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4-(5-{2-[5-(4-Cyanophenyl)-3-methylthiophen-2-yl]-3,3,4,4,5,5-hexafluorocyclopent-1-en-1-yl}-4-methylthiophen-2-yl)benzonitrile chloroform hemisolvate

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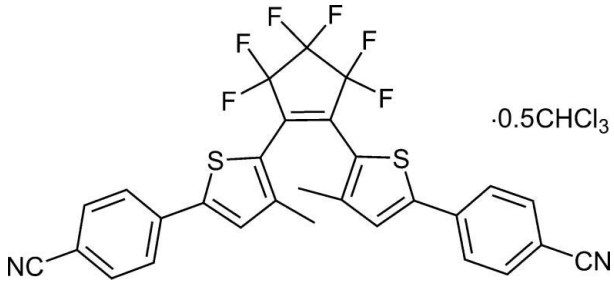
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.069; wR factor = 0.174; data-to-parameter ratio = 13.9.

The crystal structure of the title compound, $C_{29}H_{16}F_6N_2S_2\cdot 0.5CHCl_3$, consists of molecules with disordered perfluorocyclopentene rings [occupancy ratio 0.685 (3):0.315 (3)] and close F···F contacts (in the range 2.45–2.73 Å) between molecules. The short contacts are associated with the disorder. The dihedral angle between thiophene rings is 57.44 (8)°. The 5-(4-cyanophenyl)-3-methyl-2-thienyl groups of adjacent molecules are parallel, leading to zigzag chains of molecules along [101]. The dihedral angles between each thiophene ring and its adjacent cyanobenzene ring are 8.9 (2) and 7.15 (10)°.

Related literature

For applications of substituted thienylperfluorocyclopentenes as switches, see: Waldeck (1991); Pu *et al.* (2006); Dulic *et al.* (2007). For related structures, see: Irie *et al.* (1995, 2000); Morimitsu *et al.* (2002); Mori *et al.* (2011).



Experimental

Crystal data

$C_{29}H_{16}F_6N_2S_2\cdot 0.5CHCl_3$
M_r = 630.24
Monoclinic, $C2/c$
a = 18.4237 (4) Å
b = 15.7594 (6) Å
c = 20.9299 (7) Å
β = 113.280 (2)°
V = 5582.2 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 150 K
0.40 × 0.30 × 0.30 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*DENZO*/*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.857, T_{max} = 0.890
10636 measured reflections
6329 independent reflections
4168 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.174
S = 1.04
6329 reflections
455 parameters
92 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO*/*SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP99* for Windows (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MW2111).

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