

Supporting Information

for

Photophysical properties of free-base and manganese(III) N-confused porphyrins

Li-Li Wang,¹ Su-Hong Peng,^{2,3} Hui Wang,^{*,1} Liang-Nian Ji,^{1,4} and Hai-Yang Liu^{*,2}

¹ State Key Laboratory of Optoelectronics Materials and Technologies, Sun Yat-Sen University,

Guangzhou 510275, China

² Department of Chemistry, South China University of Technology, Guangzhou 510641, China

³ College of Chemistry and Bioengineering, Yichun University, Yichun 336000, China

⁴ School of Chemistry and Chemical Engineering/MOE Laboratory of Bioinorganic and Synthetic

Chemistry, Sun Yat-Sen University, Guangzhou 510275, China

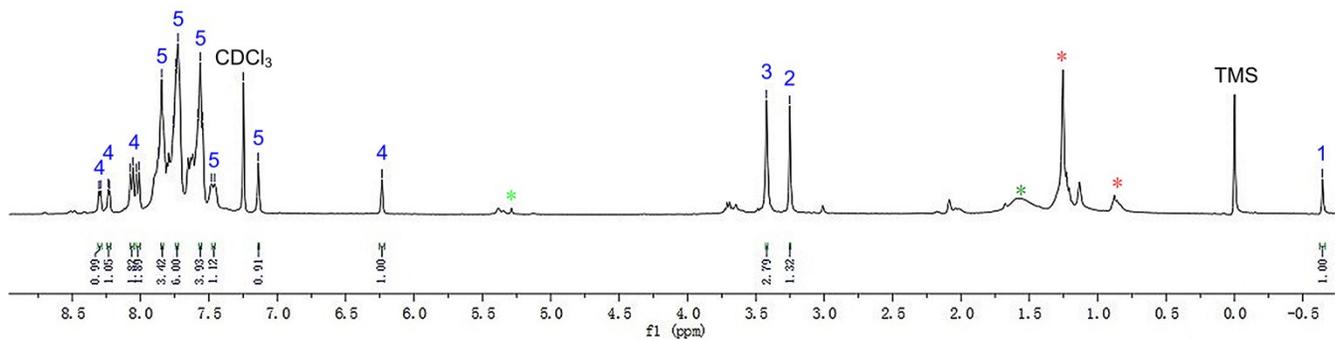


Fig. S2 ^1H NMR spectrum of NCH_3NCTPP with *para*-Cl recorded in CDCl_3 .

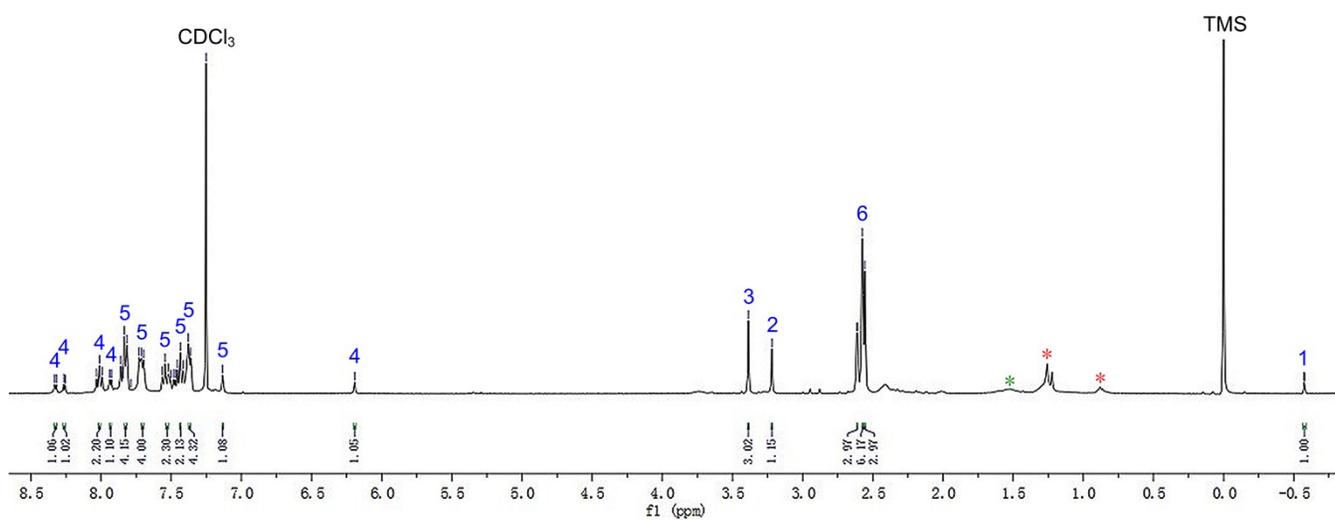


Fig. S3 ^1H NMR spectrum of NCH_3NCTPP with *para*- CH_3 recorded in CDCl_3 .

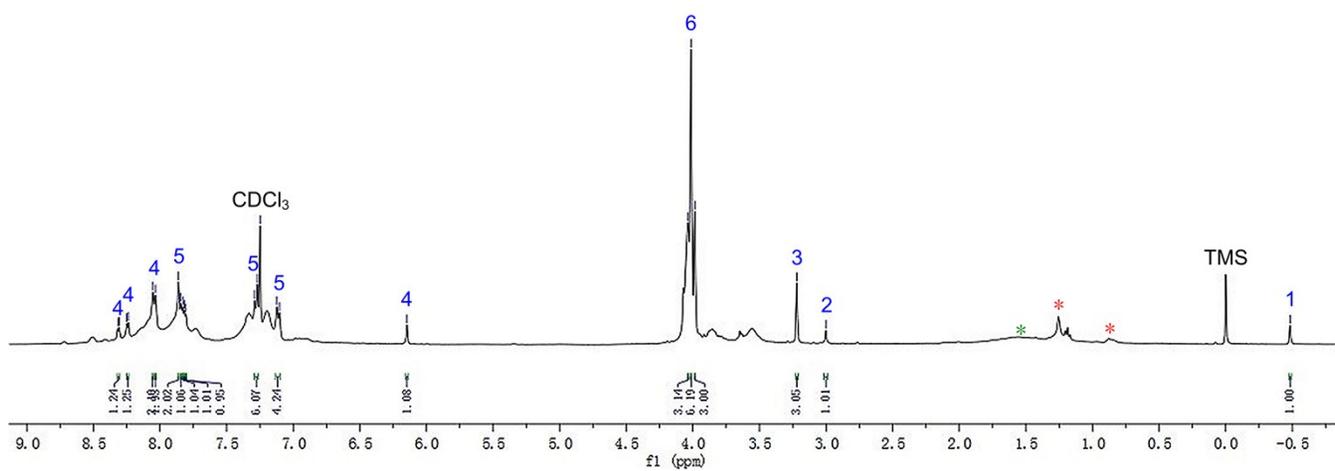


Fig. S4 ^1H NMR spectrum of NCH_3NCTPP with *para*- OCH_3 recorded in CDCl_3 .

2. Nanosecond Transient Absorption Measurement of N-confused Porphyrins.

The triplet state dynamics of Mn(Cl)NCH₃NCTPPs and NCTPP with *para*-H were measured using laser flash photolysis apparatus with 532-nm excitation.³ The triplet absorption decay curves were well fitted with a single-exponential function convoluted with a Gaussian response function. The triplet quantum yield of NCTPP with *para*-H was calculated to be 0.30, using TPP in toluene as a reference ($\Phi_{T(\text{std})} = 0.80$, $\epsilon_{T(\text{std})} \approx 35000 \text{ M}^{-1}\text{cm}^{-1}$).^{3, 4} The T₁-state lifetime of NCTPP with *para*-H in deaerated toluene is fitted to be 47.5 μs , which is in agreement with the earlier report.⁵ Unfortunately, the ⁷T₁-state absorption of Mn(Cl)NCH₃NCTPPs in deaerated DCM were not detected by using the same experimental apparatus.

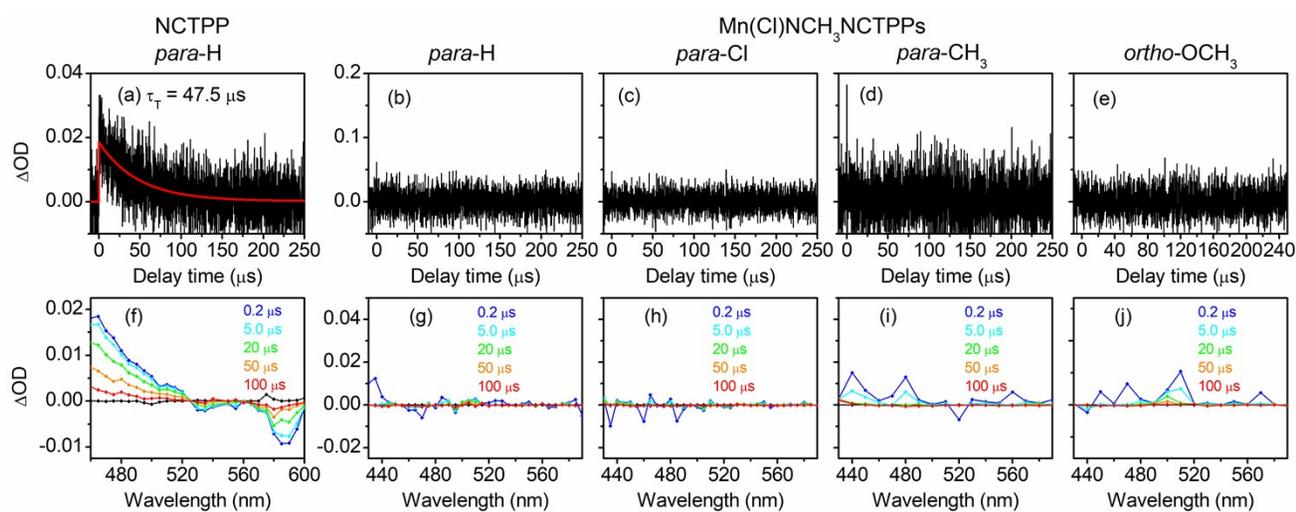


Fig. S7 Triplet kinetics (a–e) and spectra (f–j) of NCTPP with *para*-H in deaerated toluene and four Mn(Cl)NCH₃NCTPPs in deaerated DCM. Sample concentration was about 34 μM .

3. Steady-state Absorption Spectra of Solvents.

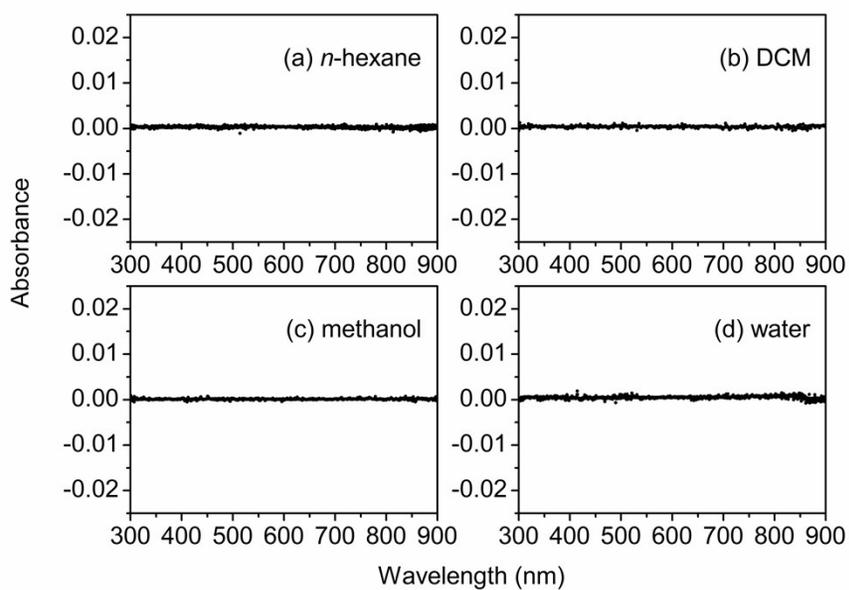


Fig. S8 Steady-state absorption spectra of solvents: (a) *n*-hexane, (b) DCM, (c) methanol, and (d) water.

References

1. S.-H. Peng, M. H. R. Mahmood, H.-B. Zou, S.-B. Yang and H.-Y. Liu, *J. Mol. Catal. A: Chem.*, 2014, 395, 180-185.
2. H. E. Gottlieb, V. Kotlyar and A. Nudelman, *J. Org. Chem.*, 1997, 62, 7512-7515.
3. W. Shao, H. Wang, S. He, L. Shi, K. Peng, Y. Lin, L. Zhang, L. Ji and H. Liu, *J. Phys. Chem. B*, 2012, 116, 14228-14234.
4. A. C. Pelegrino, M. M. Carolina, A. F. Gotardo, A. R. Simioni, M. D. Assis and A. C. Tedesco, *Photochem. Photobiol.*, 2005, 81, 771-776.
5. E. A. Alemán, C. S. Rajesh, C. J. Ziegler and D. A. Modarelli, *J. Phys. Chem. A*, 2006, 110, 8605-8612.