Electronic Supplementary Material (ESI) for Dalton Transactions.
This journal is © The Royal Society of Chemistry 2020

Supporting Information

pH-sensitive subphthalocyanines and subazaphthalocyanines

Ivan A. Skvortsov,[a, b] Petr Zimcik,[b] Pavel A. Stuzhin,[a]* Veronika Novakova[b]*

[a] Research Institute of Macroheterocycles, Ivanovo State University of Chemistry and Technology, Sheremetevsky Avenue 7, Ivanovo RF-153000, Russia

[b] Faculty of Pharmacy in Hradec Kralove, Charles University, Ak. Heyrovskeho 1203, Hradec Kralove 50005, Czech Republic

Content

Switching studies in acetone

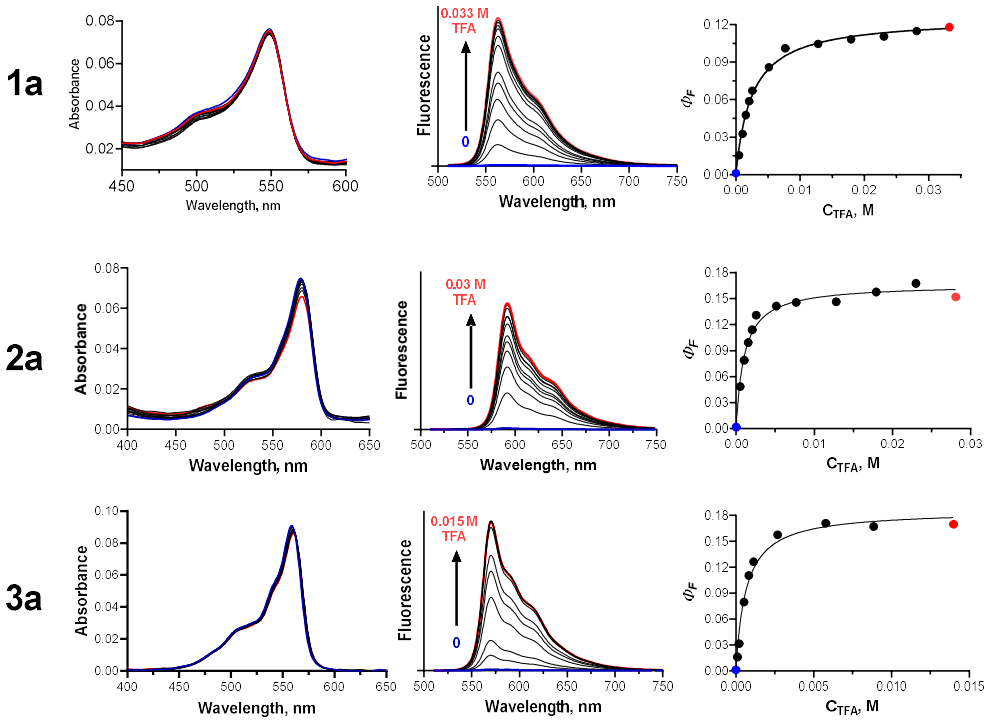


Fig. S1: Changes in absorption spectra and fluorescence emission spectra upon addition of TFA, and dependence of Φ_F of **1a**-**3a** (c = 1 μM) in acetone on the concentration of TFA. The solid lines in graphs on the right side represent the least-square fits to the experimental points.

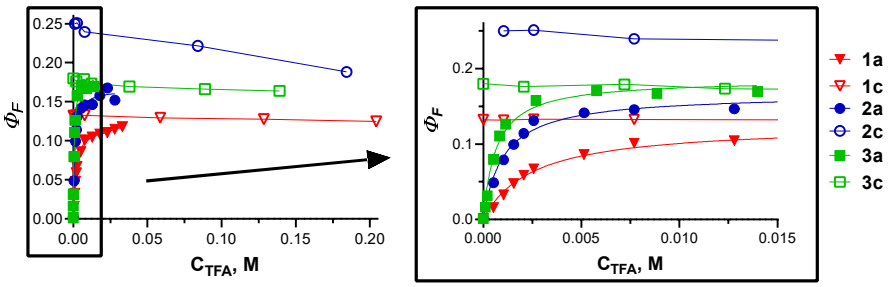


Fig. S2: Dependence of Φ_F of **1a**-**3a** and **1c**-**3c** (c = 1 μM) in acetone on the concentration of TFA. The solid lines for **1a**-**3a** represent the least-square fits to the experimental points, for **1c**-**3c** represent connecting lines.

Decomposition studies

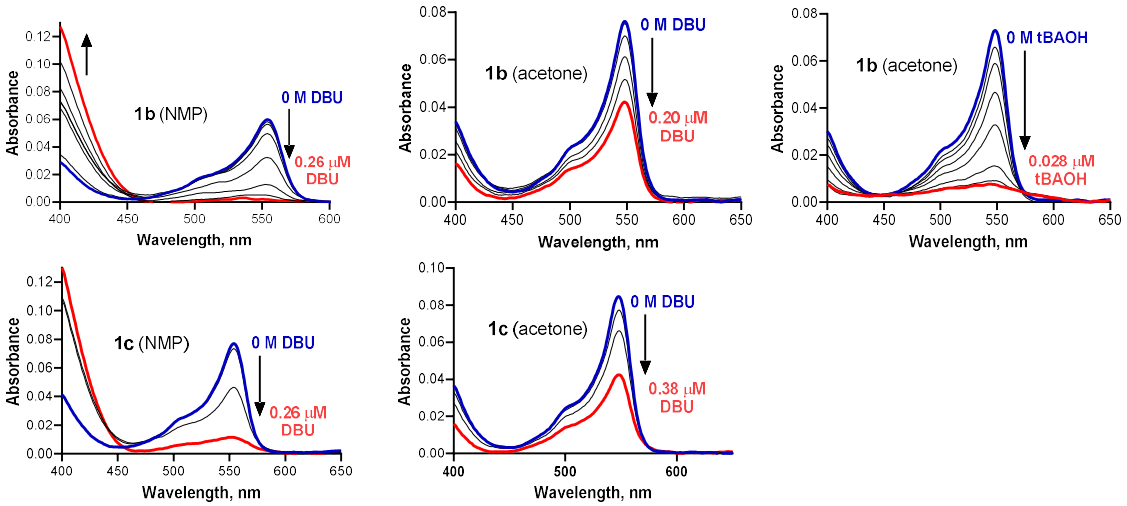


Fig. S3: Changes in absorption spectra of SubPyzPzs **1a** and **1c** (in acetone or N-methyl-2-pyrrolidone (NMP), c = 1 μM) upon addition of a base (1,8-diazabicyclo(5.4.0)undec-7-ene (DBU) or tetrabutylammonium hydroxide (tbaOH).

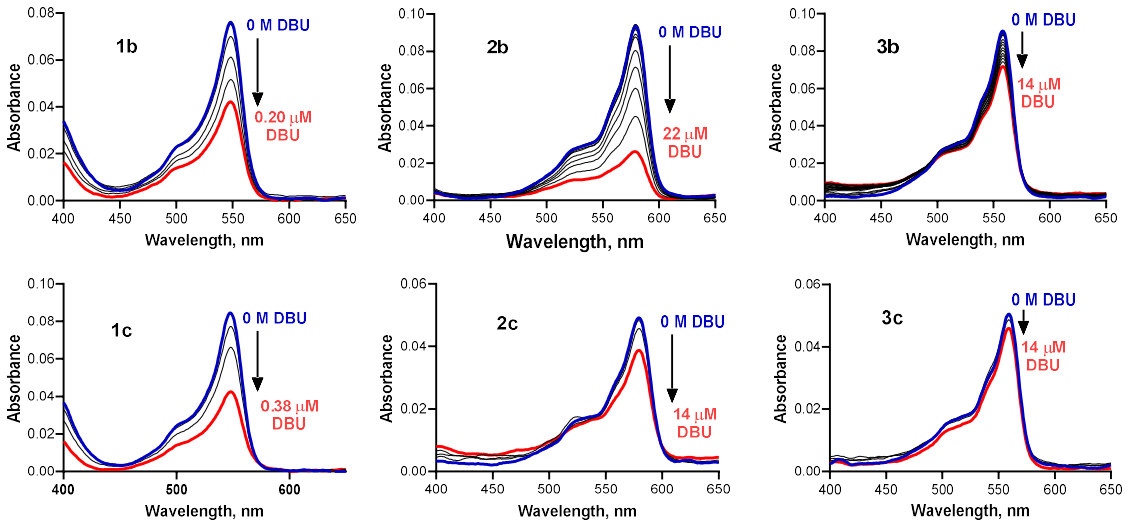


Fig. S4: Changes in absorption spectra of SubPcs and SubPyzPzs (in acetone, c = 1 μM) upon addition of 1,8-diazabicyclo(5.4.0)undec-7-ene (DBU).

NMR spectra

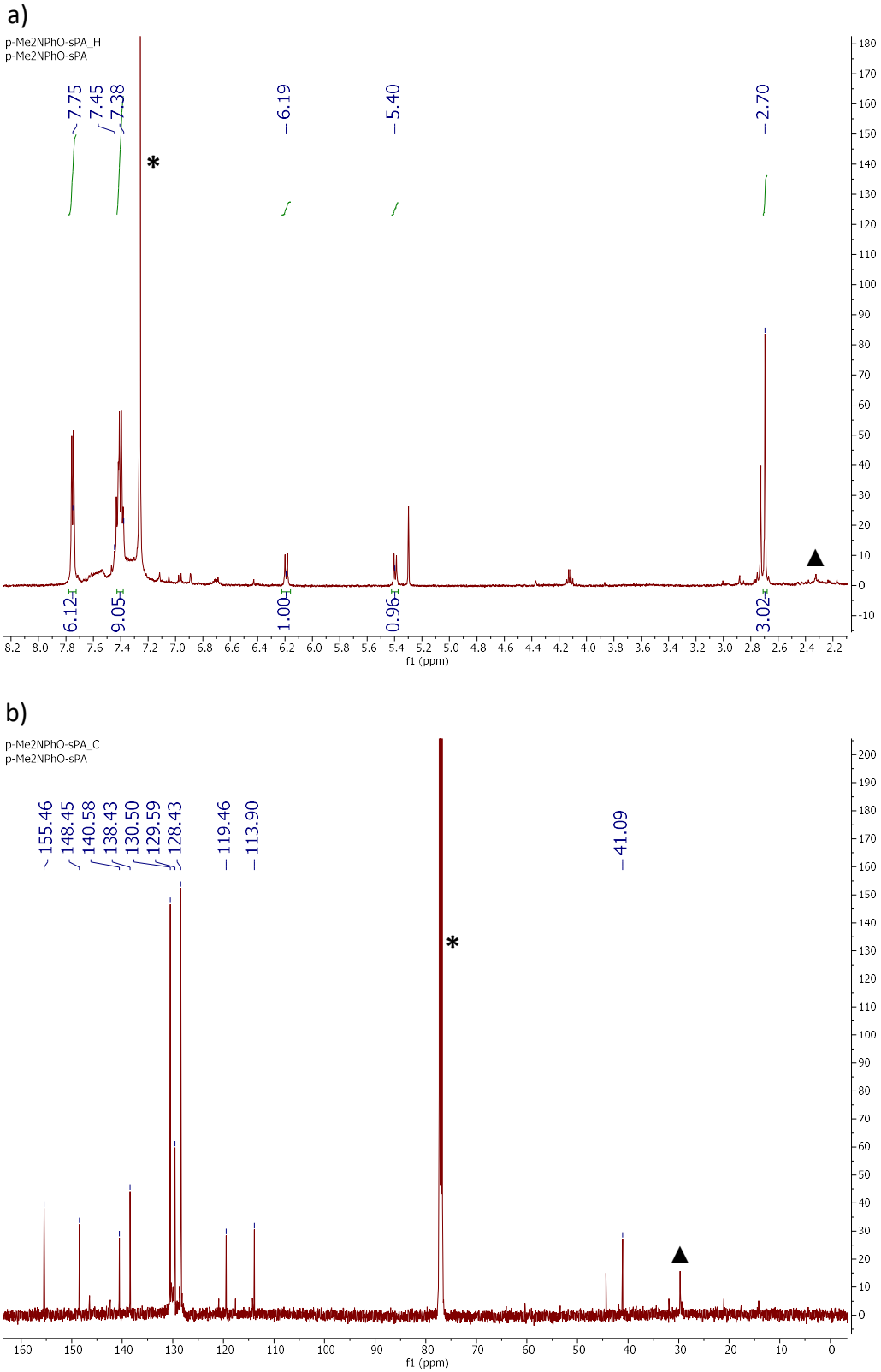
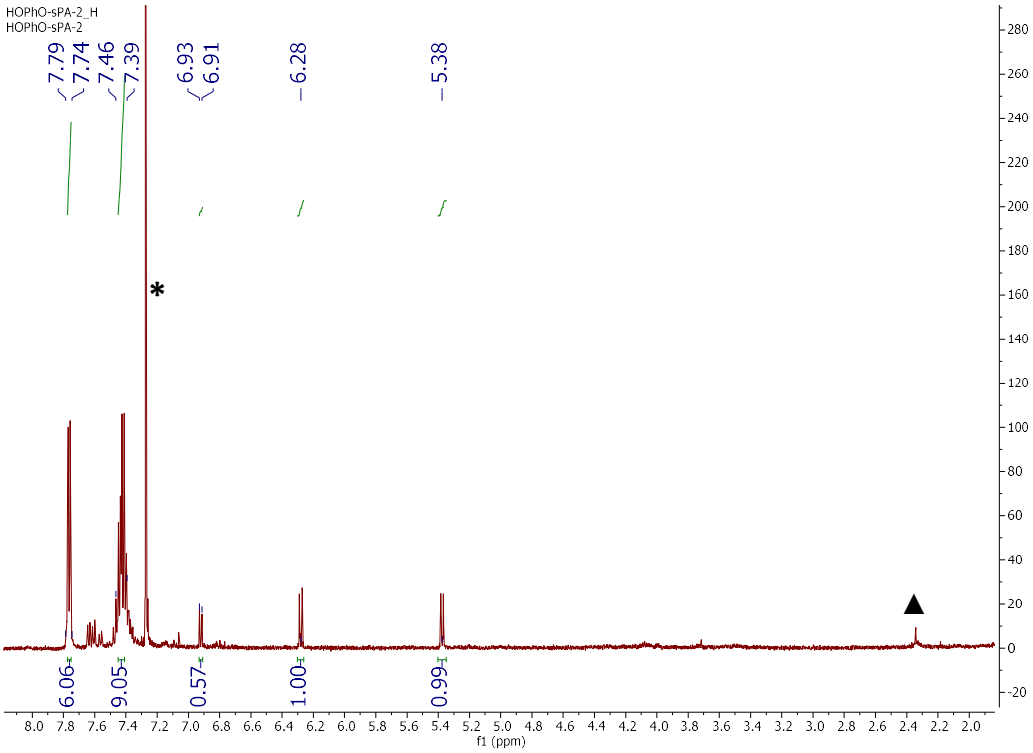


Fig. S5: ^{1}H NMR (500 MHz) (a) and ^{13}C NMR (126 MHz) (b) spectra of compound **1a** in $CDCl_3$. Asterisk (*) and triangle (▲) indicate residuals of non-deuterated solvent and acetone, respectively.

a)



b)

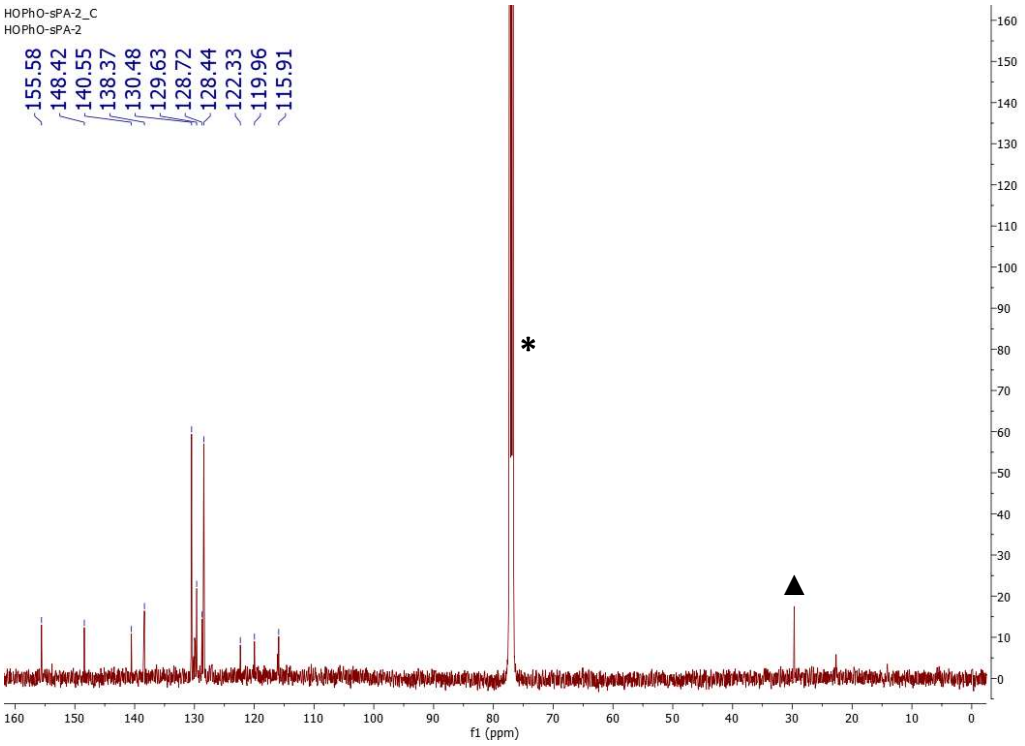


Fig. S6: ^{1}H NMR (500 MHz) (a) and ^{13}C NMR (126 MHz) (b) spectra of compound **1b** in $CDCl_3$. Asterisk (*) and triangle (▲) indicate residuals of non-deuterated solvent and acetone, respectively.

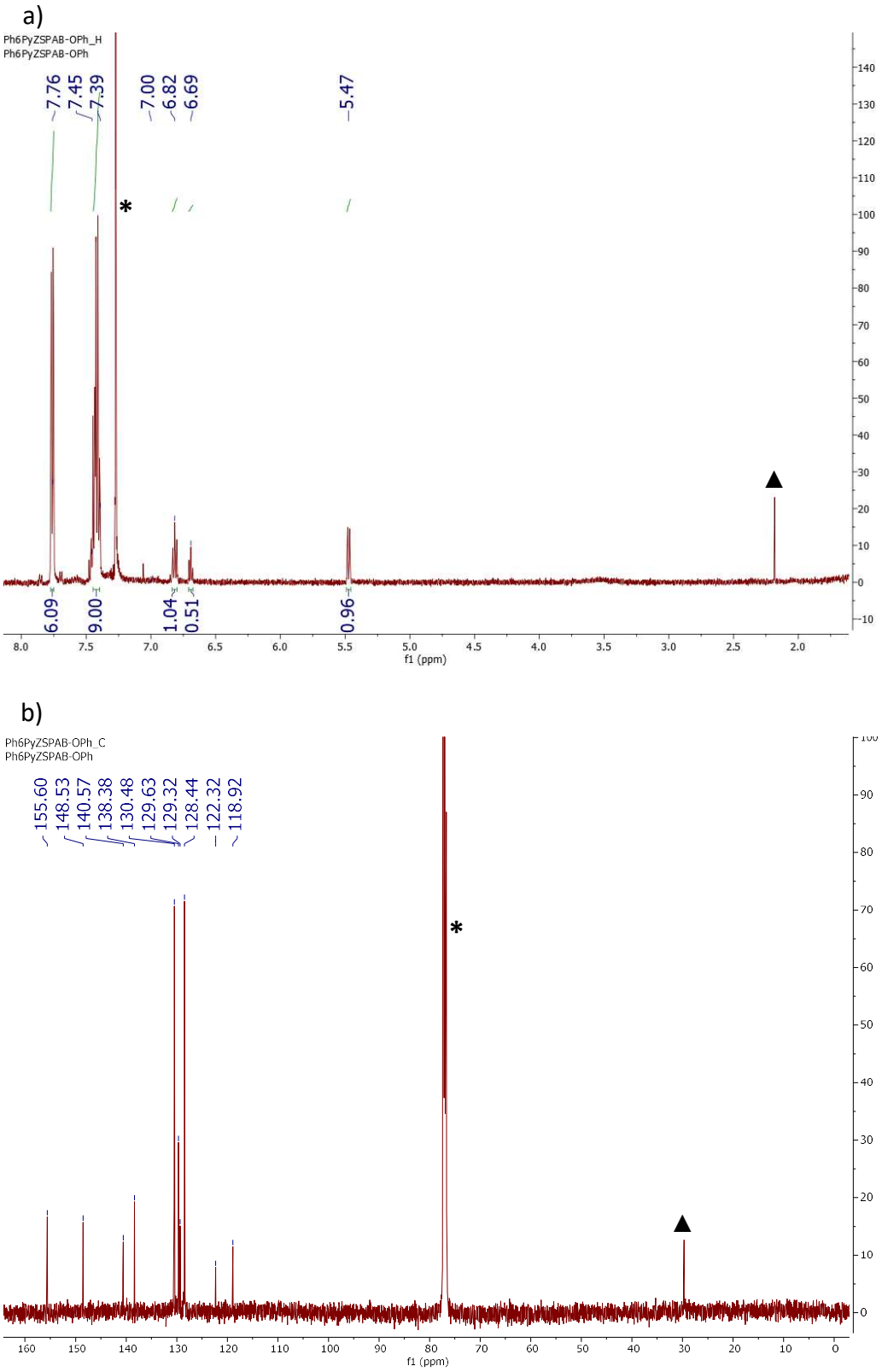


Fig. S7: ^{1}H NMR (500 MHz) (a) and ^{13}C NMR (126 MHz) (b) spectra of compound **1c** in $CDCl_3$. Asterisk (*) and triangle (▲) indicate residuals of non-deuterated solvent and acetone, respectively.

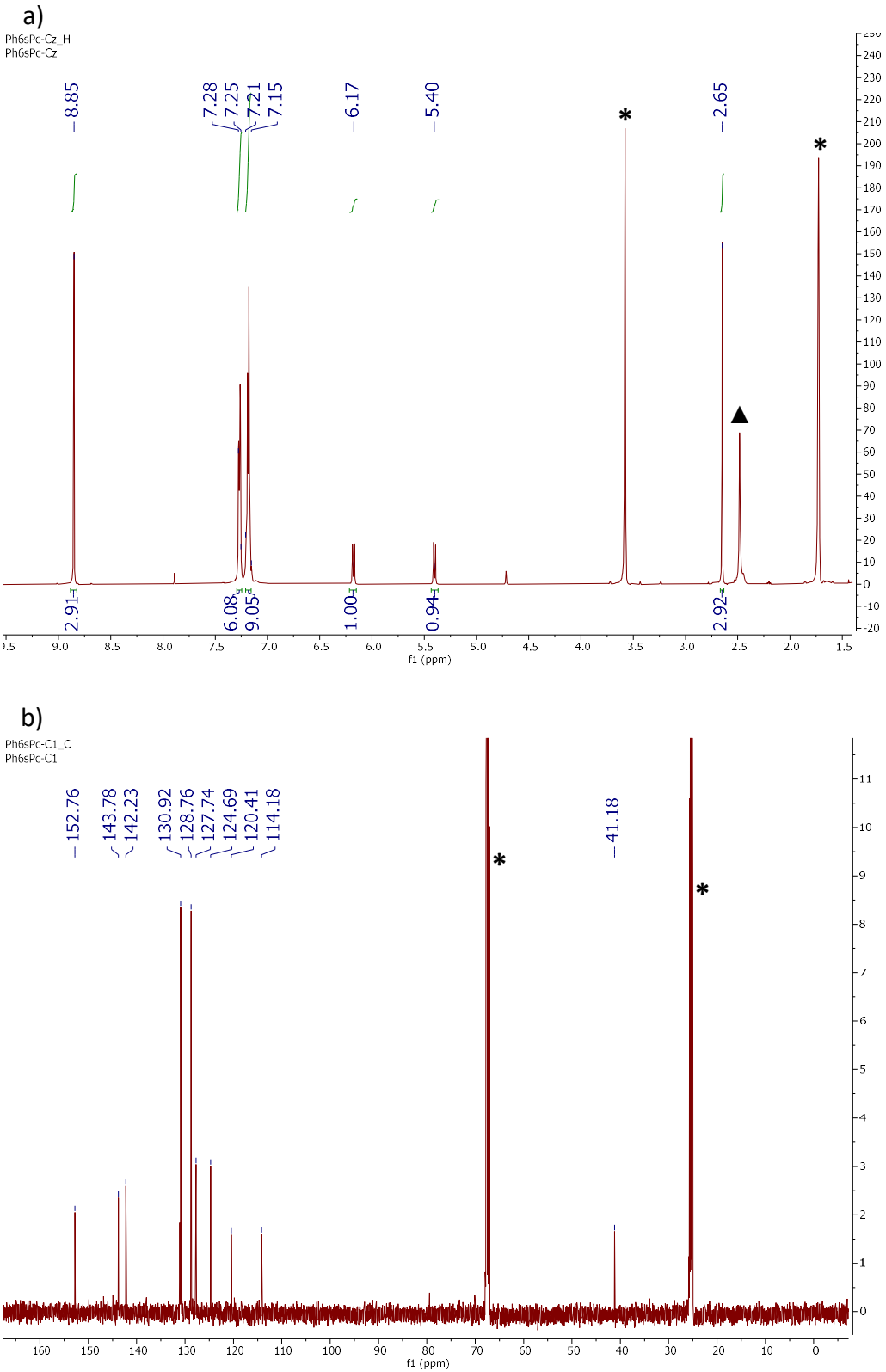


Fig. S8: ^{1}H NMR (500 MHz) (a) and ^{13}C NMR (126 MHz) (b) spectra of compound **2a** in THF-d_8. Asterisk (*) and triangle (▲) indicate residuals of non-deuterated solvent and water, respectively.

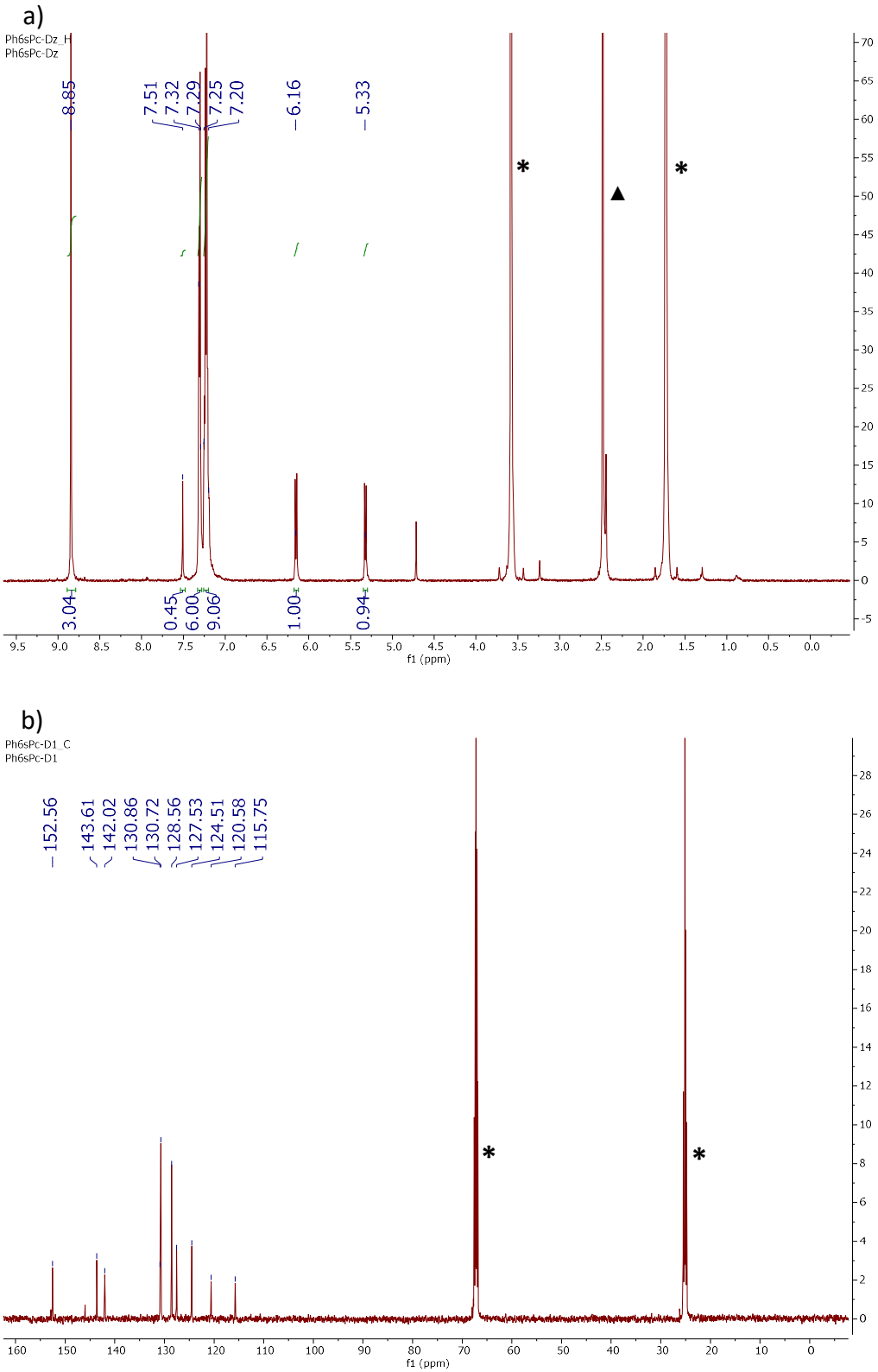


Fig. S9: ^{1}H NMR (500 MHz) (a) and ^{13}C NMR (126 MHz) (b) spectra of compound **2b** in THF-d_8. Asterisk (*) and triangle (▲) indicate residuals of non-deuterated solvent and water, respectively.

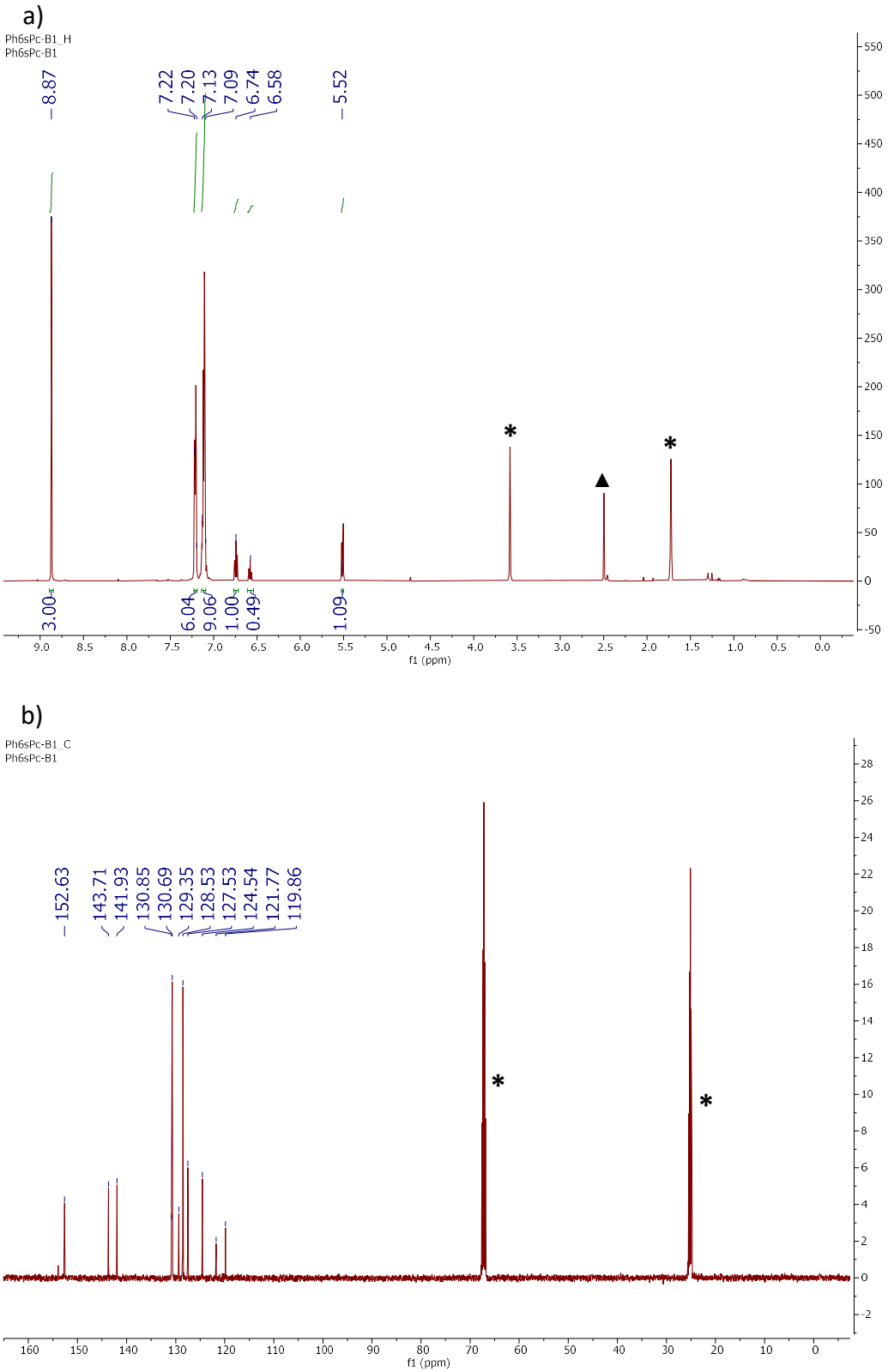


Fig. S10: ^{1}H NMR (500 MHz) (a) and ^{13}C NMR (126 MHz) (b) spectra of compound **2c** in THF-d_8. Asterisk (*) and triangle (▲) indicate residuals of non-deuterated solvent and water, respectively.