

Electronic Supporting Information

Porphothionolactones: Synthesis, structure, physical, and chemical properties of a chemodosimeter for hypochlorite[‡]

Yi Yu, Brigitte Czepukojc, Claus Jacob, Yue Jiang, Matthias Zeller,
Christian Brückner* and Jun-Long Zhang*

* Beijing National Laboratory for Molecular Sciences, State Key Laboratory of Rare Earth Materials Chemistry and Applications, College of Chemistry and Molecular Engineering, Peking University, ChengFu Road 202, Beijing 100871, P.R. China.

Fax: (+86) 10-62767034; E-mail: zhangjunlong@pku.edu.cn

* Department of Chemistry, University of Connecticut, Storrs, CT 06269-3060 USA.

Fax: (+01) 860-486-2981; E-mail: c.bruckner@uconn.edu

Table of Contents

Figure S1. ¹ H NMR spectrum of 5a in CDCl ₃ .	2
Figure S2. ¹ H NMR spectrum of 5b in CDCl ₃ .	2
Figure S3. ¹ H NMR spectrum of 5c in CDCl ₃ .	3
Figure S4. ¹ H NMR spectrum of 5d in CDCl ₃ .	3
Figure S5. ¹³ C NMR spectrum of 5a in CDCl ₃ .	4
Figure S6. ¹³ C NMR spectrum of 5b in CDCl ₃ .	4
Figure S7. ¹³ C NMR spectrum of 5c in CDCl ₃ .	5
Figure S8. ¹³ C NMR spectrum of 5d in CDCl ₃ .	5
Figure S9. ¹⁹ F NMR spectrum of 5a in CDCl ₃ .	6
Figure S10. Normalized UV-vis absorption spectra of 4a and 5a in DCM.	6
Figure S11. Normalized UV-vis absorption spectra of 4b and 5b in DCM.	7
Figure S12. Normalized UV-vis absorption spectra of 4c and 5c in DCM.	7
Figure S13. Normalized UV-vis absorption spectra of 4d and 5d in DCM.	8
Figure S14. Fluorescence emission spectra of 4a and 5a in DCM (5×10^{-6} M, $\lambda_{\text{ex}} = \lambda_{\text{Soret}}$).	8
Figure S15. Fluorescence emission spectra of 4b and 5b in DCM (5×10^{-6} M, $\lambda_{\text{ex}} = \lambda_{\text{Soret}}$).	9
Figure S16. Fluorescence emission spectra of 4c and 5c in DCM (5×10^{-6} M, $\lambda_{\text{ex}} = \lambda_{\text{Soret}}$).	9
Figure S17. Fluorescence emission spectra of 4d and 5d in DCM (5×10^{-6} M, $\lambda_{\text{ex}} = \lambda_{\text{Soret}}$).	10
Figure 18. IR spectra of 4a and 5a .	10
Figure 19. IR spectra of 4b and 5b .	11
Figure 20. IR spectra of 4c and 5c .	11
Figure 21. IR spectra of 4d and 5d .	12

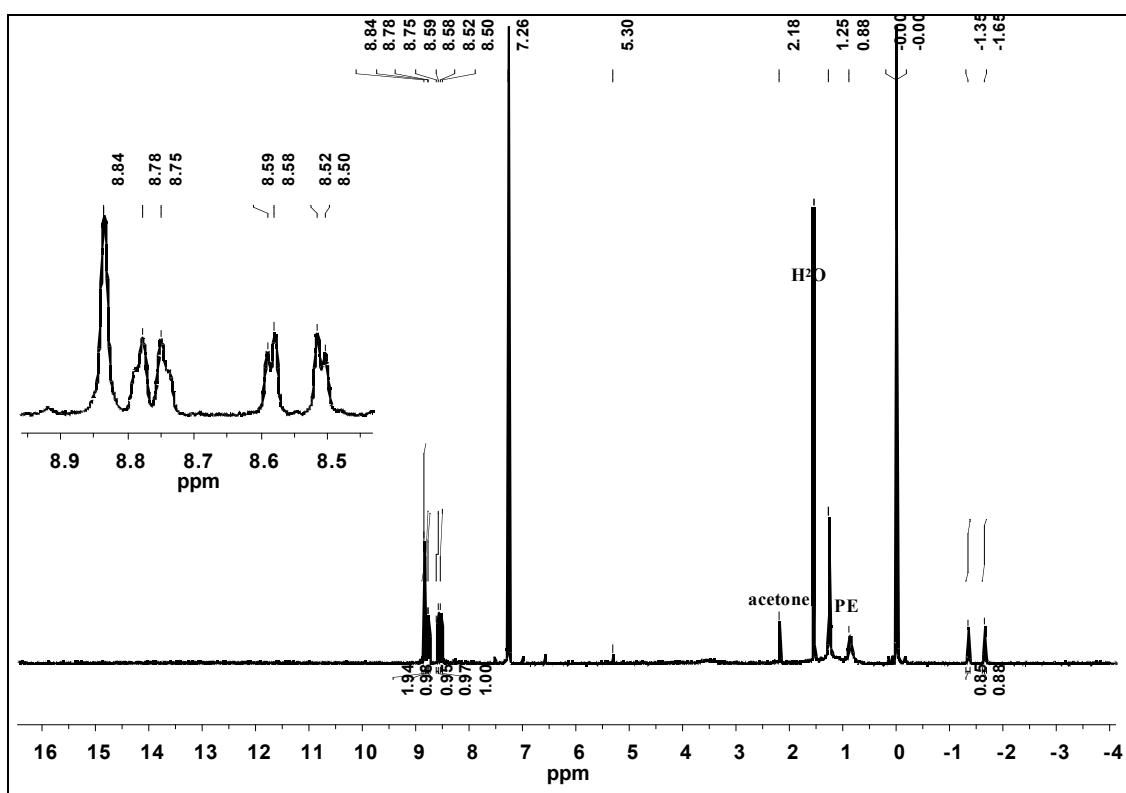


Figure S1. ¹H NMR spectrum of **5a** in CDCl₃.

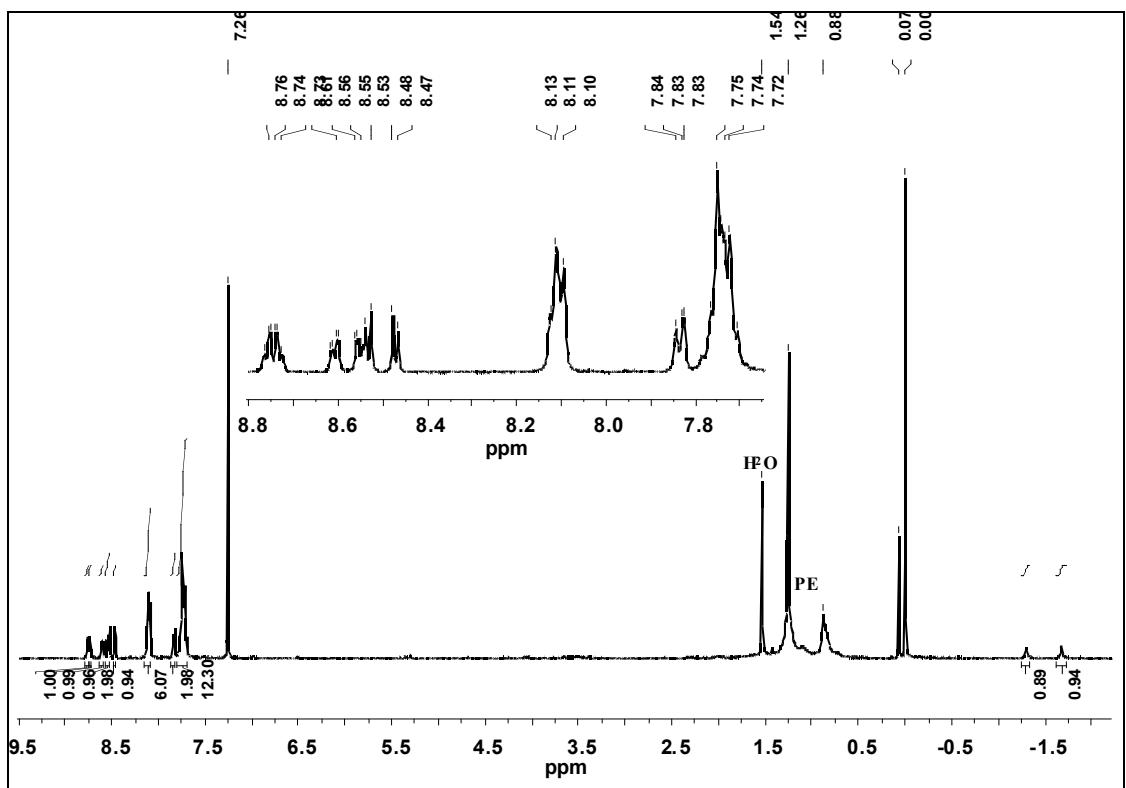


Figure S2. ¹H NMR spectrum of **5b** in CDCl₃.

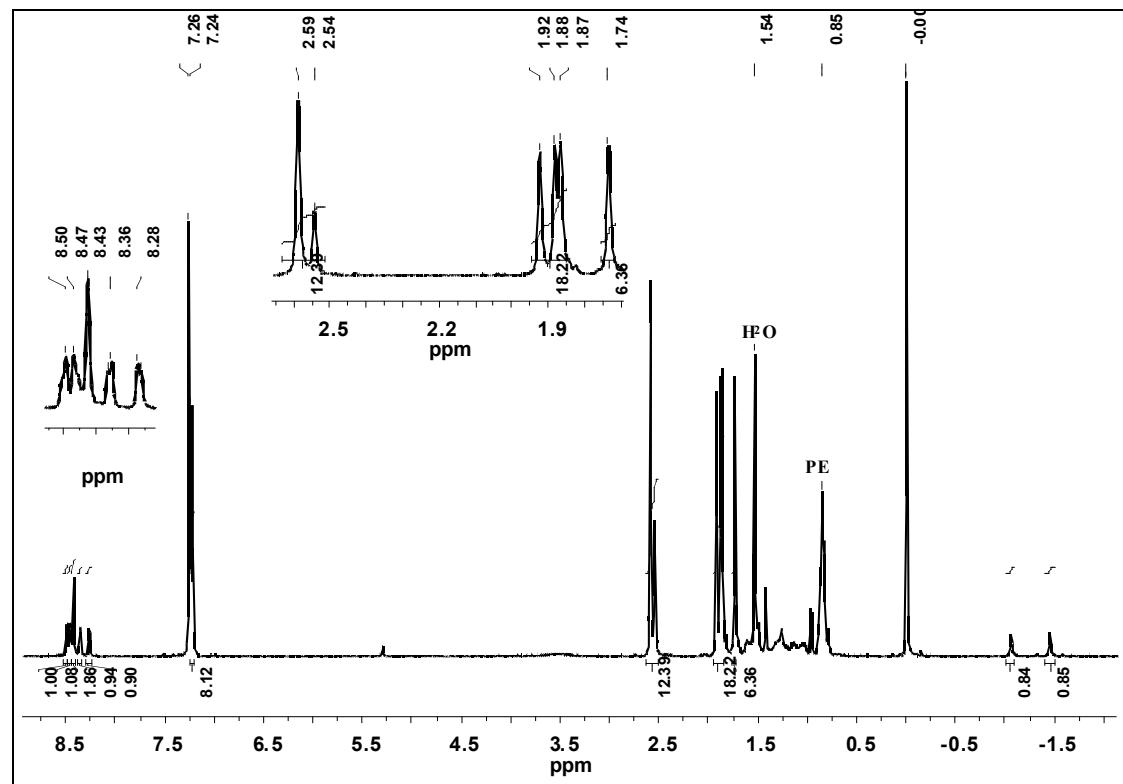


Figure S3. ^1H NMR spectrum of **5c** in CDCl_3 .

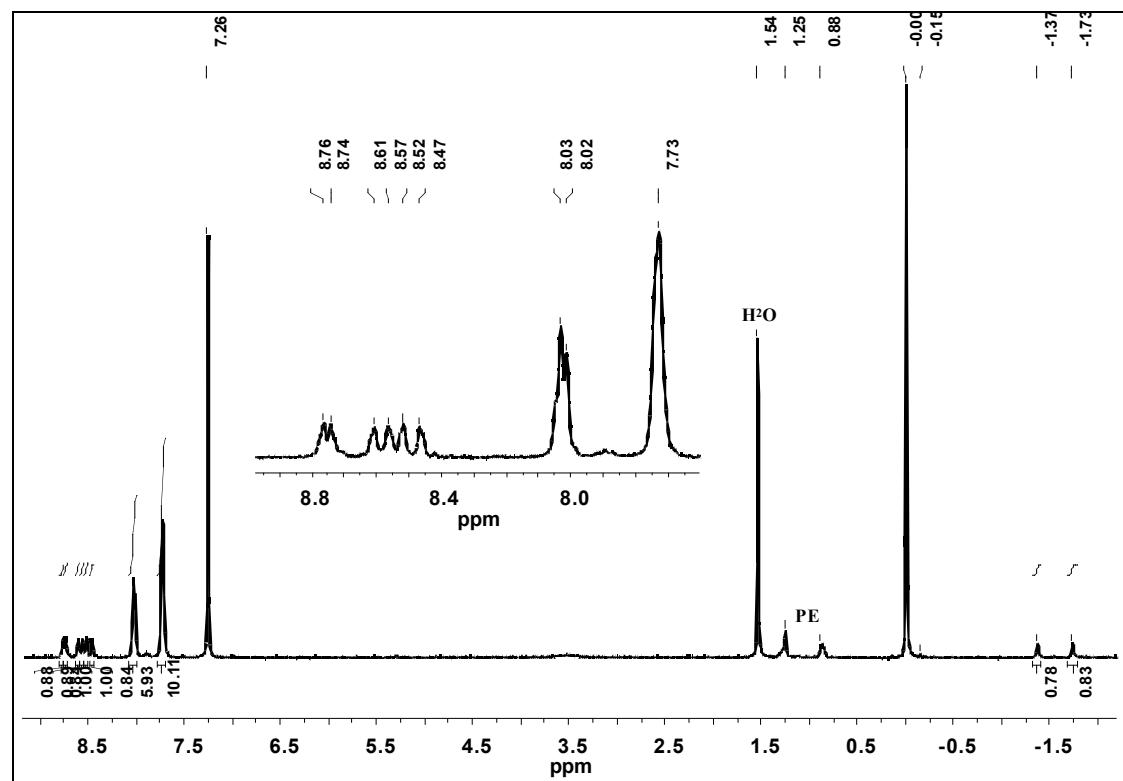


Figure S4. ^1H NMR spectrum of **5d** in CDCl_3 .

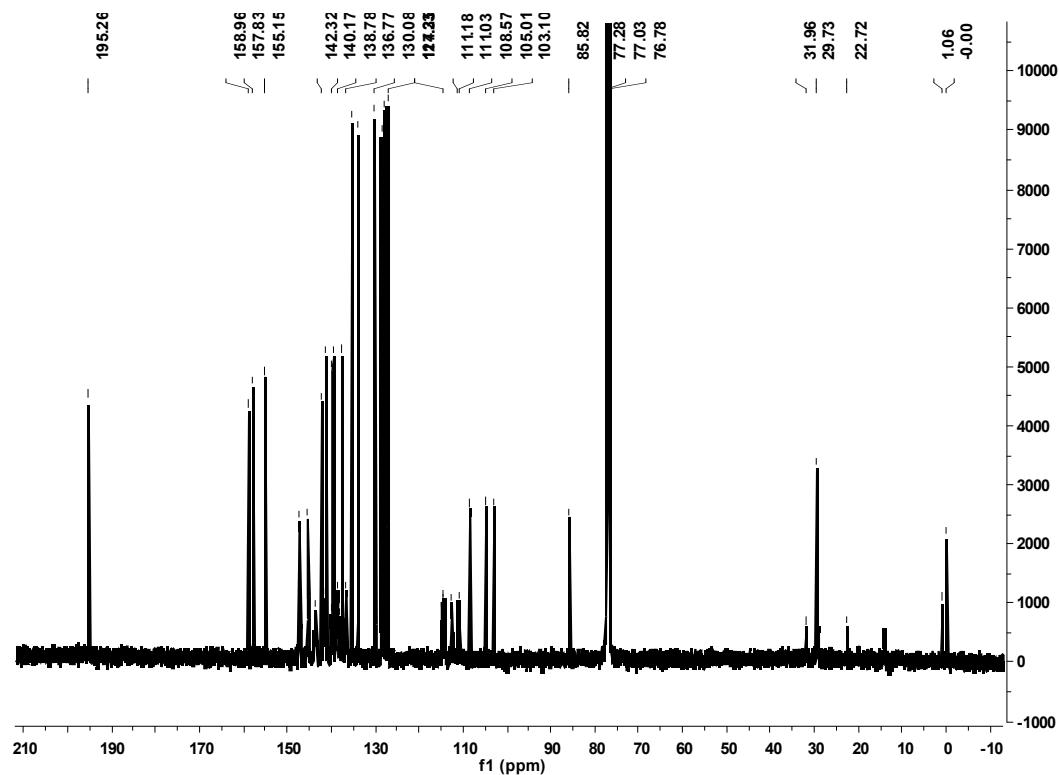


Figure S5. ¹³C NMR spectrum of **5a** in CDCl₃.

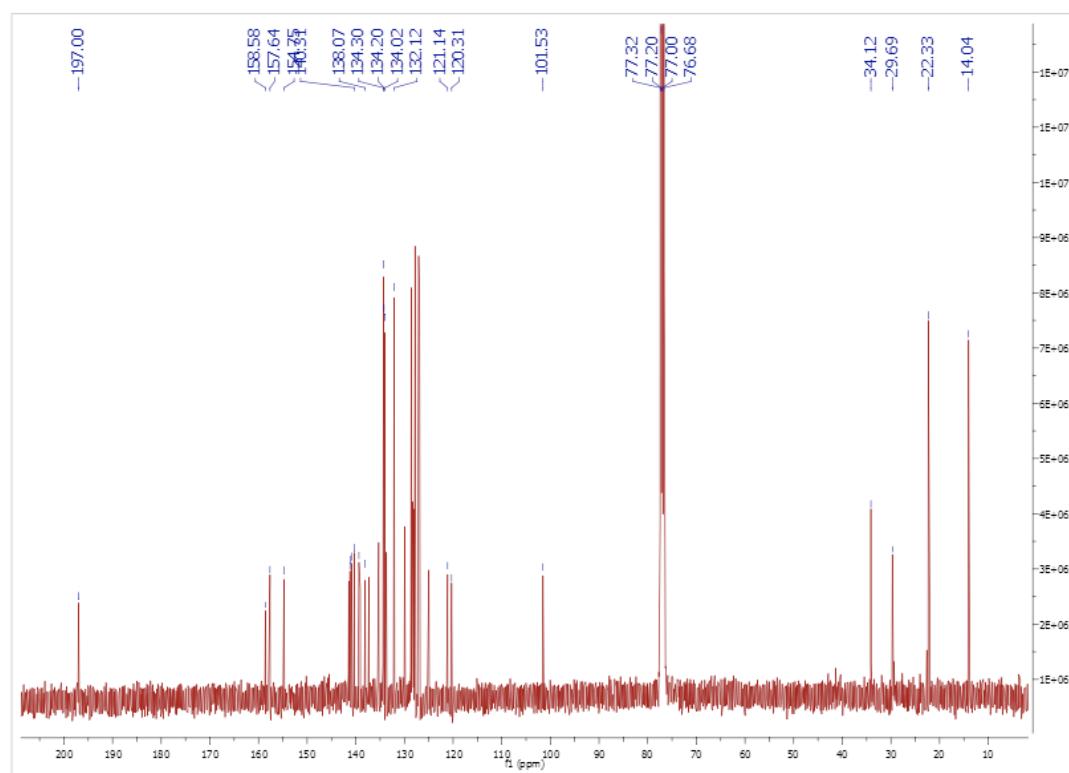


Figure S6. ¹³C NMR spectrum of **5b** in CDCl₃.

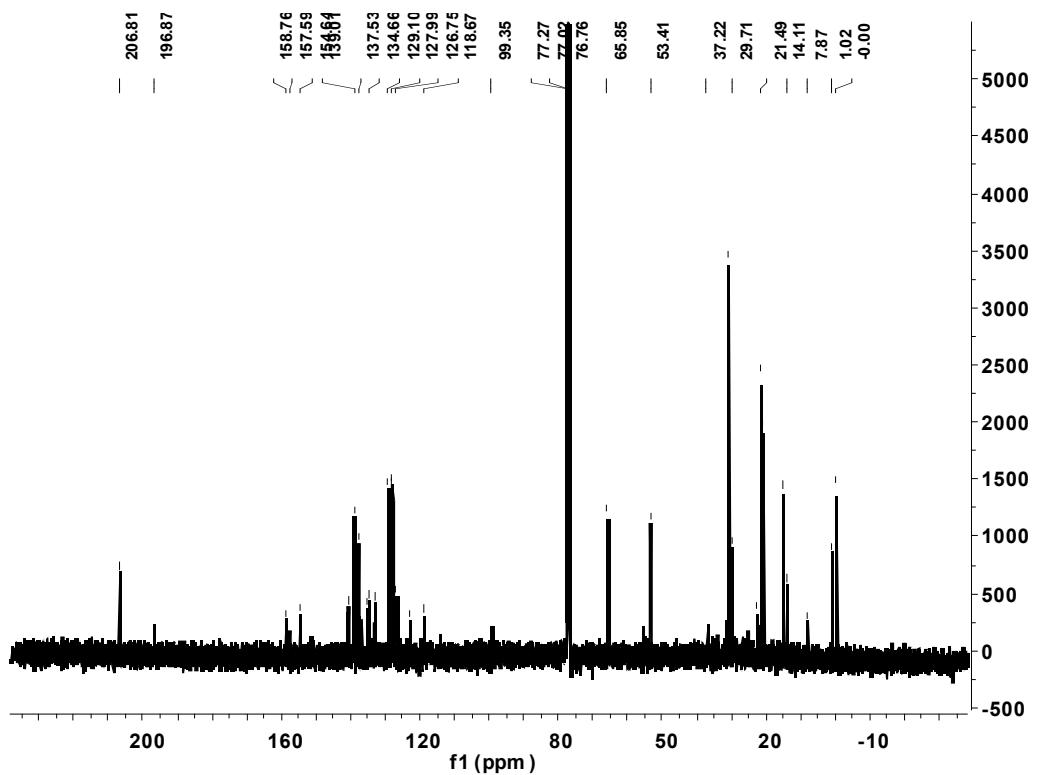


Figure S7. ^{13}C NMR spectrum of **5c** in CDCl_3 .

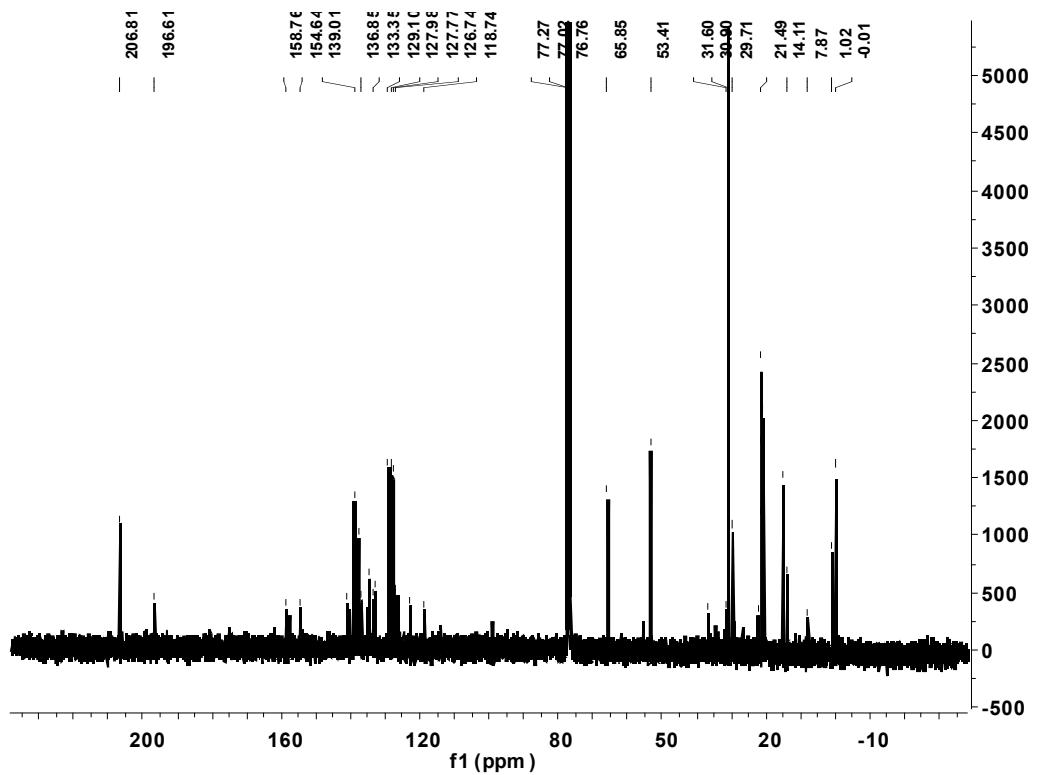


Figure S8. ^{13}C NMR spectrum of **5d** in CDCl_3 .

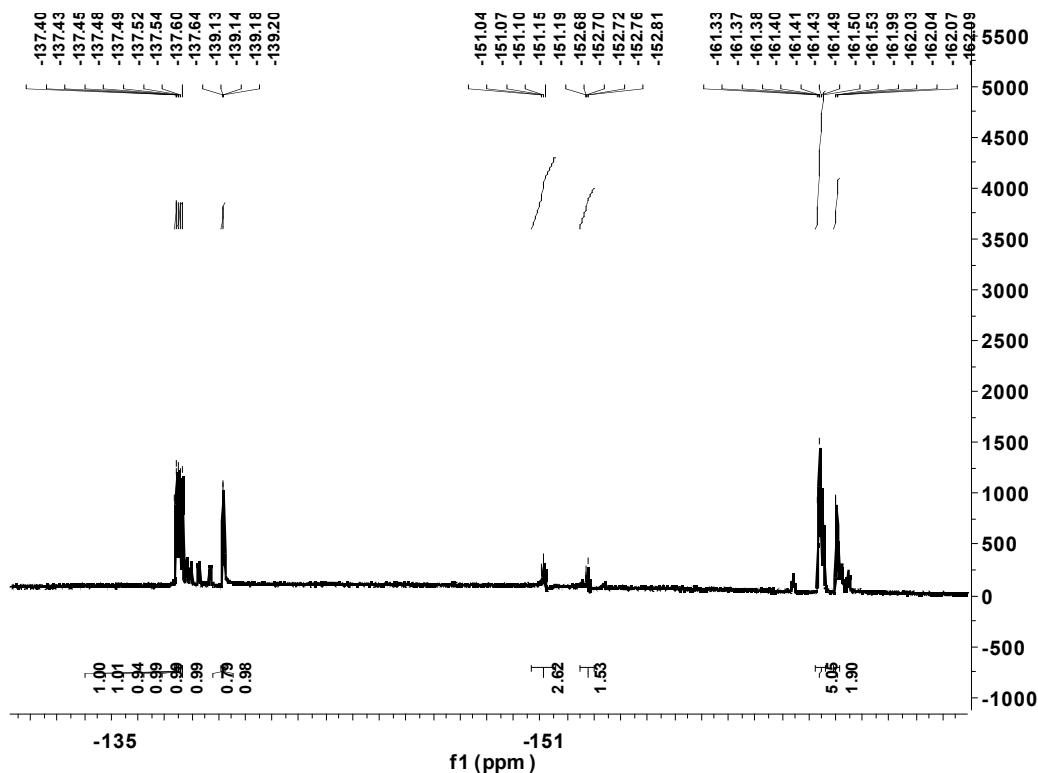


Figure S9. ^{19}F NMR spectrum of **5a** in CDCl_3 .

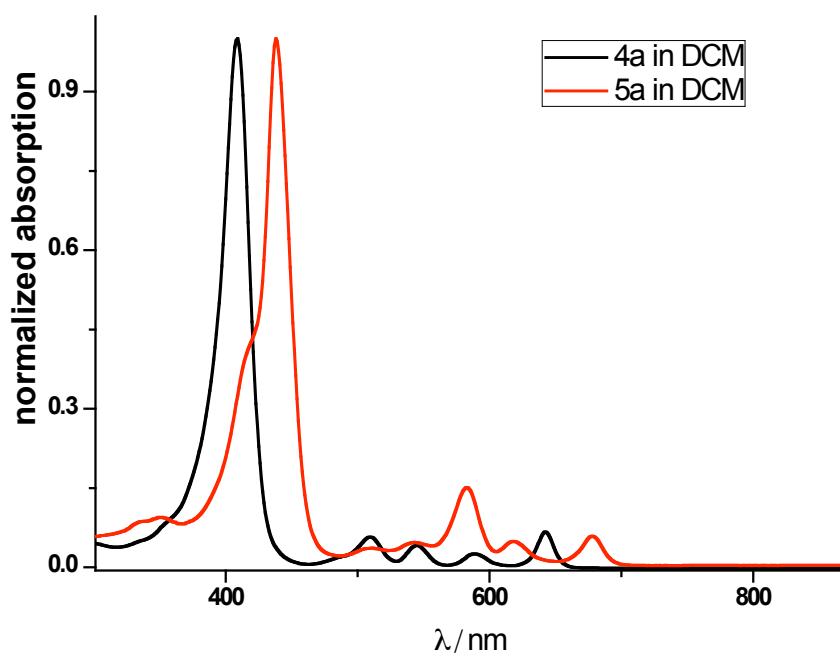


Figure S10. Normalized UV-vis absorption spectra of **4a** and **5a** in DCM.

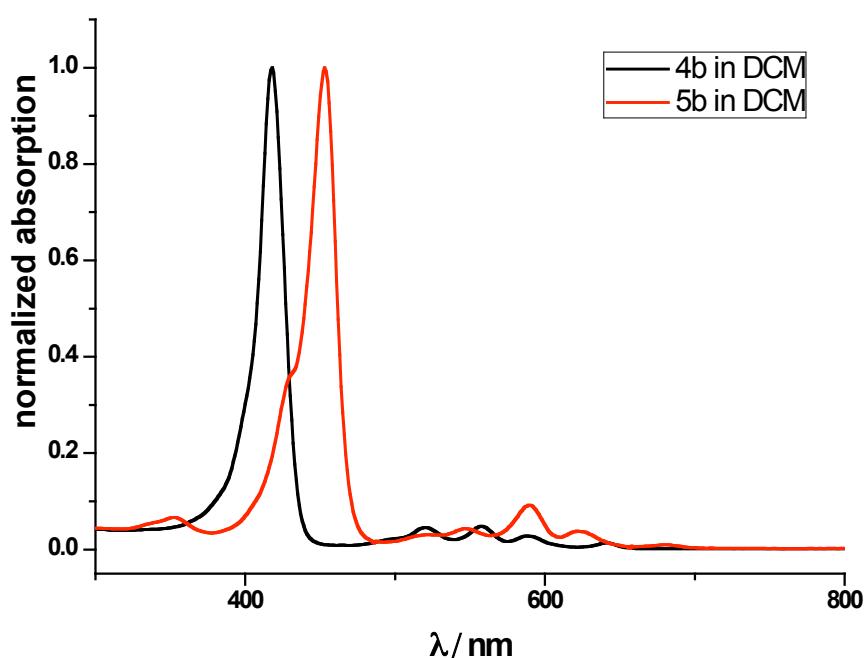


Figure S11. Normalized UV-vis absorption spectra of **4b** and **5b** in DCM.

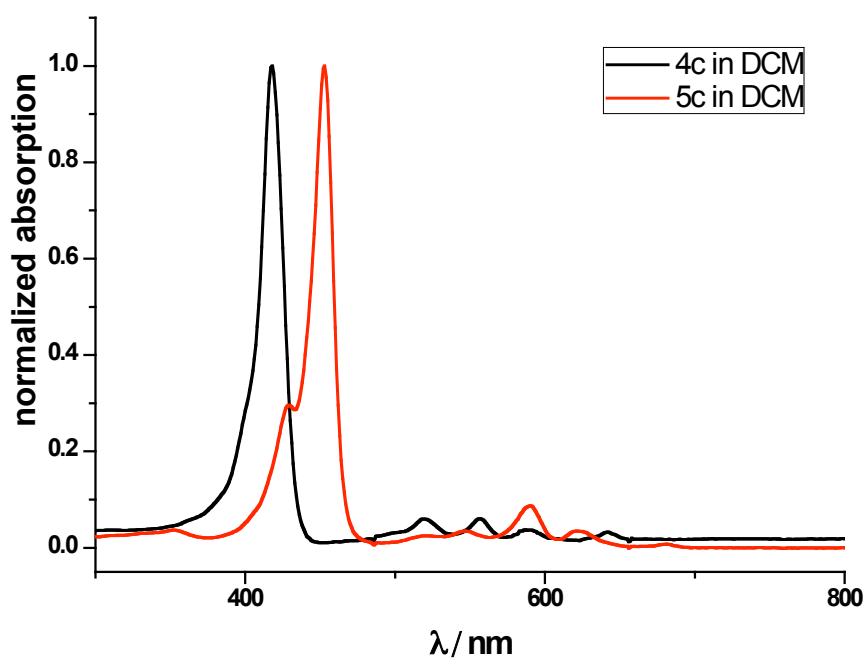


Figure S12. Normalized UV-vis absorption spectra of **4c** and **5c** in DCM.

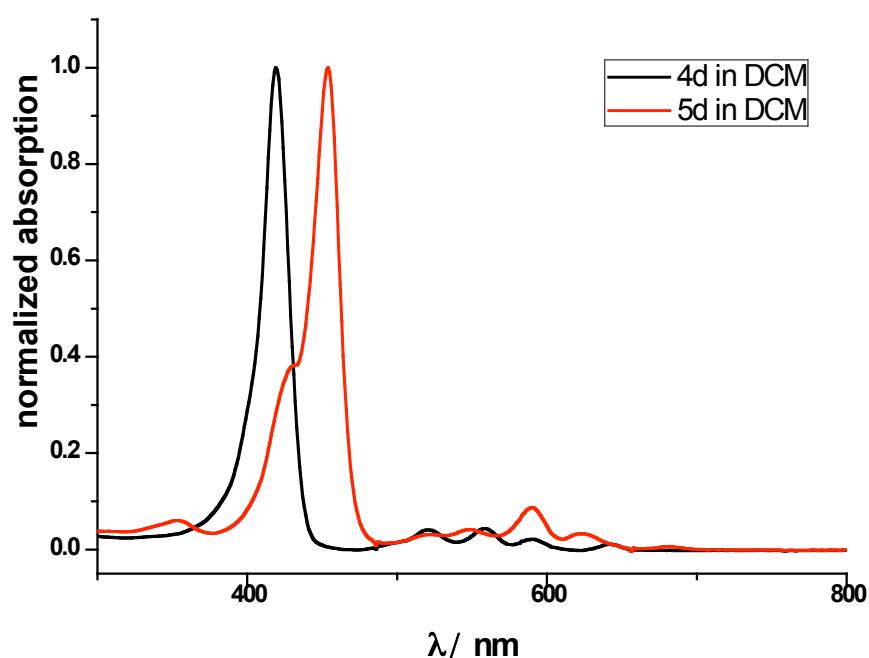


Figure S13. Normalized UV-vis absorption spectra of **4d** and **5d** in DCM.

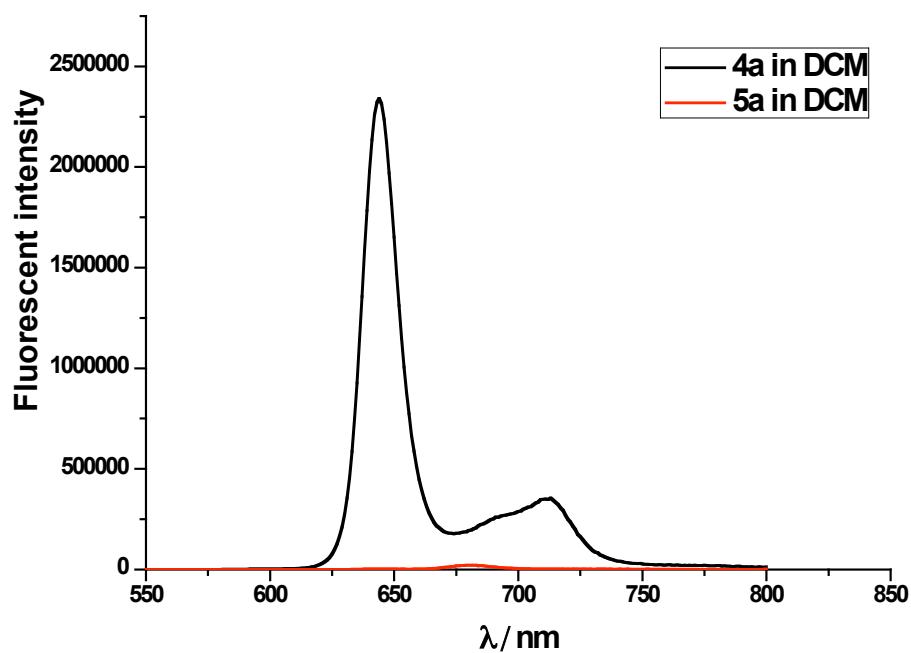


Figure S14. Fluorescence emission spectra of **4a** and **5a** in DCM (5×10^{-6} M, $\lambda_{\text{ex}} = \lambda_{\text{Soret}}$).

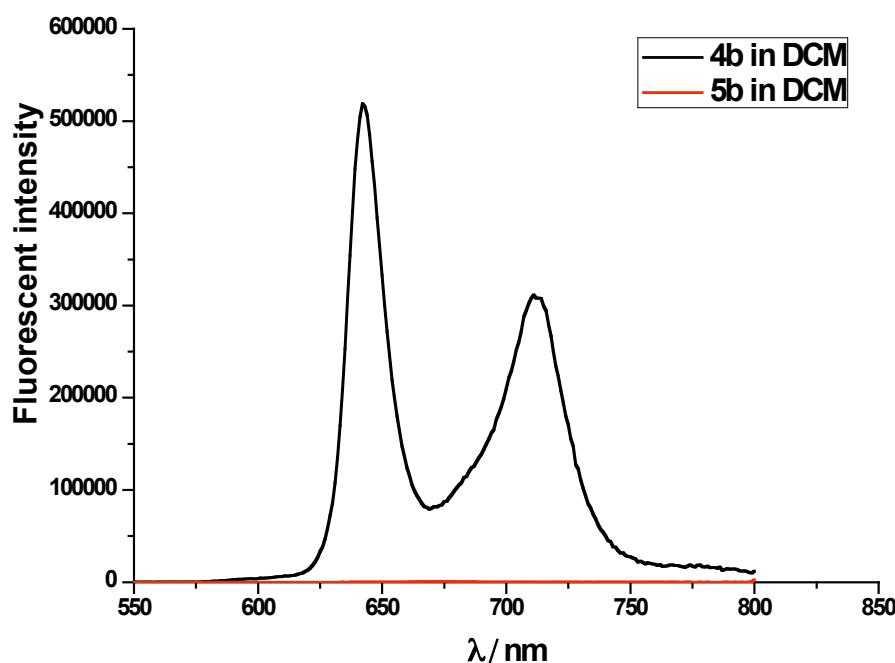


Figure S15. Fluorescence emission spectra of **4b** and **5b** in DCM (5×10^{-6} M, $\lambda_{\text{ex}} = \lambda_{\text{Soret}}$).

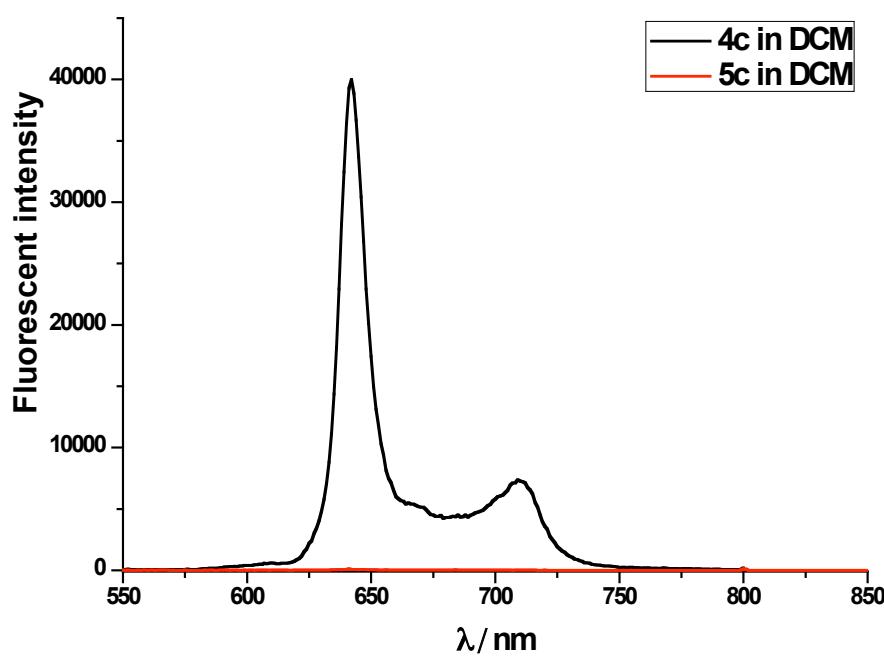


Figure S16. Fluorescence emission spectra of **4c** and **5c** in DCM (5×10^{-6} M, $\lambda_{\text{ex}} = \lambda_{\text{Soret}}$).

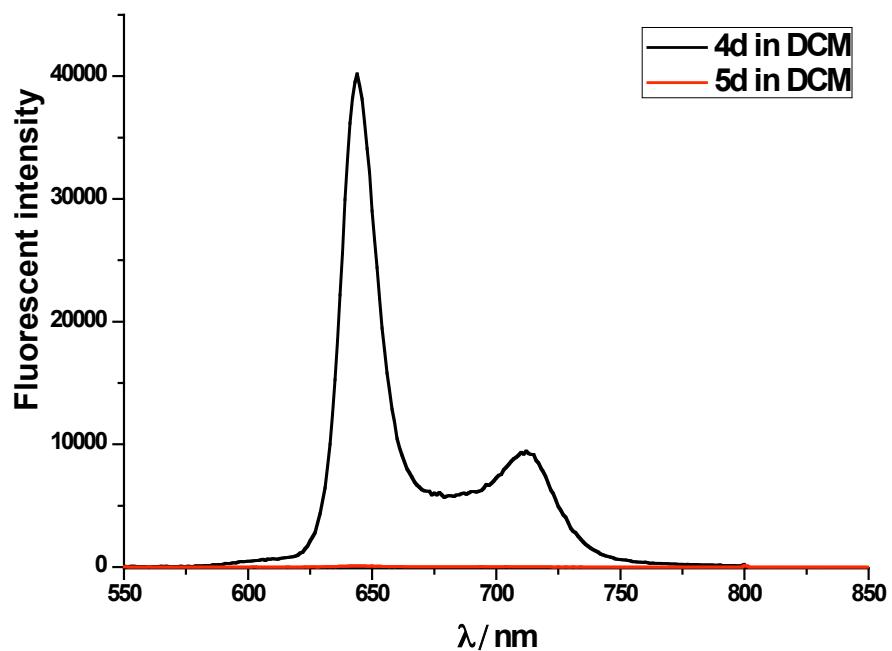


Figure S17. Fluorescence emission spectra of **4d** and **5d** in DCM (5×10^{-6} M, $\lambda_{\text{ex}} = \lambda_{\text{Soret}}$).

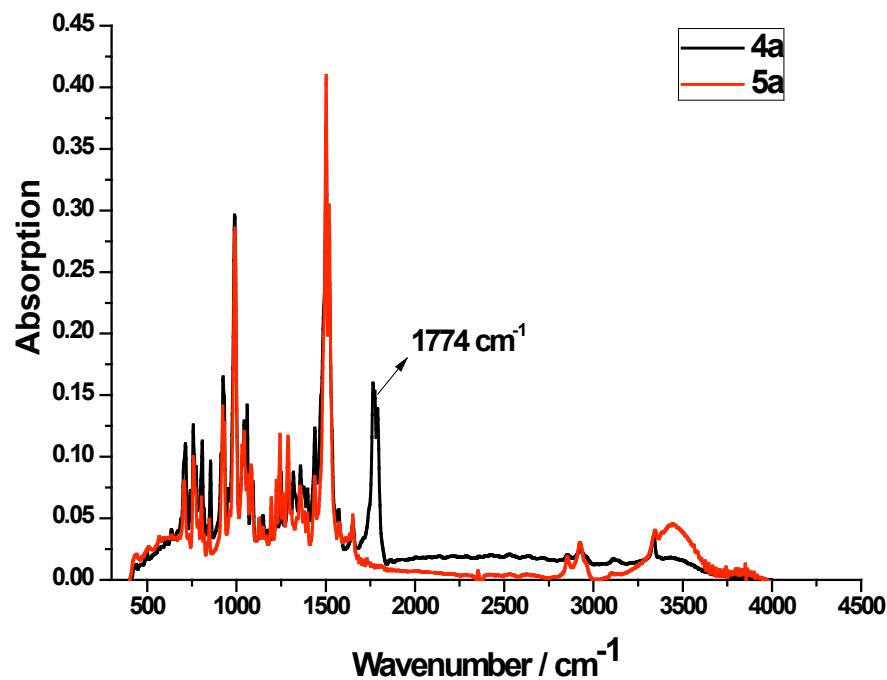


Figure S18. IR spectra of **4a** and **5a**.

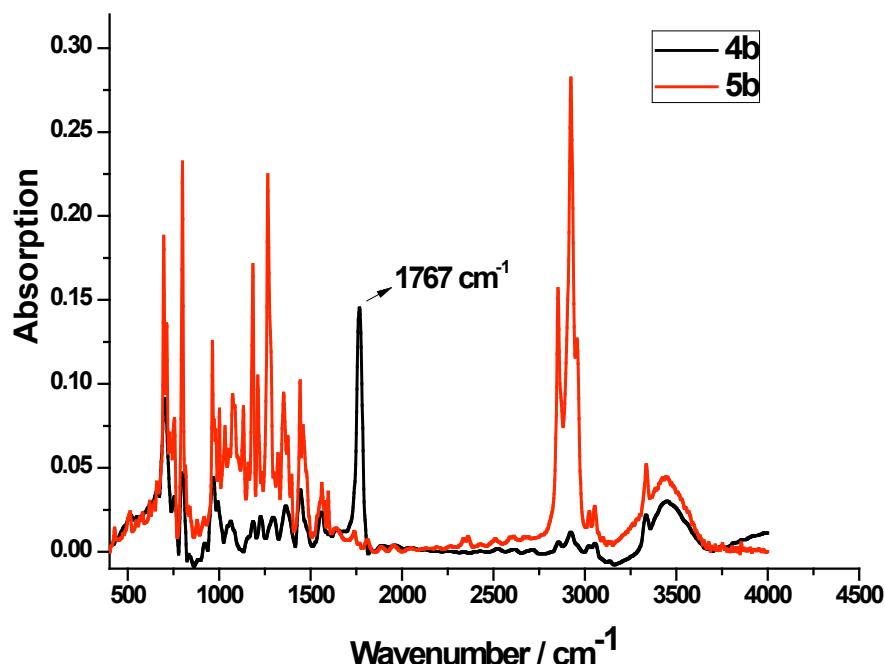


Figure S19. IR spectra of **4b** and **5b**.

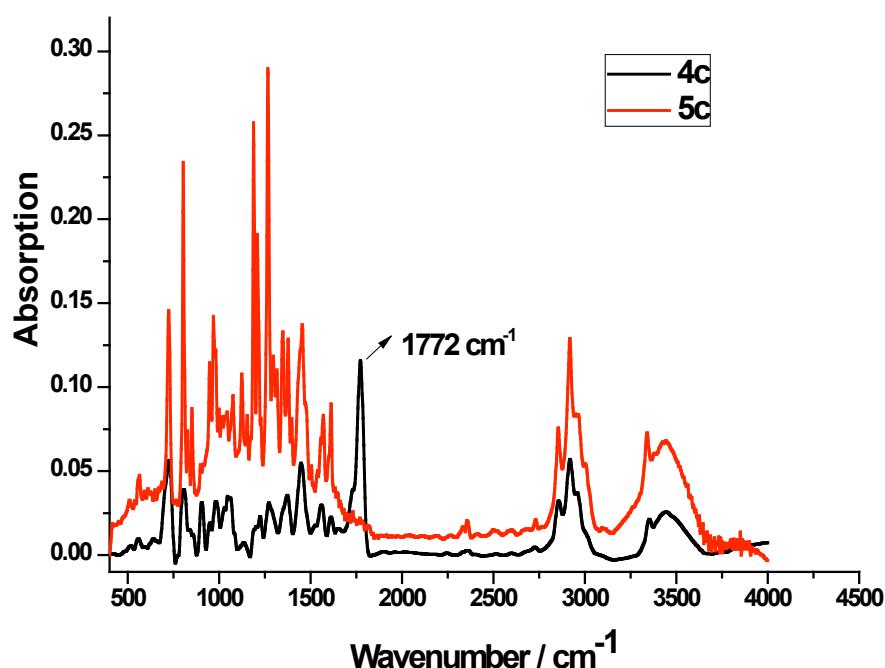


Figure S20. IR spectra of **4c** and **5c**.

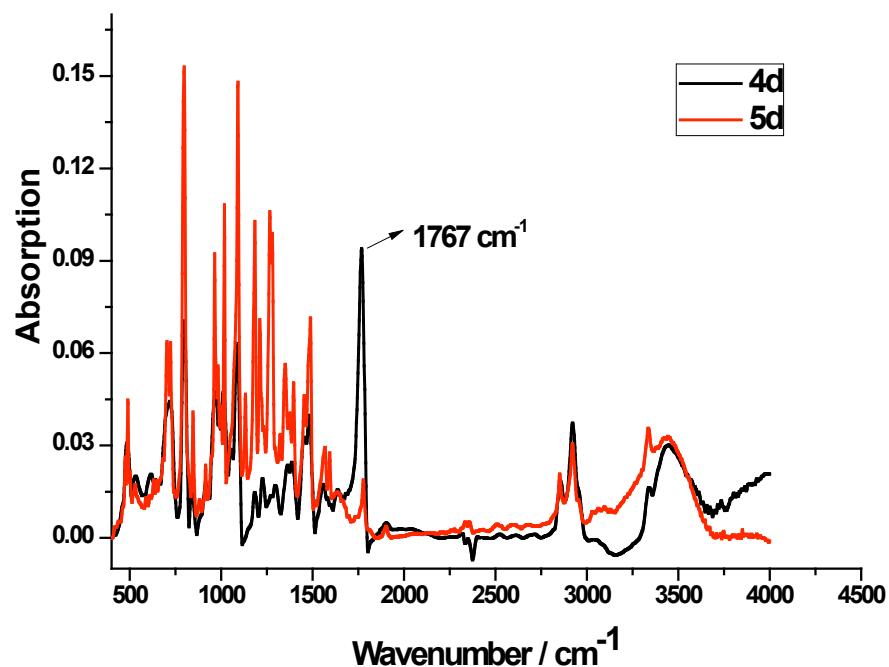


Figure S21. IR spectra of **4d** and **5d**.