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4-(4-Bromo-5-methylthiophen-2-yl)pyridine

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.007 Å
R factor = 0.049
wR factor = 0.098
Data-to-parameter ratio = 14.9

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

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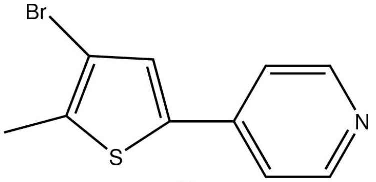
The title compound, $C_{10}H_8BrNS$, is used as a precursor to diarylethene derivatives. The dihedral angle between the thiophene and pyridine rings is 4.9 (1)°, and there is evidence for conjugation throughout the molecule. The structure is stabilized by π–π stacking interactions down the *c* axis.

Comment

Photochromic diarylethenes are among the most promising materials for optical memories and other optoelectronic devices (Irie, 2000). The title compound, (I), can be used to produce 1,2-bis[2-methyl-5-(4-pyridyl)-3-thienyl]perfluorocyclopentene and other photochromic diarylethene derivatives (Nakashima *et al.*, 1996; Alvaro & Lehn, 1999; Sasai *et al.*, 2000; Matsuda *et al.*, 2004). The dihedral angle between the pyridine and thiophene ring planes is 4.9 (1)° [5.2 (1)° if the thiophene ring is extended to include the Br and methyl C atoms], suggesting a considerable degree of conjugation throughout the molecule.



(I)

Compound (I) can be compared to the structure of the related compound 1,2-bis[5-(4-pyridyl)-3-thienyl]perfluorocyclopentene [(*A*); Matsuda *et al.*, 2001]. This system contains two discrete 4-pyridylthienyl groups linked through a cyclopentene ring and crystallizes with two molecules in the asymmetric unit. The C1—C6 bond in (I) [1.456 (6) Å] is shorter than the equivalent bonds in (*A*) [1.463 (4), 1.469 (4), 1.470 (4) and 1.478 (4) Å]. Furthermore, the dihedral angles between the pyridine and thiophene rings in (*A*) range from 3.8 (1) to 27.8 (1)°, suggesting that steric interactions within and between the molecules of (*A*) may be of greater importance than for (I). The structure is stabilized by columnar π–π stacking interactions down the *c* axis. The distance between molecular planes in the columns is 3.426 (5) Å, with adjacent molecules stacked in an obverse fashion (Fig. 2).

Experimental

The title compound was prepared according to the procedure of Gilat *et al.* (1993). Crystals were obtained by evaporation of a solution in chloroform. ^{1}H NMR ($CDCl_3$): δ 8.59 (*d*, 2H), 7.41 (*d*, 1H), 7.39 (*d*, 1H), 7.32 (*s*, 1H), 2.45 (*s*, 3H).

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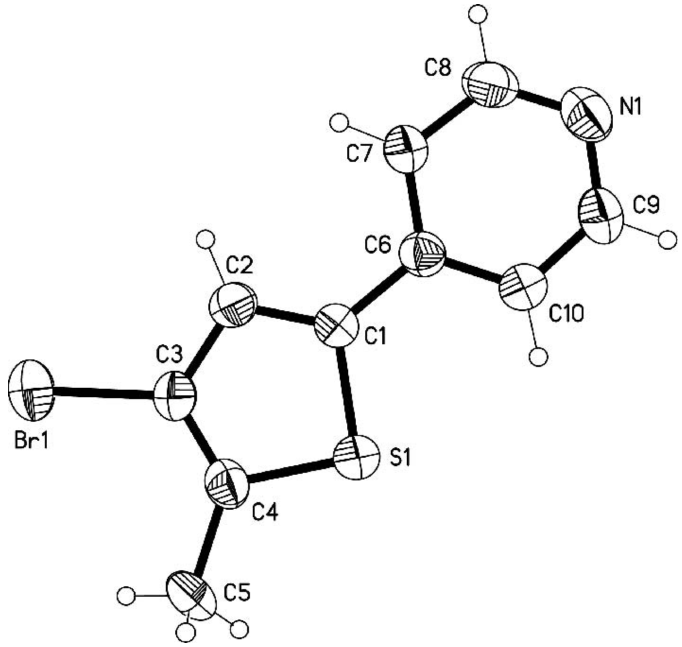

Figure 1
View of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 35% probability level. H atoms are represented by circles of arbitrary radius.

Crystal data

$C_{10}H_8BrNS$
M_r = 254.14
Orthorhombic, *Pbca*
a = 12.726 (4) Å
b = 11.629 (4) Å
c = 13.705 (5) Å
V = 2028.3 (11) Å^3
Z = 8
D_x = 1.665 Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 47 reflections
θ = 5.1–12.5°
μ = 4.21 mm^{-1}
T = 295 (2) K
Prism, yellow
0.4 × 0.4 × 0.3 mm

Data collection

Bruker *P*4 diffractometer
ω scans
Absorption correction: multi-scan (North *et al.*, 1968)
$T_{\min}$ = 0.217, $T_{\max}$ = 0.283
2321 measured reflections
1776 independent reflections
1028 reflections with $I > 2\sigma(I)$

$R_{\rm int}$ = 0.049
$\theta_{\max}$ = 25.0°
$h = -1 \rightarrow 15$
$k = -1 \rightarrow 13$
$l = -16 \rightarrow 1$
3 standard reflections every 97 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.098
S = 1.04
1776 reflections
119 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.001P)^2 + 3.5P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 0.26 e Å^{-3}
$\Delta\rho_{\min}$ = −0.30 e Å^{-3}

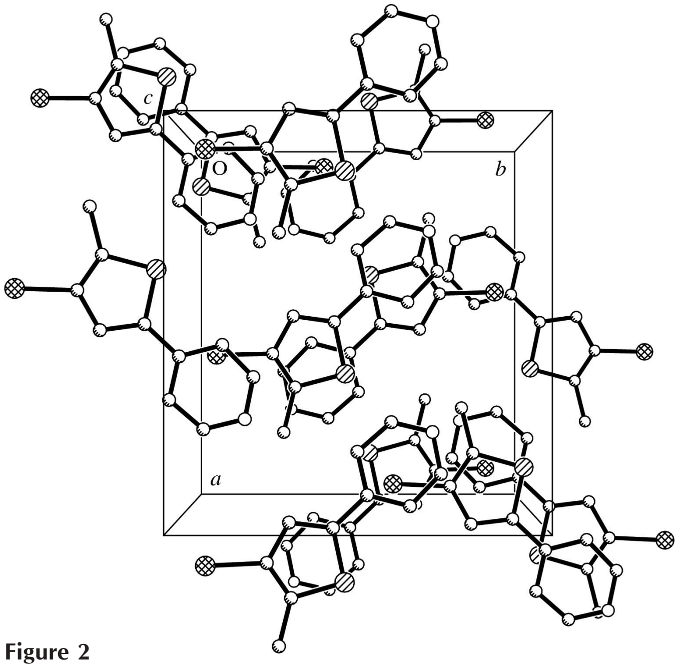

Figure 2
A view, down the *c* axis, of the molecular packing of (I). H atoms have been omitted.

All H atoms were refined using a riding model, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for aromatic, and C—H = 0.96 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for methyl C atoms.

Data collection: *XSCANS* (Bruker, 1997); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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References

Alvaro, F. A. & Lehn, J.-M. (1999). *Chem. Eur. J.* **5**, 3285–3292.
Bruker (1997). *XSCANS* (Version 2.2) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Gilat, S. L., Kawai, S. H. & Lehn, J.-M. (1993). *J. Chem. Soc. Chem. Commun.* pp. 1439–1442.
Irie, M. (2000). *Chem. Rev.* **100**, 1685–1716.
Matsuda, K., Takayama, K. & Irie, M. (2001). *Chem. Commun.* pp. 363–364.
Matsuda, K., Takayama, K. & Irie, M. (2004). *Inorg. Chem.* **43**, 482–489.
Nakashima, N., Deguchi, Y. & Irie, M. (1996). *Chem. Lett.* **25**, 817–818.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sasai, R., Ogiso, H., Shindachi, I., Shichi, T. & Takagi, K. (2000). *Tetrahedron*, **56**, 6979–6984.