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Planar 2-(2-hydroxyphenyl)benzothiazole-based dyes functionalized via triple bonds as exceedingly efficient solid-state fluorophores

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Measurement Conditions and Instruments

UV absorption spectra were obtained on a UV-vis spectrophotometer (U-3310). The fluorescence spectra were recorded on a fluorospectrophotometer (F-7000). The fluorescence quantum yield (Φ_f) in solution was determined by using quinine sulfate (Φ_f = 0.55 in 0.1M H_2SO_4) as a standard. Φ_f of the crystals were determined with a PTI C-701 calibrated integrating sphere system.

The single crystals of compounds HBT-H and HBT-Me were obtained by the slow diffusion of their respective CH_2Cl_2/hexane solution for several days at room temperature. The data collection was done at room temperature on a Bruker SMART APEX-II CCD area detector using graphite-monochromated Mo Ka radiation (λ=0.71073 Å). Data reduction and integration were done by the INTEGRATE program of the $APEX_2$ software. Semi-empirical absorption correction was applied using the SCALE program. The structure was solved by direct method and refined by the full matrix least-squares method on F_2 using SHELX."

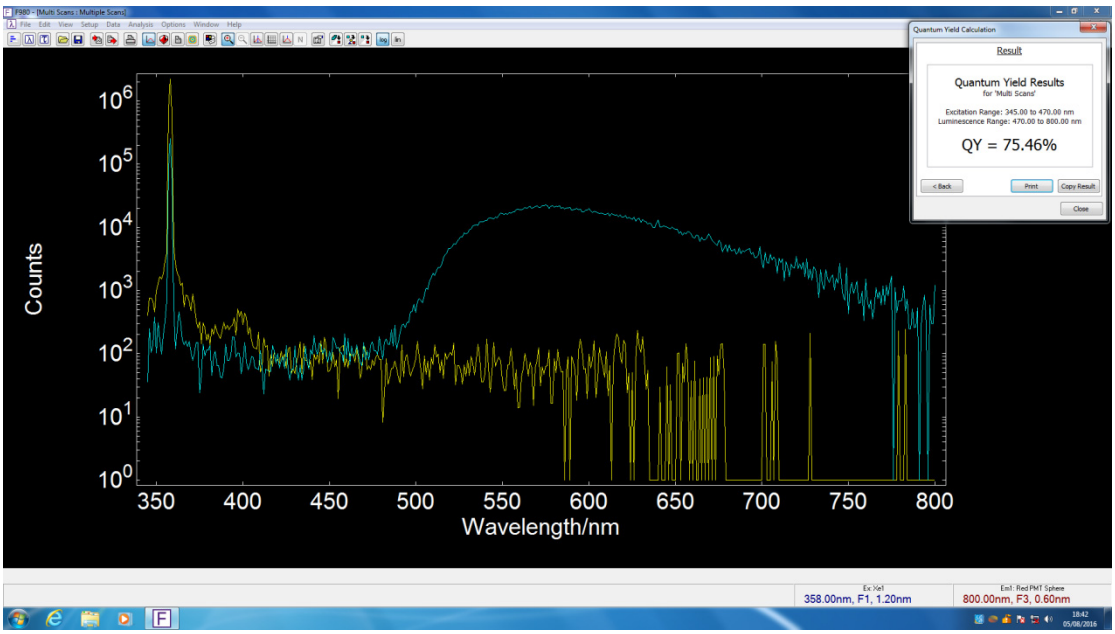

Fig. S1 the Φ_f of HBT-H crystal measured by integrating sphere.

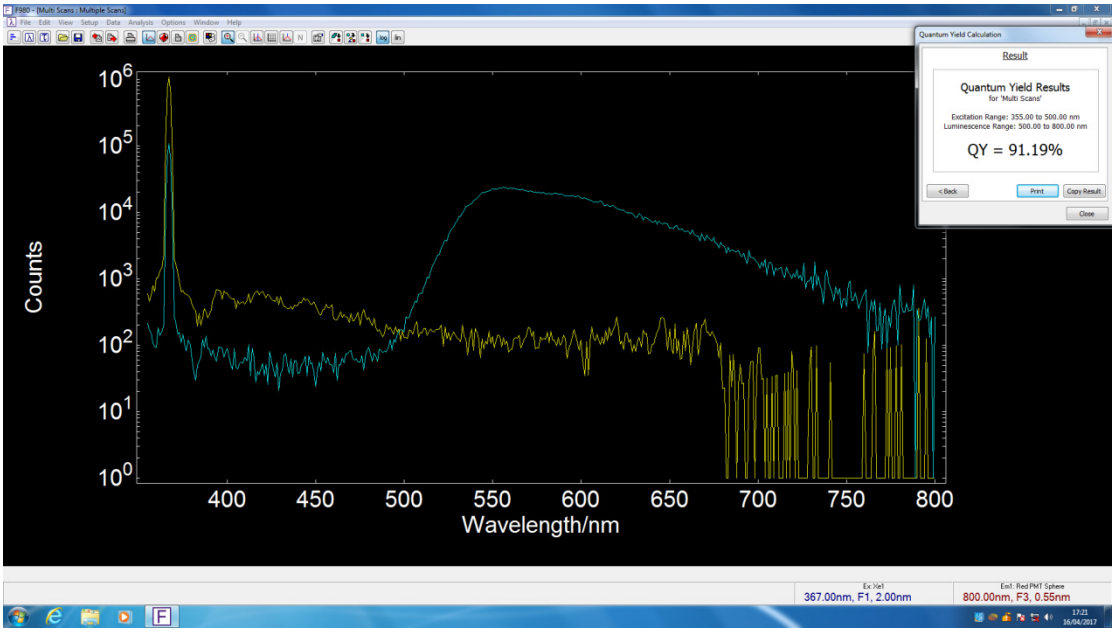

Fig. S2 the Φ_f of HBT-Me crystal measured by integrating sphere.

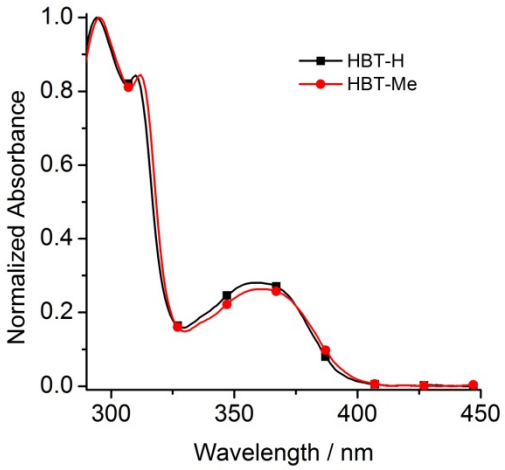

Fig. S3 Absorption spectra of HBT-H and HBT-Me in toluene.

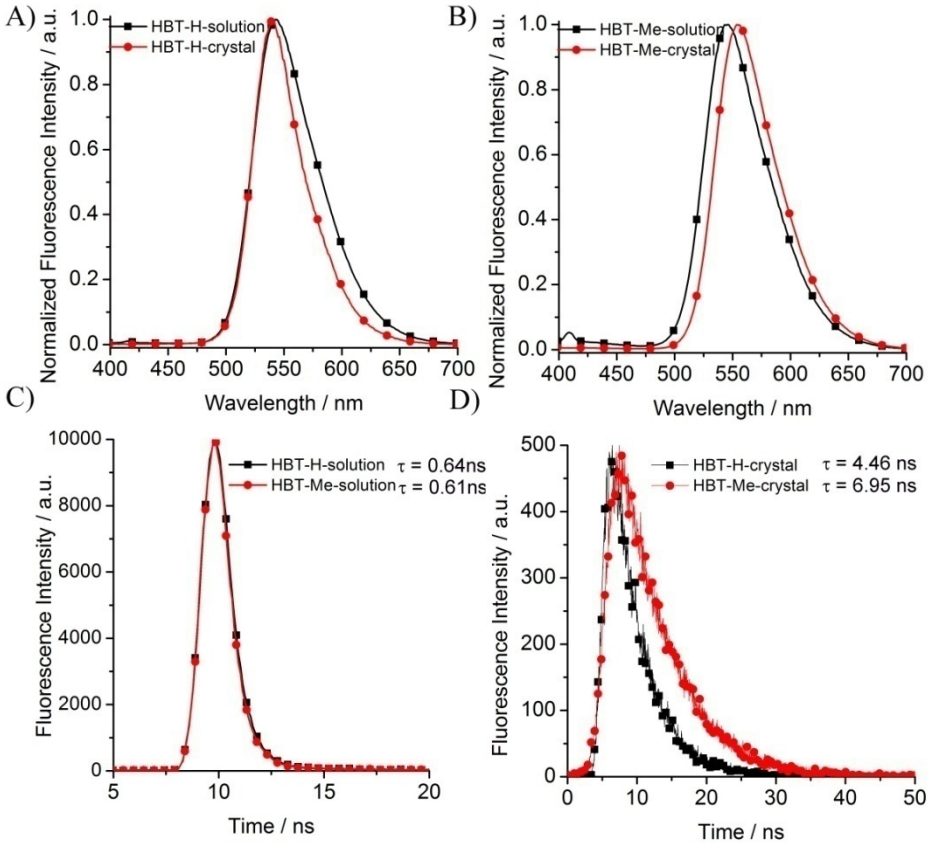

Fig. S4 Fluorescence spectra of a) HBT-H and b) HBT-Me in toluene solutions and in the crystalline state. Fluorescence lifetimes (τ) of HBT-H and HBT-Me c) in toluene solutions and d) in the crystalline state. The sample was excited at 360 nm and the emission kinetic data were collected at their respective keto-emission wavelength.

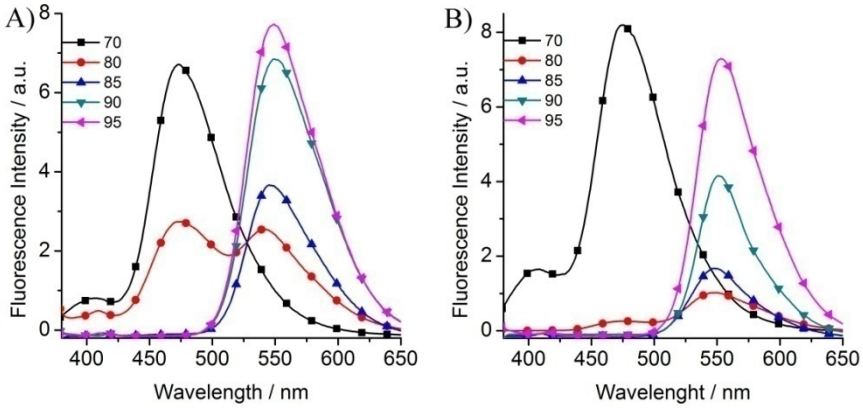

Fig. S5 Changes in fluorescence spectra of a) HBT-H and b) HBT-Me as the amount of water in THF was increased. λ_{em}=360 nm for HBT-H and HBT-Me.

Table S1. Crystal data and structure refinement for HBT-H (CCDC number 1482414.

Empirical formula	C21 H13 N O S
Formula weight	327.38
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 4.5363(4) A alpha = 90 deg.
	b = 10.1250(8) A beta = 90 deg.
	c = 34.375(3) A gamma = 90 deg.
Volume	1578.8(2) A^3
Z, Calculated density	4, 1.377 Mg/m^3
Absorption coefficient	0.211 mm^-1
F(000)	680
Crystal size	0.43 x 0.17 x 0.15 mm
Theta range for data collection	2.33 to 25.02 deg.
Limiting indices	-5<=h<=5, -11<=k<=12, -40<=l<=38
Reflections collected / unique	8041 / 2782 [R(int) = 0.0448]
Completeness to theta = 25.02	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9690 and 0.9147
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2782 / 0 / 217
Goodness-of-fit on F^2	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0446, wR2 = 0.0649
R indices (all data)	R1 = 0.0680, wR2 = 0.0684
Absolute structure parameter	-0.10(10)
Largest diff. peak and hole	0.213 and -0.178 e.A^-3

Table S2. Crystal data and structure refinement for HBT-Me (CCDC number 1482415).

Empirical formula	C22 H15 N O S
Formula weight	341.41
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 8.0270(8) A alpha = 90 deg.
	b = 5.9177(5) A beta = 90.1860(10) deg.
	c = 35.133(3) A gamma = 90 deg.
Volume	1668.8(3) A^3
Z, Calculated density	4, 1.359 Mg/m^3
Absorption coefficient	0.203 mm^-1
F(000)	712

Crystal size	0.40 x 0.35 x 0.30 mm
Theta range for data collection	2.32 to 25.02 deg.
Limiting indices	-8<=h<=9, -7<=k<=4, -38<=l<=41
Reflections collected / unique	7857 / 2925 [R(int) = 0.0433]
Completeness to theta = 25.02	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9416 and 0.9232
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2925 / 0 / 228
Goodness-of-fit on F^2	1.056
Final R indices [I>2sigma(I)]	R1 = 0.0570, wR2 = 0.1308
R indices (all data)	R1 = 0.0799, wR2 = 0.1411
Extinction coefficient	0.0122(14)
Largest diff. peak and hole	0.248 and -0.236 e.A^-3