Supporting Information

for

Synthesis of Functionalized Ethynylphenothiazine Fluorophores

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Tables of data collection parameters, bond lengths and angles, positional and thermal parameter, and least-squares planes for **7a**.

Table 1. Crystal data and structure refinement for **7a**.

Identification code	Kraemer11 Mueller M2251 5/00
Empirical formula	C17 H11 N S
Formula weight	261.33
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	orthorhombic
Space group	Pbca
Unit cell dimensions	a = 10.086(2) A alpha = 90 deg. b = 9.620(5) A beta = 90 deg. c = 27.859(6) A gamma = 90 deg.
Volume	2703(2) A^3
Z	8
Density (calculated)	1.284 Mg/m^3
Absorption coefficient	0.223 mm^-1
F(000)	1088
Crystal size	0.57 x 0.47 x 0.27 mm
Theta range for data collection	2.92 to 24.03 deg.
Index ranges	-11<=h<=11, -10<=k<=10, -31<=l<=31
Reflections collected	4228
Independent reflections	2113 [R(int) = 0.0250]
Absorption correction	Semi-empirical
Max. and min. transmission	0.9997 and 0.9721

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2113 / 0 / 173
Goodness-of-fit on F^2	1.115
Final R indices [I>2sigma(I)]	R1 = 0.0454, wR2 = 0.0917
R indices (all data)	R1 = 0.0772, wR2 = 0.1049
Largest diff. peak and hole	0.155 and -0.125 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **7a**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1)	4148(1)	2039(1)	1153(1)	64(1)
N(1)	6241(2)	-94(2)	1068(1)	65(1)
C(1)	5176(2)	1799(3)	649(1)	55(1)
C(2)	5063(2)	2649(3)	256(1)	58(1)
C(3)	5775(2)	2400(3)	-162(1)	61(1)
C(4)	6603(3)	1249(3)	-170(1)	70(1)
C(5)	6777(2)	434(3)	227(1)	67(1)
C(6)	6081(2)	692(3)	647(1)	58(1)
C(7)	6247(2)	599(3)	1512(1)	60(1)
C(8)	7128(3)	271(3)	1877(1)	76(1)
C(9)	7095(3)	965(3)	2307(1)	79(1)
C(10)	6195(3)	2028(3)	2394(1)	68(1)
C(11)	5313(3)	2370(3)	2027(1)	63(1)
C(12)	5332(2)	1667(3)	1598(1)	57(1)
C(13)	5668(3)	3311(3)	-567(1)	71(1)
C(14)	5609(4)	4049(4)	-894(1)	97(1)
C(15)	7029(3)	-1373(3)	1036(1)	87(1)
C(16)	6190(3)	2755(4)	2839(1)	79(1)
C(17)	6213(4)	3365(4)	3202(1)	97(1)

Table 3. Selected bond lengths [A] and angles [deg] for **7a**.

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [A] and angles [deg] for **7a**.

S(1)-C(12)	1.757(3)
S(1)-C(1)	1.762(3)
N(1)-C(6)	1.404(3)
N(1)-C(7)	1.407(3)
N(1)-C(15)	1.467(3)
C(1)-C(2)	1.370(3)
C(1)-C(6)	1.403(3)
C(2)-C(3)	1.389(3)
C(3)-C(4)	1.387(4)
C(3)-C(13)	1.433(4)
C(4)-C(5)	1.366(4)
C(5)-C(6)	1.387(4)
C(7)-C(8)	1.386(3)
C(7)-C(12)	1.401(3)
C(8)-C(9)	1.373(4)
C(9)-C(10)	1.389(4)
C(10)-C(11)	1.395(4)
C(10)-C(16)	1.422(4)
C(11)-C(12)	1.374(4)
C(13)-C(14)	1.156(4)
C(16)-C(17)	1.169(4)
C(12)-S(1)-C(1)	97.82(12)
C(6)-N(1)-C(7)	118.7(2)
C(6)-N(1)-C(15)	117.6(2)
C(7)-N(1)-C(15)	116.6(2)
C(2)-C(1)-C(6)	120.3(2)
C(2)-C(1)-S(1)	120.7(2)
C(6)-C(1)-S(1)	119.0(2)
C(1)-C(2)-C(3)	121.6(2)
C(4)-C(3)-C(2)	117.5(3)
C(4)-C(3)-C(13)	121.4(3)
C(2)-C(3)-C(13)	121.1(2)
C(5)-C(4)-C(3)	121.5(3)
C(4)-C(5)-C(6)	121.0(3)
C(5)-C(6)-C(1)	117.9(3)
C(5)-C(6)-N(1)	123.4(2)
C(1)-C(6)-N(1)	118.7(2)
C(8)-C(7)-C(12)	117.7(3)
C(8)-C(7)-N(1)	122.7(2)
C(12)-C(7)-N(1)	119.6(2)
C(9)-C(8)-C(7)	120.9(3)
C(8)-C(9)-C(10)	121.8(3)
C(9)-C(10)-C(11)	117.5(3)
C(9)-C(10)-C(16)	121.1(3)
C(11)-C(10)-C(16)	121.4(3)
C(12)-C(11)-C(10)	120.9(3)
C(11)-C(12)-C(7)	121.2(3)
C(11)-C(12)-S(1)	120.2(2)
C(7)-C(12)-S(1)	118.5(2)
C(14)-C(13)-C(3)	178.6(4)
C(17)-C(16)-C(10)	178.4(4)

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for **7a**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1)	47(1)	68(1)	77(1)	3(1)	4(1)	12(1)
N(1)	54(1)	43(1)	97(2)	-10(1)	-6(1)	7(1)
C(1)	41(1)	47(2)	76(2)	-13(1)	-1(1)	1(1)
C(2)	49(1)	49(2)	74(2)	-14(1)	-1(1)	2(1)
C(3)	51(1)	59(2)	72(2)	-21(1)	2(1)	-7(1)
C(4)	54(2)	73(2)	84(2)	-29(2)	5(2)	-5(2)
C(5)	47(2)	57(2)	96(2)	-28(2)	0(2)	8(1)
C(6)	46(1)	42(1)	86(2)	-12(1)	-8(1)	-2(1)
C(7)	49(2)	45(2)	86(2)	3(1)	-2(1)	1(1)
C(8)	69(2)	57(2)	101(2)	1(2)	-10(2)	15(2)
C(9)	72(2)	74(2)	90(2)	12(2)	-14(2)	9(2)
C(10)	72(2)	59(2)	73(2)	10(2)	3(2)	1(2)
C(11)	59(2)	55(2)	74(2)	13(1)	11(1)	7(1)
C(12)	49(1)	48(2)	74(2)	7(1)	6(1)	1(1)
C(13)	73(2)	72(2)	69(2)	-19(2)	7(2)	-7(2)
C(14)	126(3)	85(2)	79(2)	-9(2)	18(2)	-3(2)
C(15)	80(2)	51(2)	129(3)	-15(2)	-15(2)	18(2)
C(16)	87(2)	81(2)	69(2)	17(2)	3(2)	9(2)
C(17)	112(3)	104(3)	74(2)	10(2)	0(2)	28(2)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **7a**.

	x	y	z	U(eq)
H(2)	4497(2)	3411(3)	270(1)	69
H(4)	7049(3)	1027(3)	-452(1)	84
H(5)	7372(2)	-304(3)	215(1)	80
H(8)	7750(3)	-429(3)	1829(1)	91
H(9)	7691(3)	716(3)	2547(1)	94
H(11)	4703(3)	3082(3)	2074(1)	75
H(14)	5561(4)	4643(4)	-1157(1)	116
H(15A)	7953(3)	-1140(3)	1018(6)	104
H(15B)	6777(12)	-1882(9)	754(4)	104
H(15C)	6872(13)	-1933(9)	1316(3)	104
H(17)	6232(4)	3850(4)	3490(1)	116