Supporting Information

Unexpectedly long lifetime of the excited state of benzothiadiazole derivative and its adducts with Lewis acids

by

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Table S1. Crystal data and structure refinement for the compounds.

Identification code	**2**	**3**·2C_7H_8
Empirical formula	$C_{22}H_{16}Br_2Cl_4N_8S_2Zn$	$C_{91}H_{78}Br_2Cl_2Cu_2N_8O_2P_4S_2$
Formula weight	823.54	1861.41
Temperature/K	150(2)	150(2)
Crystal system	monoclinic	orthorhombic
Space group	$P2_1/c$	$Pna2_1$
a/Å	11.5203(9)	19.7043(12)
b/Å	18.2029(16)	18.9722(12)
c/Å	13.1842(12)	22.2962(17)
β/°	93.957(3)	90
Volume/Å^3	2758.2(4)	8335.1(10)
Z	4	4
ρ_{calc}g/cm^3	1.983	1.483
μ/mm^{-1}	4.359	1.715
F(000)	1616.0	3800.0
Crystal size/mm^3	0.15 ×0.1 ×0.05	0.23 ×0.15 ×0.14
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/ °	3.544 to 48.874	3.496 to 48.876
Reflections collected	25850	11798
Independent reflections	4555 [R_{int} = 0.0908, R_{sigma} = 0.0790]	11798 [R_{int} = 0.089, R_{sigma} = 0.3417]
Data/restraints/parameters	4555/8/358	11798/612/883
Goodness-of-fit on F^2	1.014	0.910
Final R indexes [I>=2σ (I)]	R_1 = 0.0478, wR_2 = 0.1044	R_1 = 0.0716, wR_2 = 0.1441
Final R indexes [all data]	R_1 = 0.0833, wR_2 = 0.1176	R_1 = 0.1144, wR_2 = 0.1520
Largest diff. peak/hole / e Å^{-3}	1.45/-0.91	1.36/-0.76
Flack parameter		0.43(2)