Supporting Information for

Thiophene-Substituted Aza-Bodipy as Strategic Synthon for the Design of Near-Infrared Dyes.

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X-ray Diffraction for Compound 3

Crystal data

$C_{28}H_{16}BBr_2F_2N_3S_2$	$F(000)$ = 2640
M_r = 667.19	D_x = 1.773 Mg m^{-3}
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation, λ = 1.5418 Å
Hall symbol: -P 2ybc	Cell parameters from 13101 reflections
a = 14.606 (1) Å	θ = 3.6–67.4°
b = 14.212 (1) Å	μ = 6.02 mm^{-1}
c = 25.060 (2) Å	T = 110 K
β = 106.091 (7)°	Plate, dark red
V = 4998.2 (7) Å^3	0.36 × 0.17 × 0.08 mm
Z = 8	

Data collection

Xcalibur, Atlas, Gemini ultra diffractometer	8863 independent reflections
Radiation source: Enhance Ultra (Cu) X-ray Source	8407 reflections with $I > 2.0\sigma(I)$
mirror	$R_{int} = 0.073$
Detector resolution: 10.4685 pixels mm^{-1}	$\theta_{max} = 67.5°$, $\theta_{min} = 3.6°$
ω scans	$h = -17 \rightarrow 17$
Absorption correction: analytical *CrysAlis PRO*, Agilent Technologies, Version 1.171.35.11 (release 16-05-2011 CrysAlis171 .NET) (compiled May 16 2011,17:55:39) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid. (Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897)	$k = -16 \rightarrow 16$
$T_{min} = 0.159$, $T_{max} = 0.457$	$l = -29 \rightarrow 29$
54285 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.040$	Method, part 1, Chebychev polynomial, (Watkin, 1994, *P*rince, 1982) [*w*eight] = $1.0/[A_0*T_0(x) + A_1*T_1(x) \cdots + A_{n-1}]*T_{n-1}(x)]$ where A_i are the Chebychev coefficients listed below and x = *F* /*F*max Method = Robust Weighting (*P*rince, 1982) W = [*w*eight] * [1-(delta*F*/6*sigma*F*)^2]^2 A_i are: 0.142E + 04 0.241E + 04 0.150E + 04 626. 139.
$wR(F^2) = 0.113$	$(\Delta/\sigma)_{max} = 0.002$
$S = 1.01$	$\Delta\rangle_{max} = 0.66$ e Å^{-3}
8863 reflections	$\Delta\rangle_{min} = -0.71$ e Å^{-3}
686 parameters	Extinction correction: Larson (1970), Equation 22
0 restraints	Extinction coefficient: 48 (3)