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Supporting Information for B604910A

A new series of fluorescent 5-methoxy-2-pyridylthiazoles with a pH-sensitive dual-emission

Ming-Hua Zheng,^{a,b} Jing-Yi Jin,^{a,b} Wei Sun,^a and Chun-Hua Yan*^a

^a Beijing National Laboratory for Molecular Sciences, State Key Lab of Rare Earth Materials Chemistry and Applications & PKU-HKU Joint Lab in Rare Earth Materials and Bioinorganic Chemistry, Peking University, Beijing 100871, China

^b Department of Chemistry, Yanbian University, Yanji, Jilin 133002, China



Fig. S1 Absorption of 2-MPT in different solvents



Fig. S2 Absorption of 4-MPT in different solvents



Fig. S3 Absorption of 3-MPT in different solvents



Fig. S4 Excitation spectra of MPTs in MeCN



Fig. S5 Excitation spectra of MPTs in water.



Fig. S6 Fluorescence emissions of 2-MPT in different solvents



Fig. S7 Fluorescence emissions of 4-MPT in different solvents.



Fig. S8 Fluorescence emissions of 3-MPT in different solvents



Fig. S9 Fluorescence emissions of MPTs at different concentrations in acetonitrile: (a) 2-MPT; (b) 4-MPT; (c) 3-MPT.



Fig. S10 Fluorescence emissions of MPTs at different concentrations in aqueous system: (a) 2-MPT; (b) 4-MPT; (c) 3-MPT.







c

35

40

45

30

10

10¹

100

Counts 10² ecay24

IR23 Decay24F Decay24F

Fit Results τ1 3.21ns χ2 1.053

а



b

d



f



15

1(

Fig. S11 Fluorescence decay curves of 2-MPT in (a) in n-hexane; (b) in chloroform; (c) tetrahydrofuran; (d) dichloromethane; (e) acetonitrile; (f) methanol; (g) water at 298 K.



Fig. S12 Fluorescence decay curves of 4-MPT in (a) in chloroform; (b) tetrahydrofuran; (c) dichloromethane; (d) acetonitrile; (e) methanol; (f) water at 298 K.







Fig. S13 Fluorescence decay curves of 2-MPT at pH ($\lambda_{em} = 400$ nm excited at 310 nm).



Fig. S14 Fluorescence decay curves of 2-MPT at pH 1.0-2.5 (λ_{em} = 455 nm excited at 365 nm).





Fig. S15 Fluorescence decay curves of 4-MPT at pH 1.5-6.0 ($\lambda_{em} = 400$ nm excited at 320 nm).





(e) pH=3.0

Fig. S16 Fluorescence decay curves of 4-MPT at pH 1.0-3.0 (λ_{em} = 445 nm excited at 365 nm).



Fig. S17 Minimum energy conformation calculated with Gaussian03 by using density functional theory (DFT) at the B3LYP level.