

Electronic Supporting Information

How do substituents affect silole emission?

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Table S1. Summary of crystal data and intensity collection parameters for TPS, TPS-TMSEP and TPS-2TMSEP.

	TPS	TPS-TMSEP	TPS-2TMSEP
Empirical formula	C ₂₈ H ₂₂ Si	C ₃₉ H ₃₄ Si ₂	C ₅₀ H ₄₆ Si ₃
Mol wt	386.55	558.84	731.16
Crystal dimensions, mm	0.32 × 0.18 × 0.07	0.22 × 0.19 × 0.17	0.25 × 0.05 × 0.04
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	P2 (1)/c	P2 (1)/c	I2/a
a, Å	9.29560 (10)	18.8276 (4)	11.2522 (2)
b, Å	16.8937 (5)	11.9360 (3)	24.9636 (4)
c, Å	14.1056 (3)	15.0270 (3)	18.4374 (4)
α, deg	90	90	90
β, deg	108.130	104.794 (2)	104.987 (2)
γ, deg	90	90	90
V, Å ³	2105.13 (8)	3265.01 (13)	5002.81 (16)
Z	4	4	4
D _{calcd.} , g cm ⁻³	1.220	1.137	1.196
F ₀₀₀	816	1184	1888
Temp, (K)	173.00 (14)	173.00 (14)	173.00 (14)
Radation (λ), Å	1.5418	1.5418	1.5418
μ (Mo Kα) mm ⁻¹	1.045	1.160	3.084
2θ _{max} , deg (completeness)	66.50 (98.8%)	66.50 (97.0%)	66.50 (98.0%)
No. of collected reflns.	10945	17680	15006
No. of unique reflns.(R _{int})	3742 (0.0295)	5703 (0.0765)	4381 (0.0259)
R ₁ , wR ₂ [obs I > 2σ (I)]	0.0318, 0.0839	0.0570, 0.1425	0.0587, 0.1619
R ₁ , wR ₂ (all data)	0.0344, 0.0860	0.0714, 0.1556	0.0611, 0.1644
Residual peak/hole e.Å ⁻³	0.238/-0.225	0.521/-0.304	0.685/-0.502
Transmission ratio	1.00/0.68	1.00/0.37	1.00/0.28
Goodness-of-fit on F ²	1.006	1.003	1.013

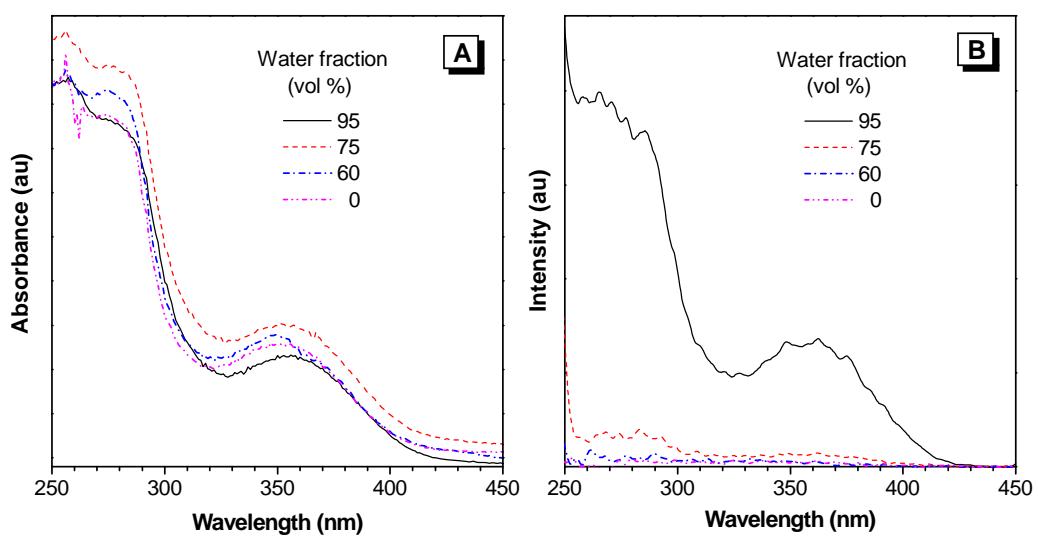


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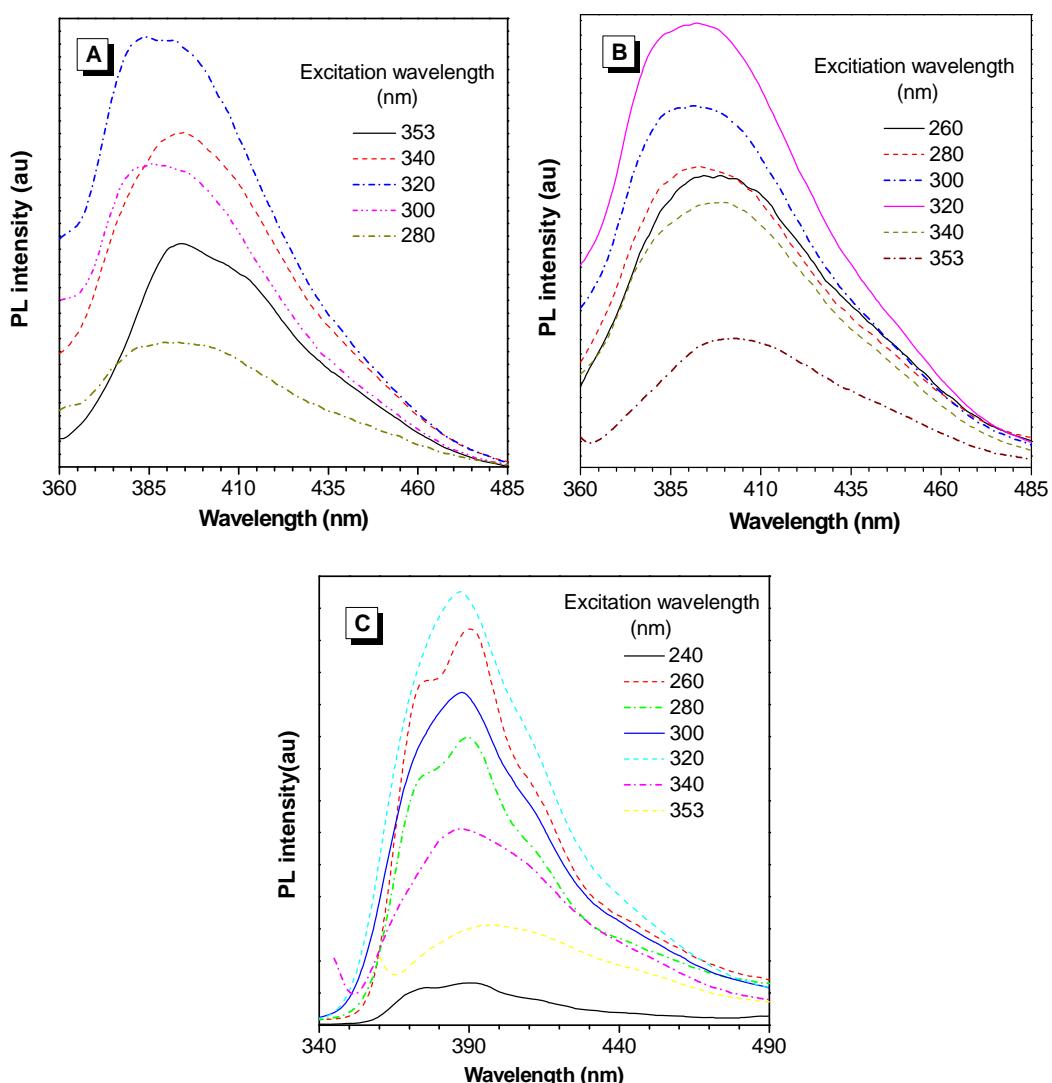


Figure S2. PL spectra of TPS-TMSEP in (A) THF, (B) THF/water mixture (40/60, v/v) and (C) chloroform at different excitation wavelengths. Concentration: 10 μ M.