Electronic Supplementary Material (ESI) for New Journal of Chemistry

Supplementary Information

Vapor phase pH induced fluorescence switching of a dimethylaminostyryl terpyridine derivative in thin films

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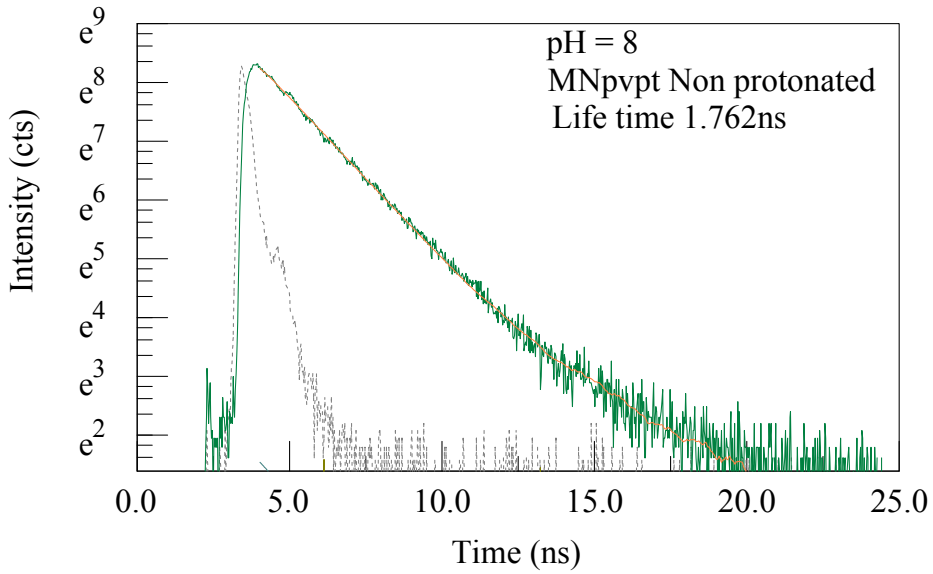
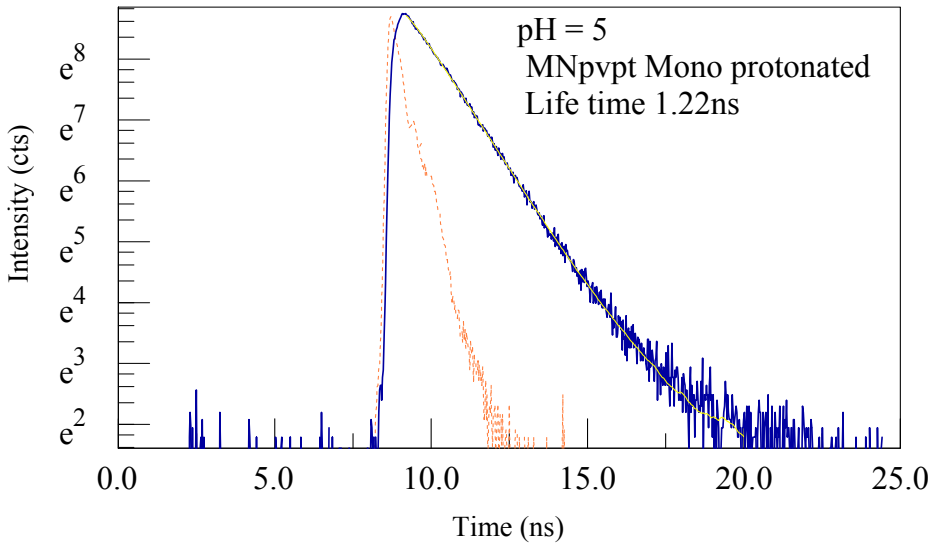
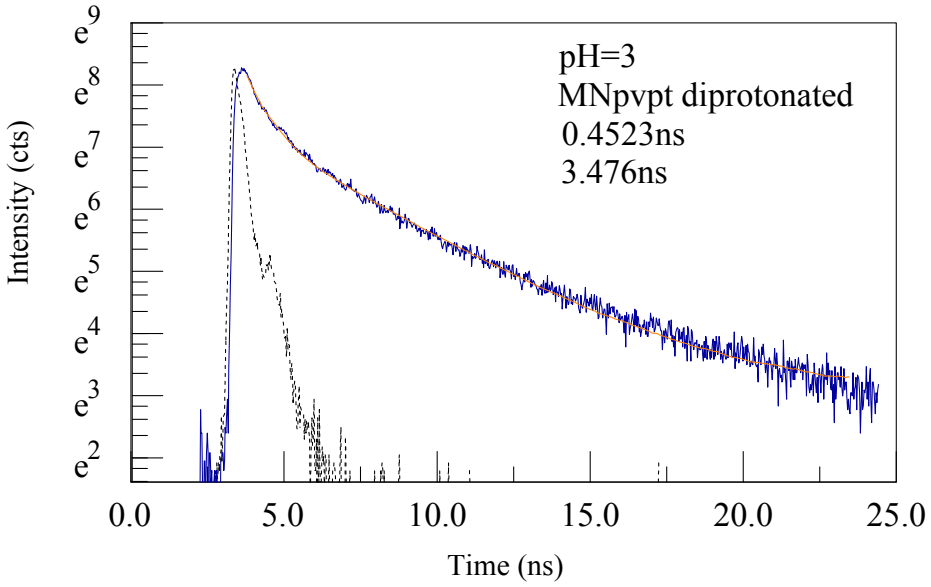
Lifetime data for MNpvpt ligand at different pH's recorded using single photon counting. Shown below is the scatter (dotted line), decay and the fit .



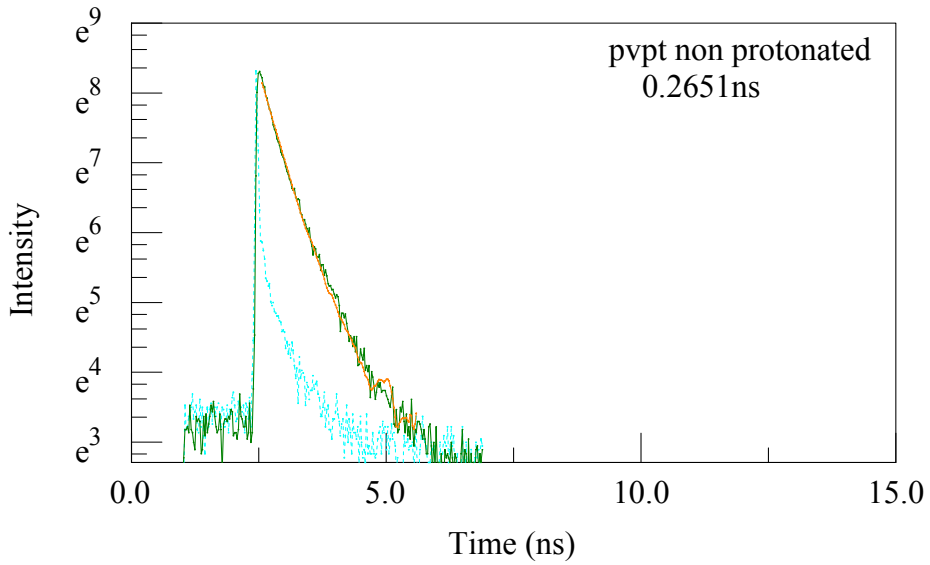


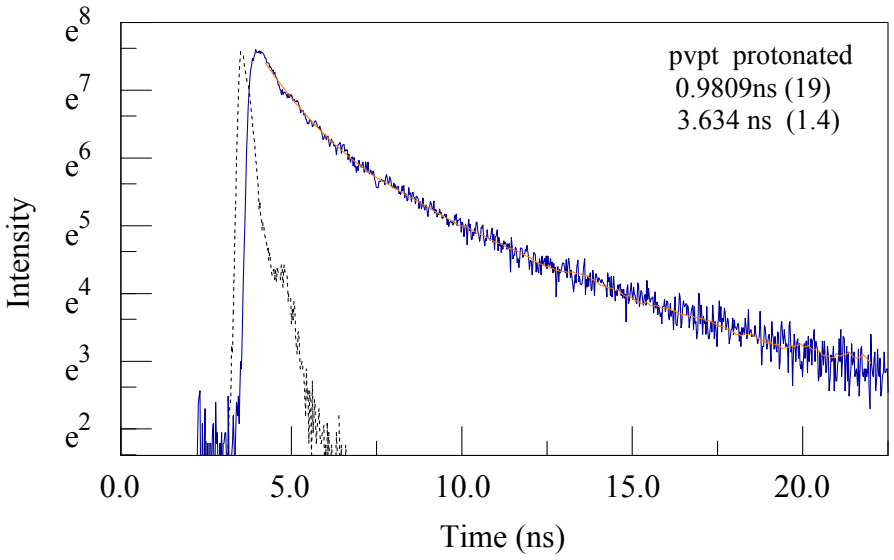


Life-time	Pre-exponential factor
0.4523ns	3.77
3.476ns	0.94

$pH = pKa^{*} - \log[\tau_{protonated} / \tau_{deprotonated}]$ was used to calculate the excited state pKa of these molecules..

$\tau_{protonated}$ – Life-time of protonated form
$\tau_{deprotonated}$ – Life-time of non-protonated form



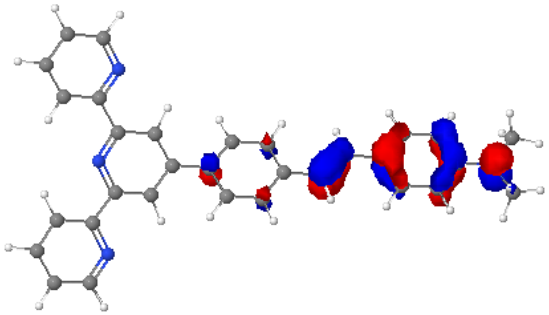


DFT calculations and molecular orbitals for MNpvpt (a) and HMNpvpt (b)

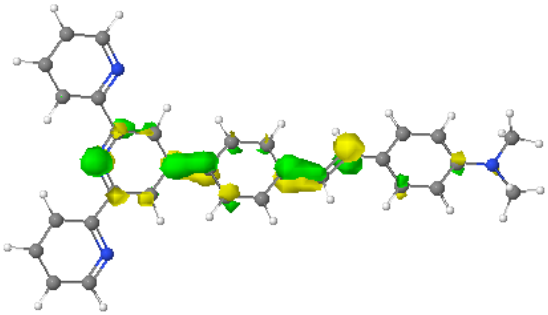
B3LYP TD-DFT calculations were employed for the molecules MNpvpt and mono-protonated MNpvpt (HMNpvpt- protonation of the dimethylamino nitrogen) using the Gaussian 03 (ref. below) software package employing the basis set (6-31G*). The geometry was fully optimized before setting up the calculations for singlet excited state molecular orbitals.

(a) MNpvpt

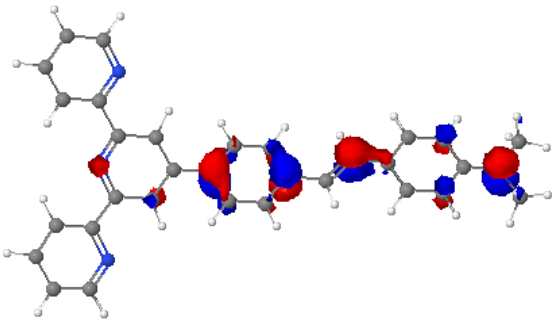
HOMO



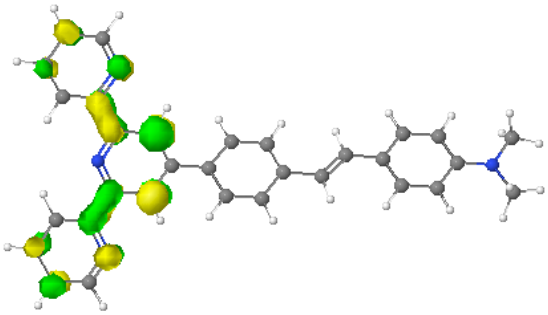
LUMO



(HOMO-1)



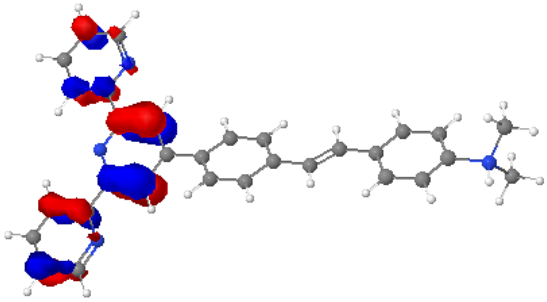
(LUMO+1)



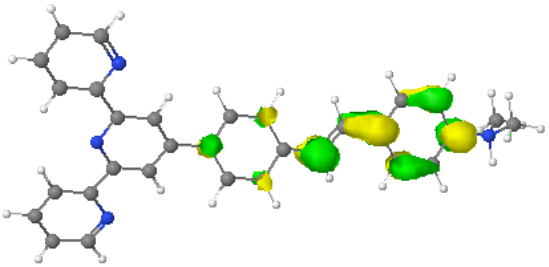
IN MNpvpt the HOMO is mostly localized on the dimethylaminonitrogen phenyl moiety and the LUMO is mostly localized on the terpyridine moiety. Upon protonation of the diemthylaminonitrogen as in HMNpvpt (shown below) the HOMO is localized on the terpyridine moiety and the LUMO is localized on the dimethylaminonitrogen phenyl moiety.

(b) HMNpvpt

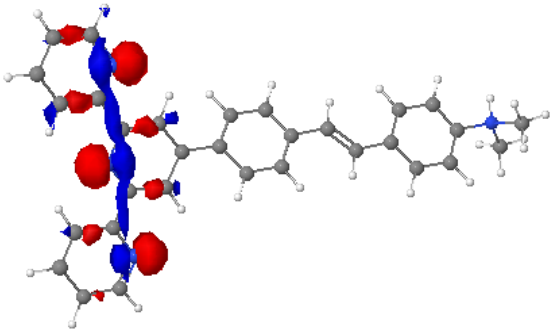
HOMO



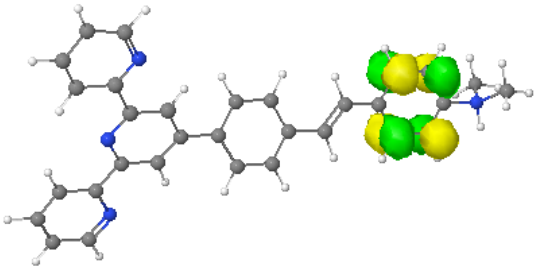
LUMO



(HOMO-1)



(LUMO+1)



Gaussian 03, Revision D.02,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
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Gaussian, Inc., Wallingford CT, 2004.