

Supplementary Information
for
Effect of cyano, ethynyl and ethylenedioxy groups on the photophysical properteies
of carbazole-based porphyrins

Chihiro Maeda,^{*a,b} Kosuke Kurihara,^a Motoki Masuda^a and Naoki Yoshioka^{*a}

*^aDepartment of Applied Chemistry, Faculty of Science and Technology, Keio University,
Kohoku-ku, Yokohama 223-8522, Japan;*

*^bDivision of Applied Chemistry, Graduate School of Natural Science and Technology, Okayama University,
Tsushima, Okayama 700-8530, Japan. E-mail: cmaeda@okayama-u.ac.jp*

Table of Contents

NMR Spectra.....	S2
Cyclic Voltammogram and Differential Pulse Voltammogram.....	S11
Calculated Electronic Transition.....	S12

Fig. S1 ^1H and ^{13}C NMR spectra of **10** in CDCl_3

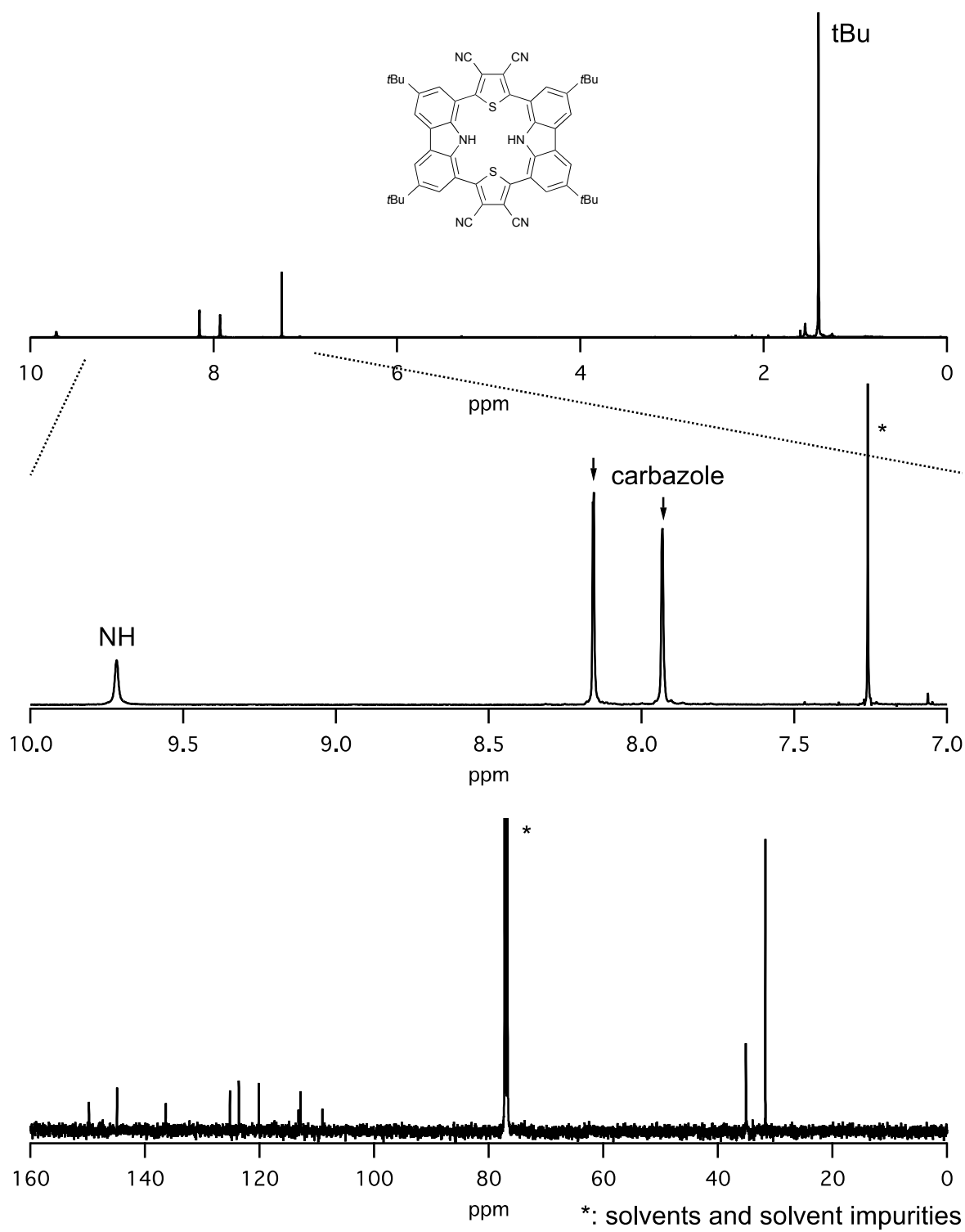


Fig. S2 ^1H and ^{13}C NMR spectra of **11** in CDCl_3

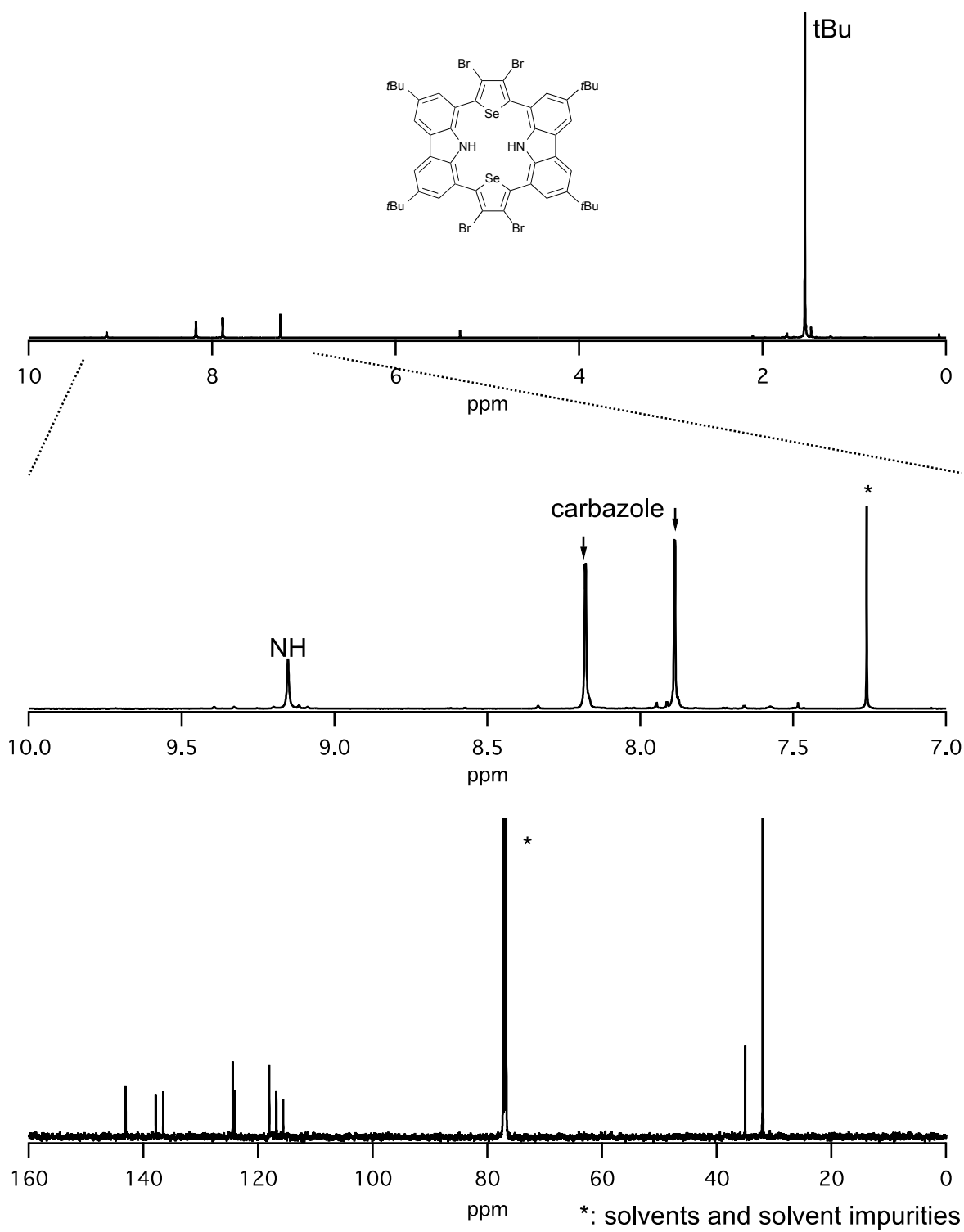


Fig. S3 ^1H and ^{13}C NMR spectra of **12** in CDCl_3

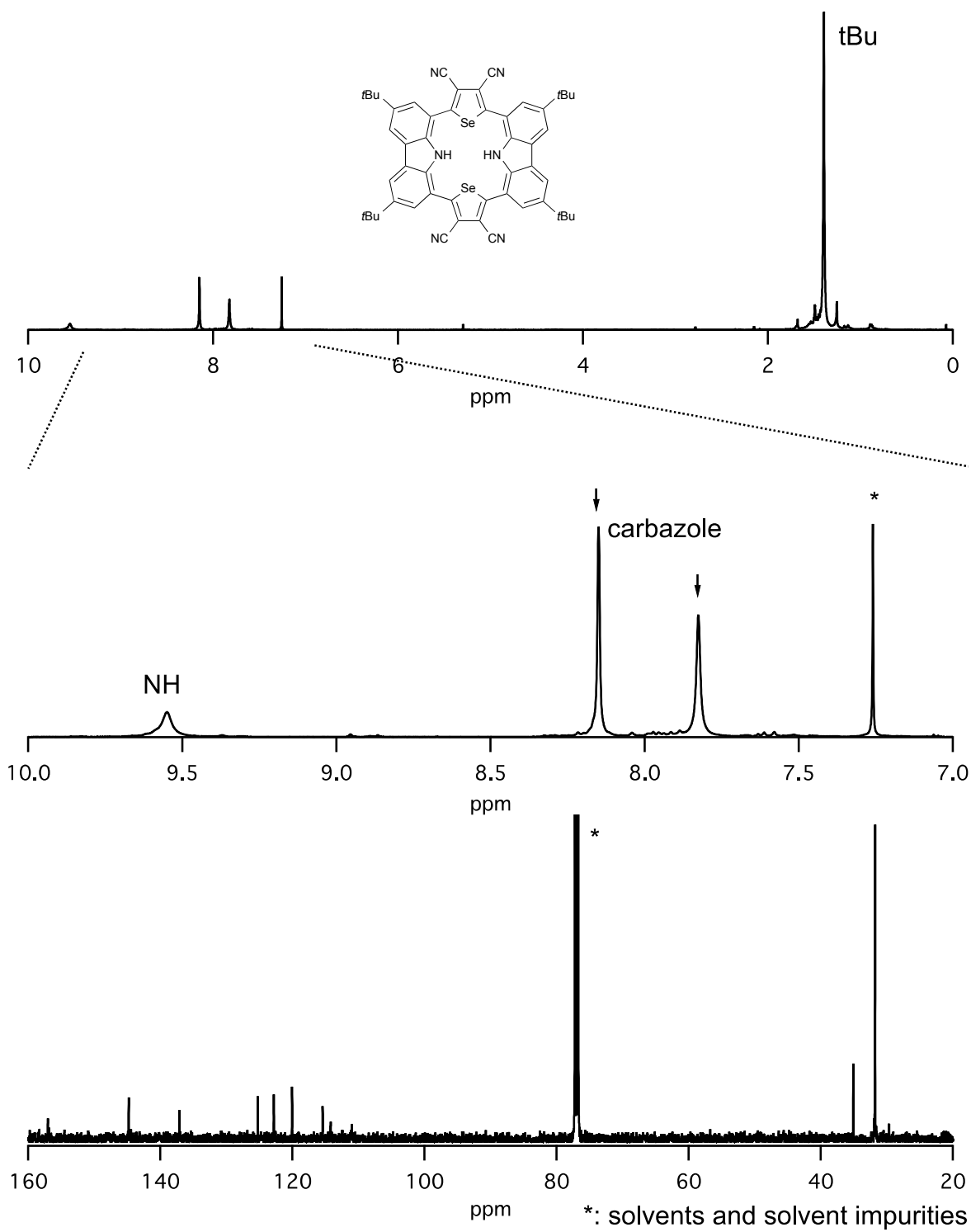


Fig. S4 ^1H and ^{13}C NMR spectra of **13** in CDCl_3

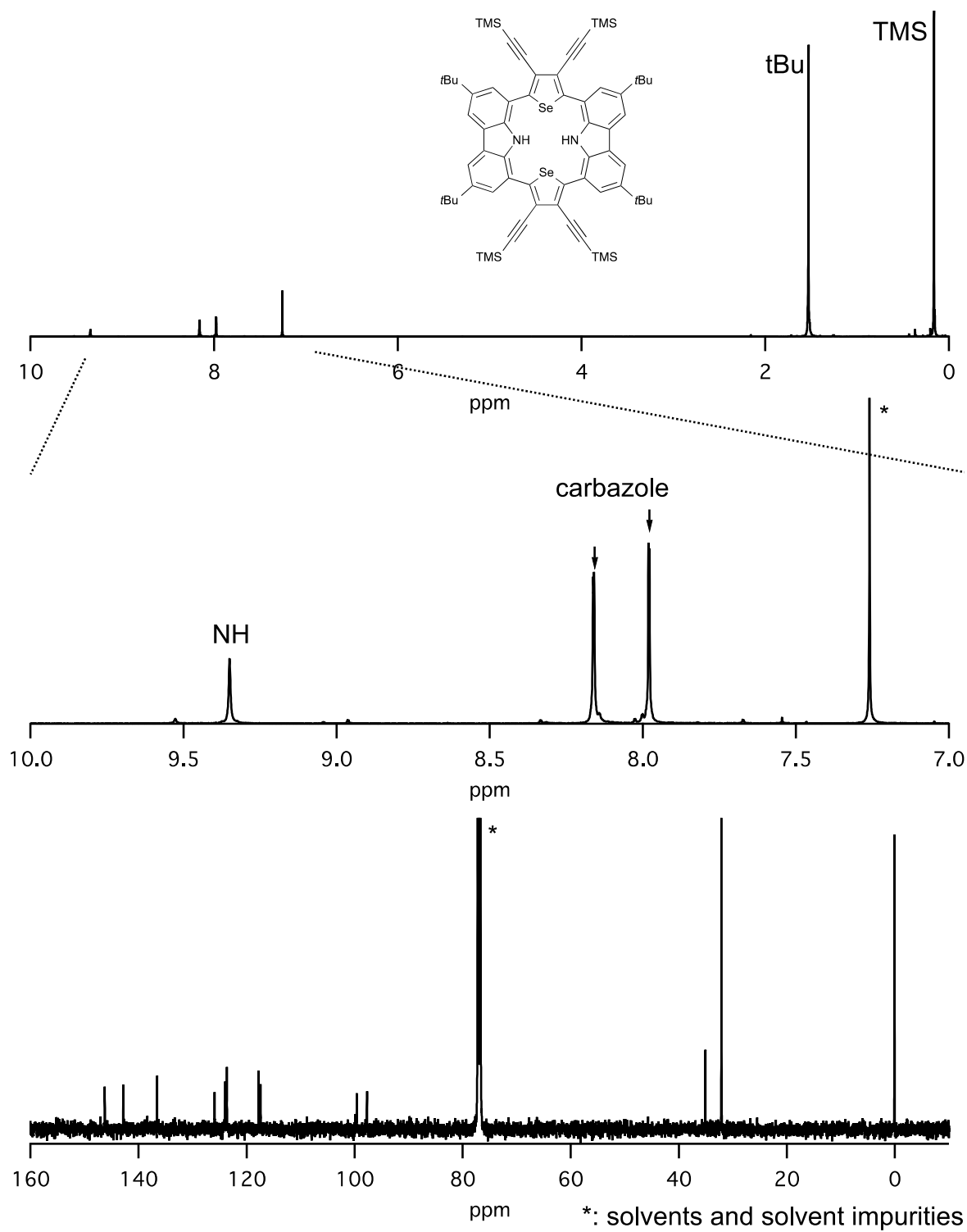


Fig. S5 ^1H and ^{13}C NMR spectra of **6** in CDCl_3

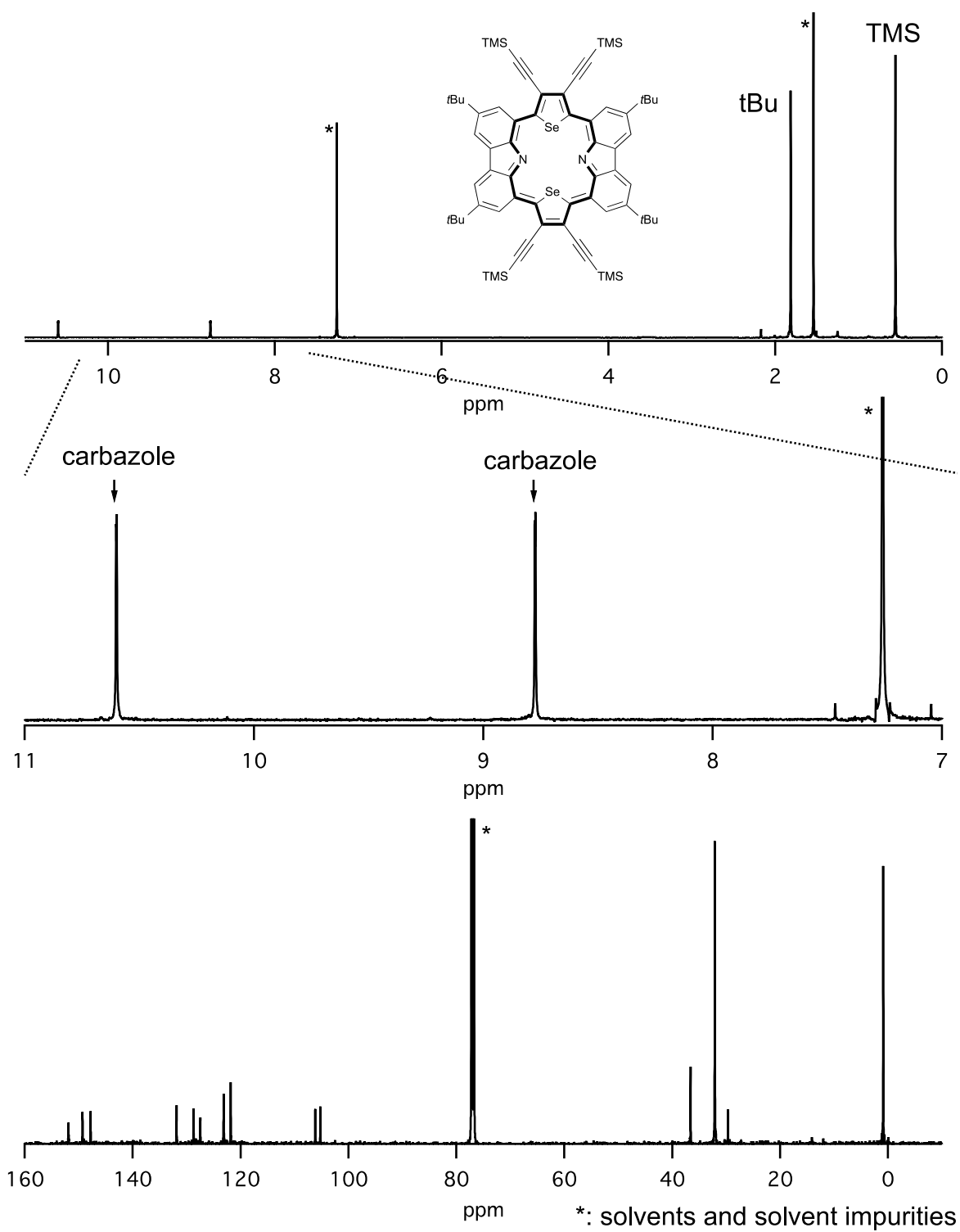


Fig. S6 ^1H and ^{13}C NMR spectra of **14** in CDCl_3

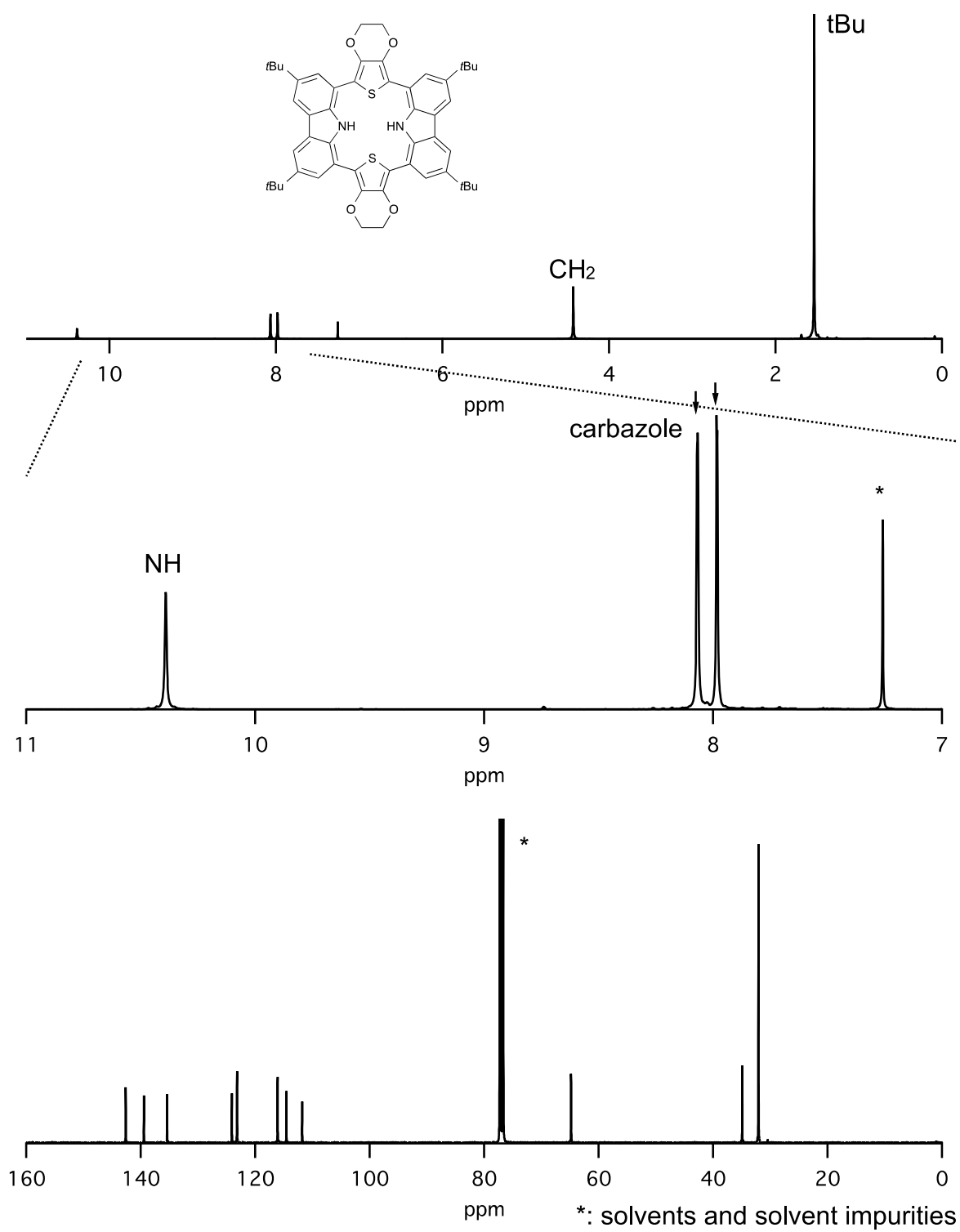


Fig. S7 ^1H NMR spectrum of **4** in CDCl_3

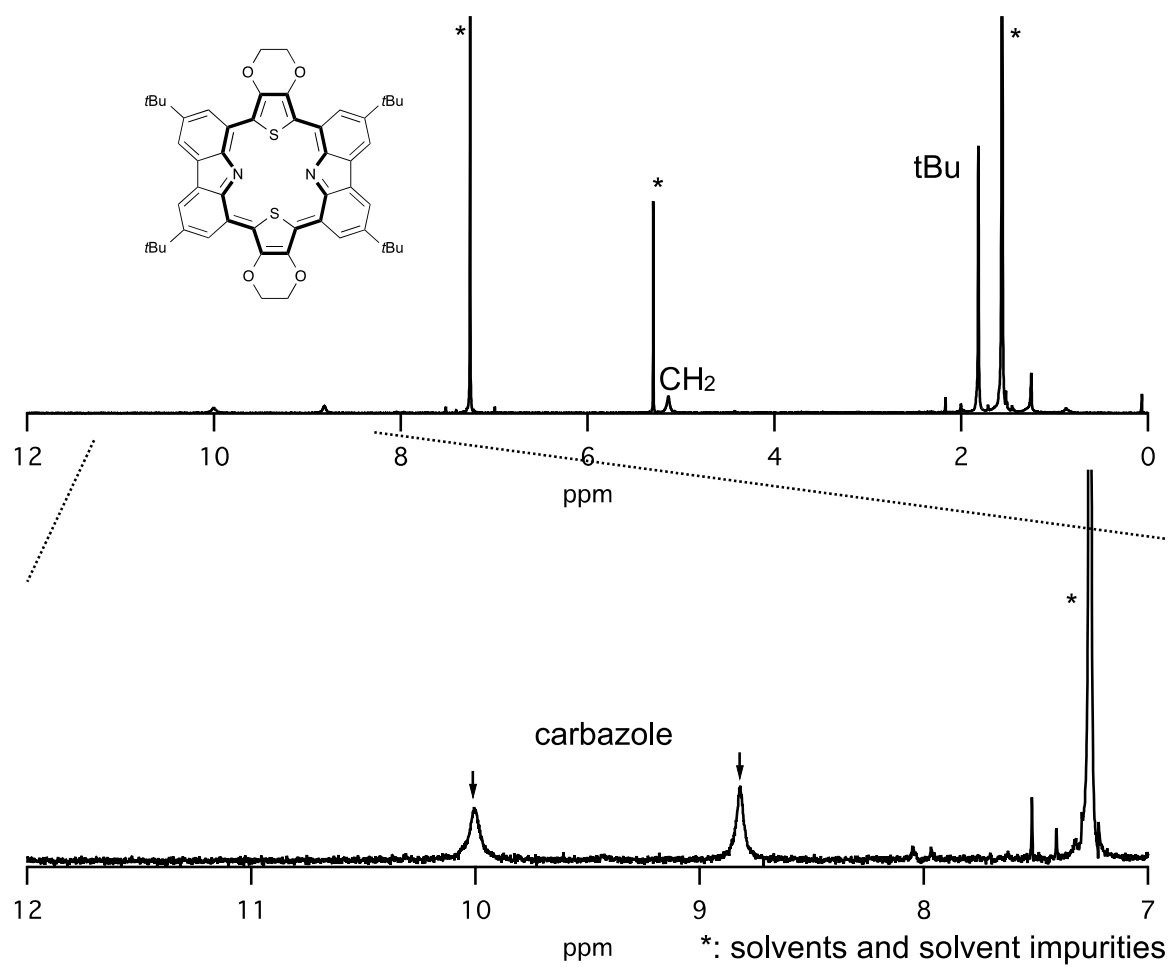


Fig. S8 ^1H and ^{13}C NMR spectra of **15** in CDCl_3

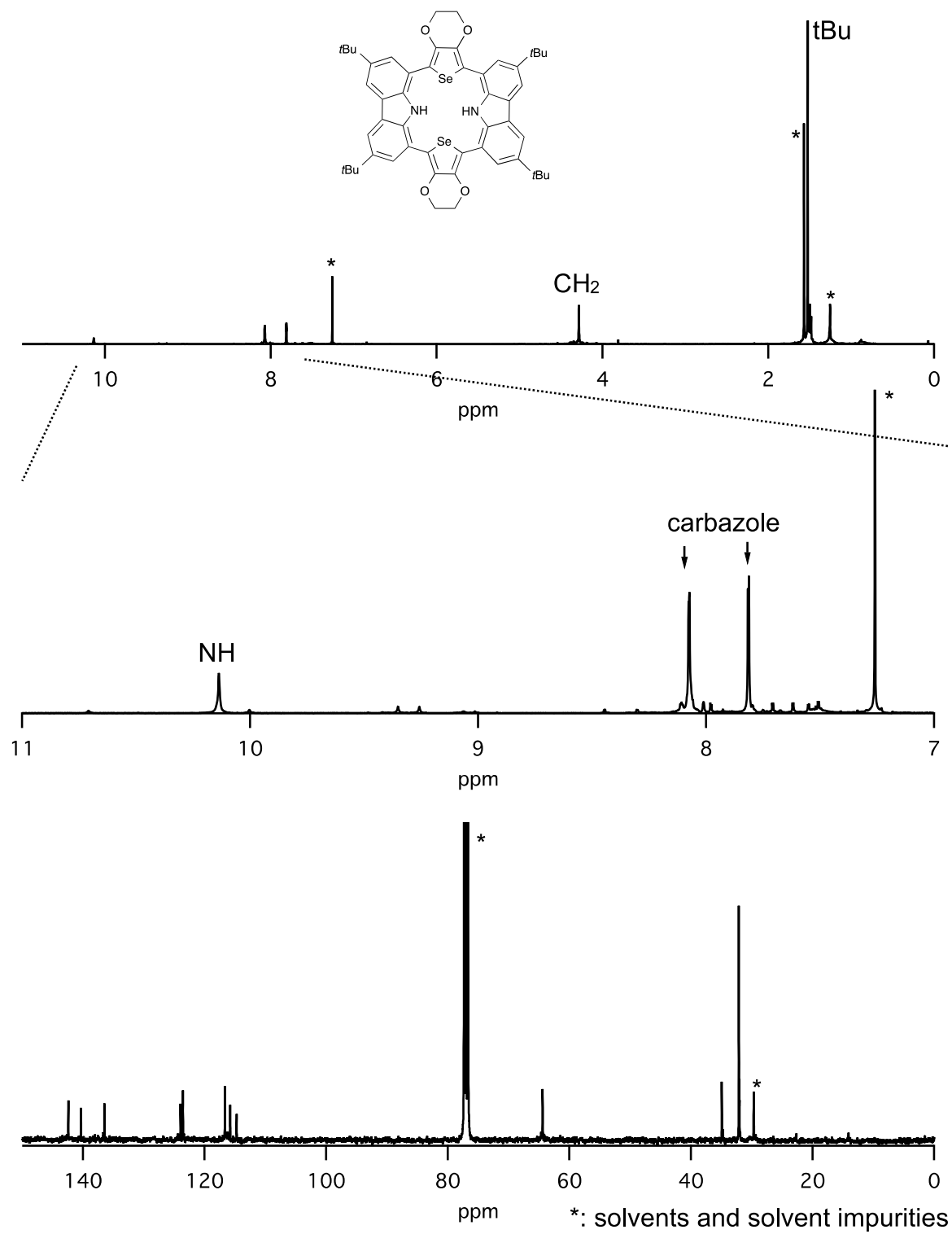


Fig. S9 ^1H NMR spectrum of **8** in CDCl_3

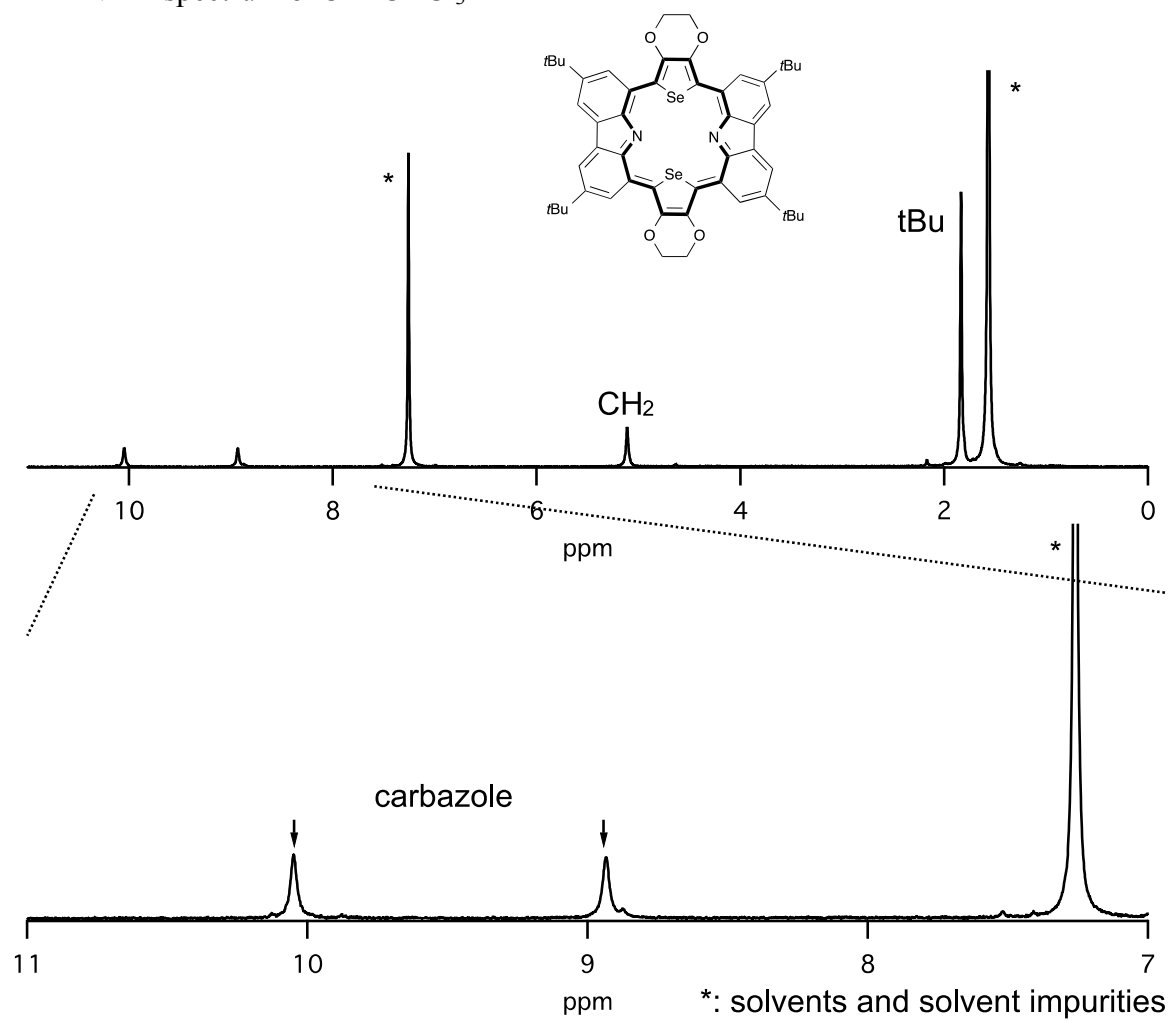


Fig. S10 Cyclic Voltammogram and Differential Pulse Voltammogram of **6** (solvent: CH₂Cl₂, supporting electrolyte: Bu₄NPF₆ (0.10 M), counter electrode: Pt, reference electrode: Ag/Ag⁺, working electrode: glassy carbon, scan rate: 0.05 V/s).

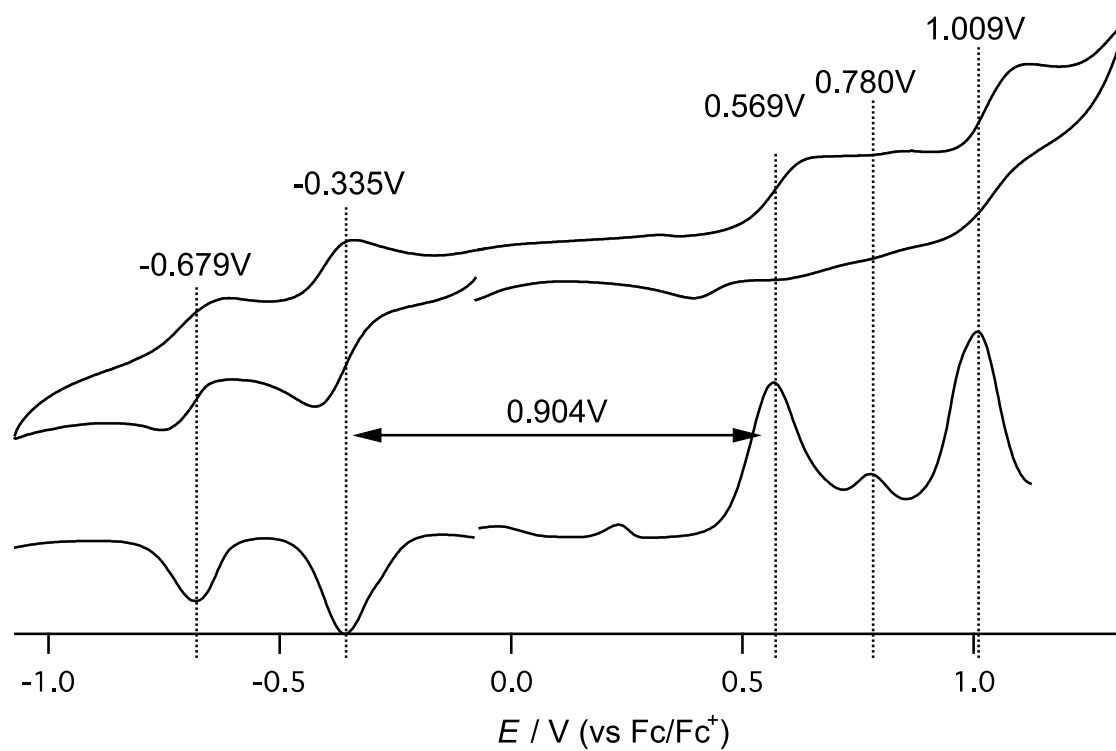


Table S1 Selected data of calculated electronic transitions in **1**

State	Transition energy (nm)	Oscillator strength	Composition of band and CI coefficients
1	1045.8	0.299554	H-1 $\rightarrow$ L (79%), H $\rightarrow$ L+1 (14%)
2	813.7	0.760098	H $\rightarrow$ L (85%)
3	630.1	0.000000	H-2 $\rightarrow$ L (95%)
4	609.5	0.023228	H-3 $\rightarrow$ L (93%)
5	457.0	0.000000	H-4 $\rightarrow$ L (84%)
6	418.4	0.000000	H-1 $\rightarrow$ L+2 (79%), H-5 $\rightarrow$ L (9%)
7	412.2	0.000000	H $\rightarrow$ L+2 (78%), H-4 $\rightarrow$ L (12%)
8	411.6	1.232244	H $\rightarrow$ L+1 (74%), H-1 $\rightarrow$ L (13%)
9	395.1	0.000000	H-7 $\rightarrow$ L (92%)
10	394.0	0.001567	H-8 $\rightarrow$ L (93%)

Table S2 Selected data of calculated electronic transitions in **2**

State	Transition energy (nm)	Oscillator strength	Composition of band and CI coefficients
1	1069.8	0.342325	H-1 $\rightarrow$ L (79%), H $\rightarrow$ L+1 (15%)
2	844.7	0.788252	H $\rightarrow$ L (85%)
3	611.3	0.000009	H-2 $\rightarrow$ L (94%)
4	592.5	0.006579	H-3 $\rightarrow$ L (93%)
5	463.5	0.000000	H-4 $\rightarrow$ L (76%), H $\rightarrow$ L+2 (18%)
6	438.8	0.000051	H-5 $\rightarrow$ L (61%), H-1 $\rightarrow$ L+2 (29%)
7	429.3	1.824787	H $\rightarrow$ L+2 (74%), H-1 $\rightarrow$ L (15%)
8	415.2	0.002586	H-1 $\rightarrow$ L+3 (62%), H-5 $\rightarrow$ L (33%)
9	414.9	0.000000	H $\rightarrow$ L+2 (71%), H-4 $\rightarrow$ L (21%)
10	406.4	2.711576	H-1 $\rightarrow$ L+1 (83%)

Table S3 Selected data of calculated electronic transitions in **3**

State	Transition energy (nm)	Oscillator strength	Composition of band and CI coefficients
1	1028.3	0.315875	H-1 $\rightarrow$ L (76%), H $\rightarrow$ L+1 (16%)
2	859.5	0.907297	H $\rightarrow$ L (86%)
3	718.7	0.000000	H-2 $\rightarrow$ L (96%)
4	700.4	0.009895	H-3 $\rightarrow$ L (93%)
5	485.8	0.000000	H-4 $\rightarrow$ L (83%)
6	434.2	1.683976	H $\rightarrow$ L+1 (76%), H-1 $\rightarrow$ L (16%)
7	418.9	0.000000	H-5 $\rightarrow$ L (43%), H-1 $\rightarrow$ L+2 (38%)
8	416.4	0.000000	H $\rightarrow$ L+2 (78%), H-4 $\rightarrow$ L (14%)
9	391.5	2.817804	H-1 $\rightarrow$ L+1 (84%)
10	389.2	0.000000	H-1 $\rightarrow$ L+2 (49%), H-5 $\rightarrow$ L (45%)