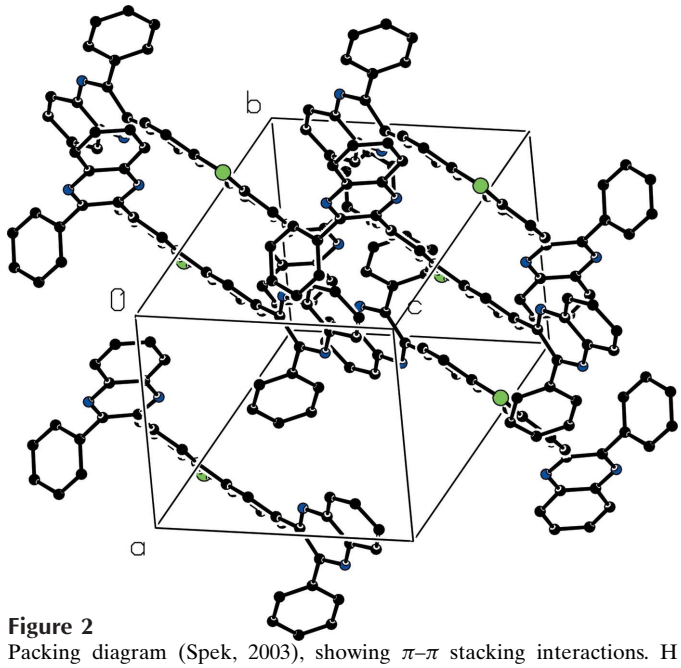


Figure 2
Packing diagram (Spek, 2003), showing π–π stacking interactions. H atoms have been omitted.

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 $(M+H)^+$; ^{1}H 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 $C_{40}H_{24}N_4S$: C, 81.06; H, 4.08; N, 9.45; Found: C, 81.15; H, 4.10; N, 9.42.

Crystal data

$C_{40}H_{24}N_4S$
M_r = 592.69
Triclinic, $P\overline{1}$
a = 9.9452 (7) Å
b = 11.6962 (9) Å
c = 12.7037 (9) Å
α = 90.480 (3)°
β = 102.645 (3)°
γ = 102.501 (2)°
V = 1405.27 (18) Å^3
Z = 2
D_x = 1.401 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 3810 reflections
θ = 2.4–25.1°
μ = 0.15 mm^{-1}
T = 100.0 (1) K
Prism, colourless
0.12 × 0.10 × 0.04 mm

Data collection

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

Refinement

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

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

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).

This work is supported by the Department of Materials Science and Enginnering, National Chiao Tung University, and Institute of Chemistry, Academia Sinica.

References

Bettenhausen, J., Greczmiel, M., Jandke M. & Strohriegl, P. (1997). *Synth. Met.* **91**, 223–228.
Bruker (2001). *SADABS*, *SMART* and *SAINT* (*APEX2* Version 1.0-27). Bruker AXS Inc., Madison, Wisconsin, USA.
Burroughes, J. H., Bradley, D. D. C., Brown, A. R., Marks, R. N., Mackay, K., Friend, R. H., Burn, P. L. & Holmes, A. B. (1990). *Nature (London)*, **347**, 539–540.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Huang, T.-H., Whang, W.-T., Shen, J. Y., Wen, Y.-S., Lin, J. T. & Wu, C.-C. (2005). *J. Mater. Chem.* Submitted.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Tang, C. W. & VanSlyke, S. A. (1987). *Appl. Phys. Lett.* **51**, 913–915.
Thomas, K. R. J., Velusamy, M., Lin, J. T., Tao, Y.-T. & Chuen, C.-H. (2005). *Chem. Mater.* **17**, 1860–1866.