Supporting Information

Photophysics of Platinum-Acetylide Substituted Hexa-peri-Benzocoronenes

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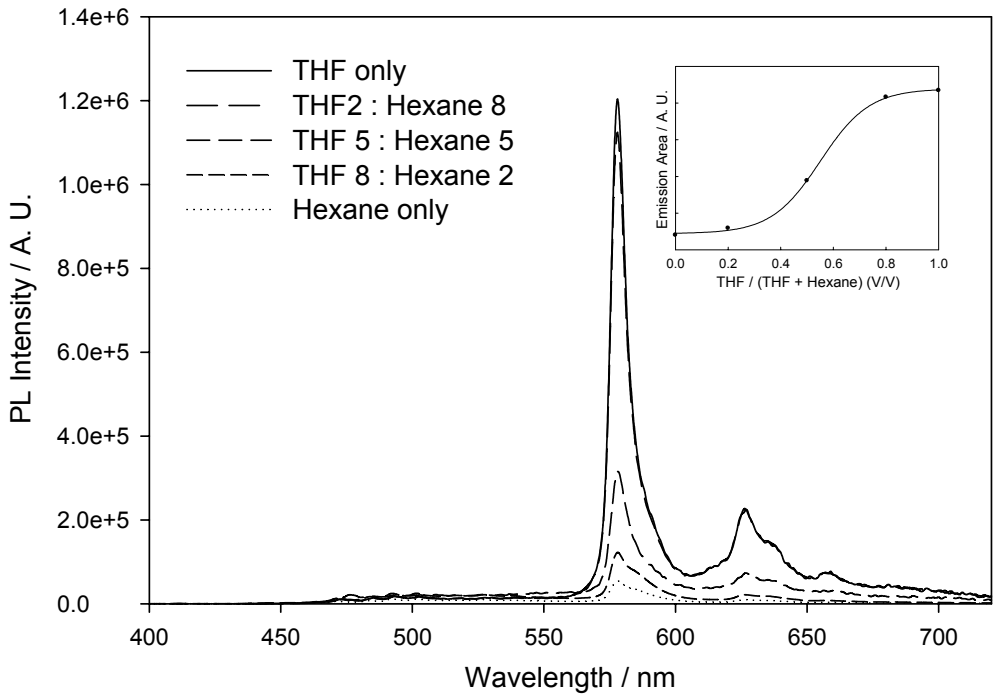
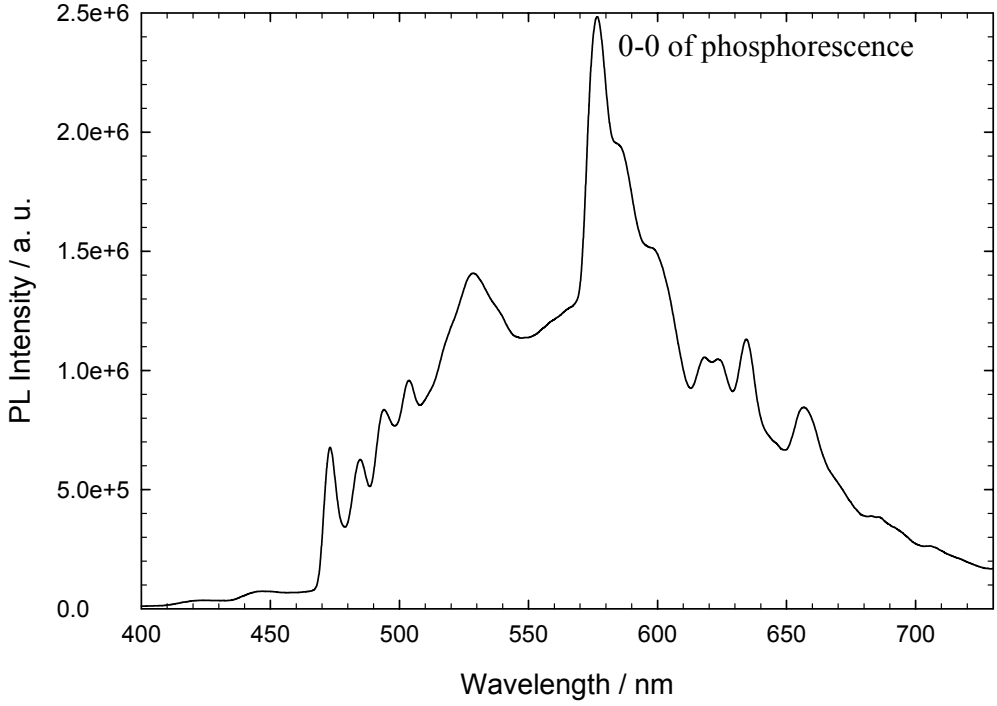
Figure S-1



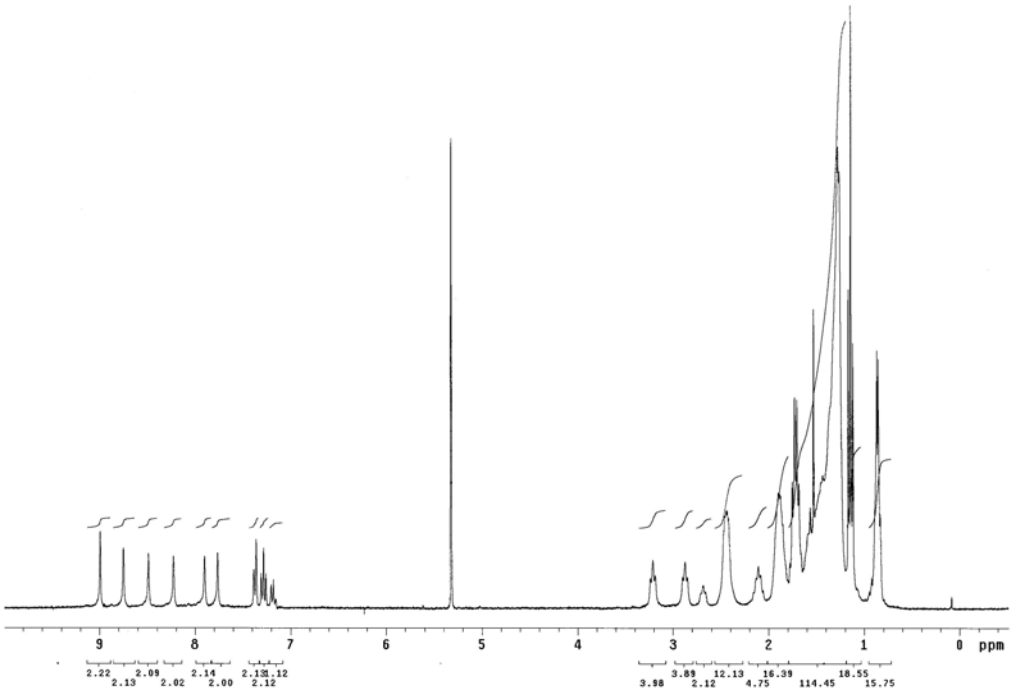
Photoluminescence spectra of complex **1** in 5 x 10^{-6} M solution of THF and hexane mixture. The measurements were taken in argon deoxygenated solution.

Figure S-2



Photoluminescence spectrum of complex **2** (c= 5 x 10^{-7} M) in a 2-methyltetrahydrofuran glass at 80 K (λ_{ex} = 360 nm). The sample solution was deoxygenated by three freeze pump thaw cycles (vacuum of 10^{-6} torr).

Figure S-3
^{1}H NMR Spectrum of Complex 1 (300 MHz, CD_2Cl_2)



^{31}P NMR Spectrum of Complex 1 (121 MHz, CD_2Cl_2)

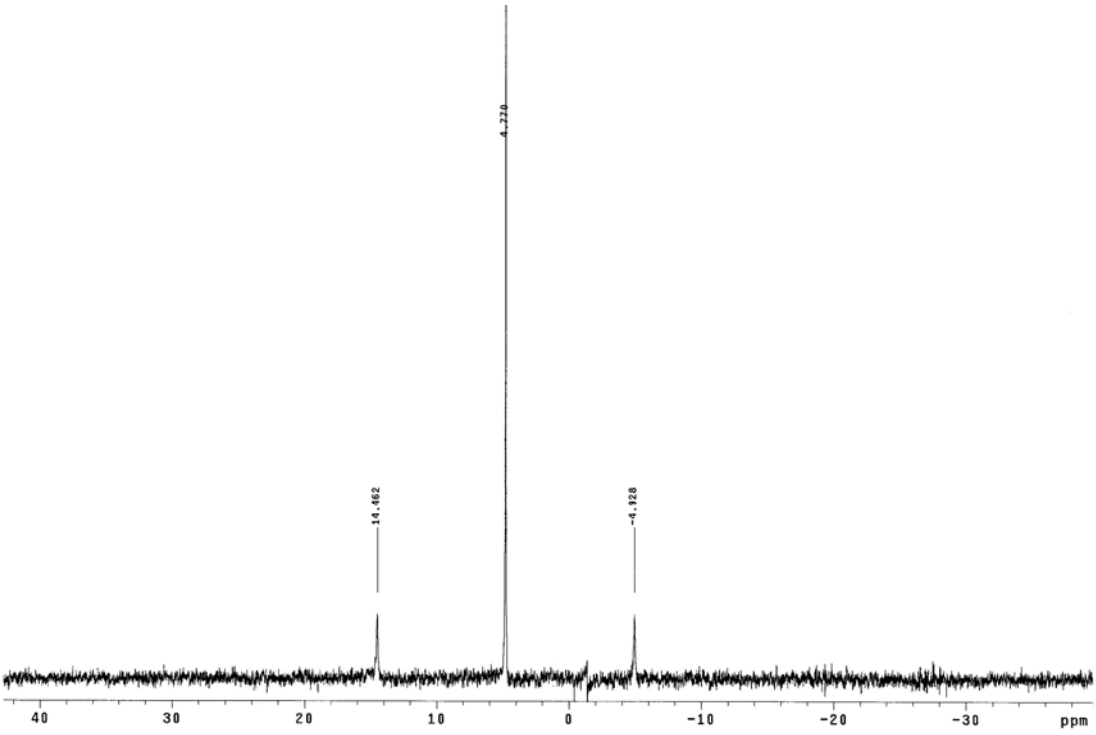
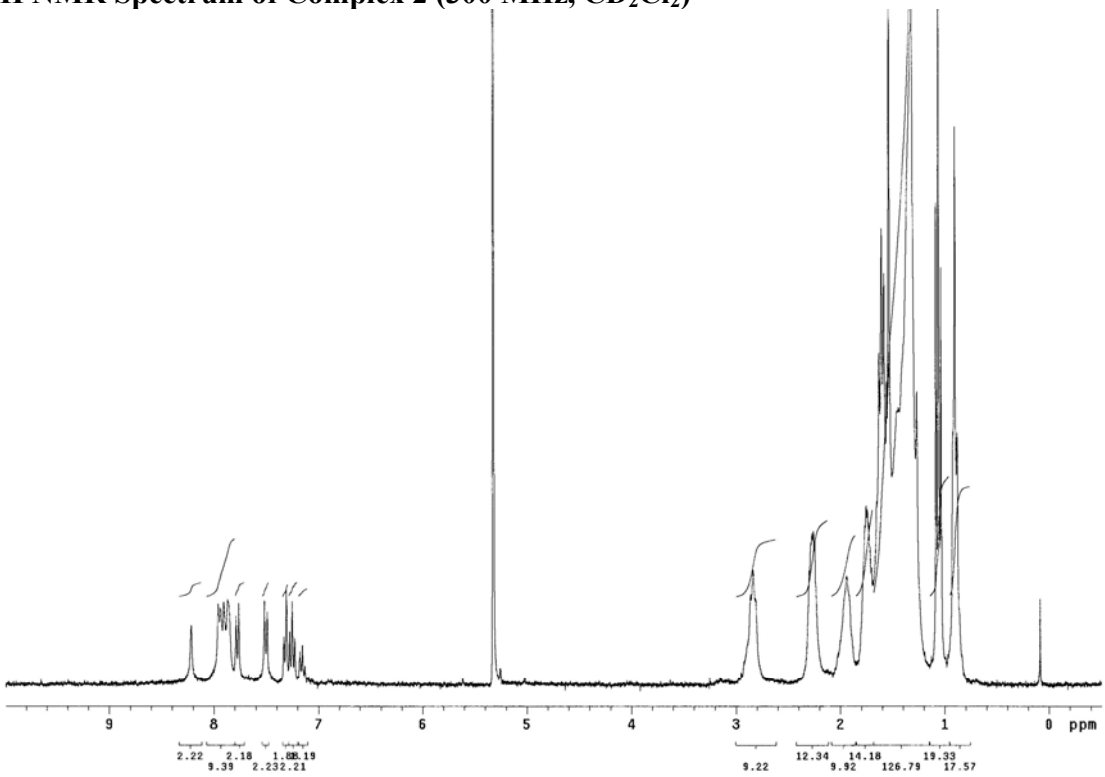


Figure S-4
^{1}H NMR Spectrum of Complex 2 (300 MHz, CD_2Cl_2)



^{31}P NMR Spectrum of Complex 2 (121 MHz, CD_2Cl_2)

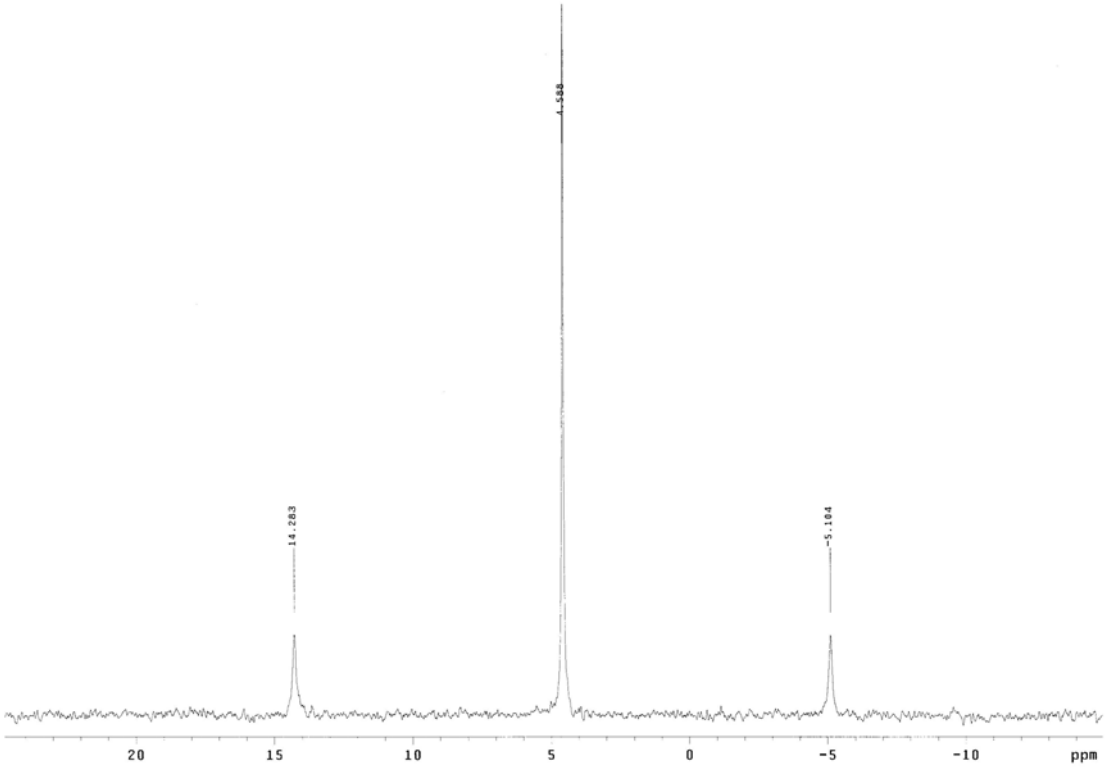


Figure S-5
^{1}H NMR Spectrum of 3 (300 MHz, $CDCl_3$)

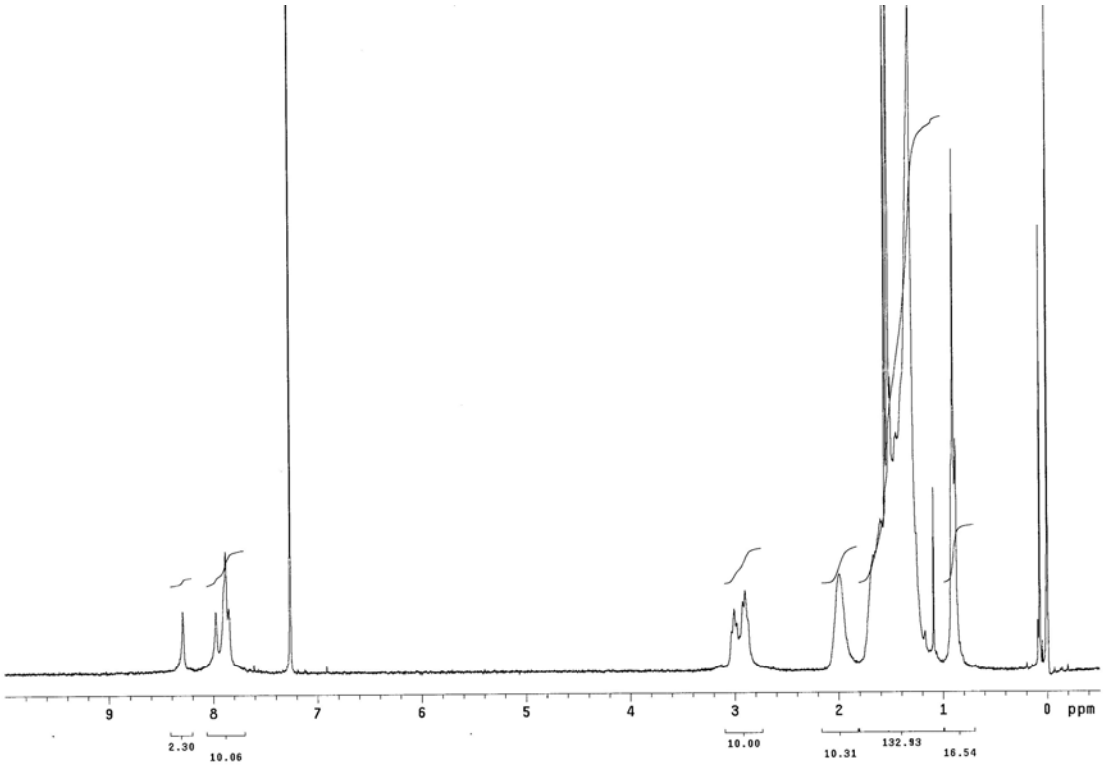


Figure S-6
^{1}H NMR Spectrum of 6 (300 MHz, $CDCl_3$)

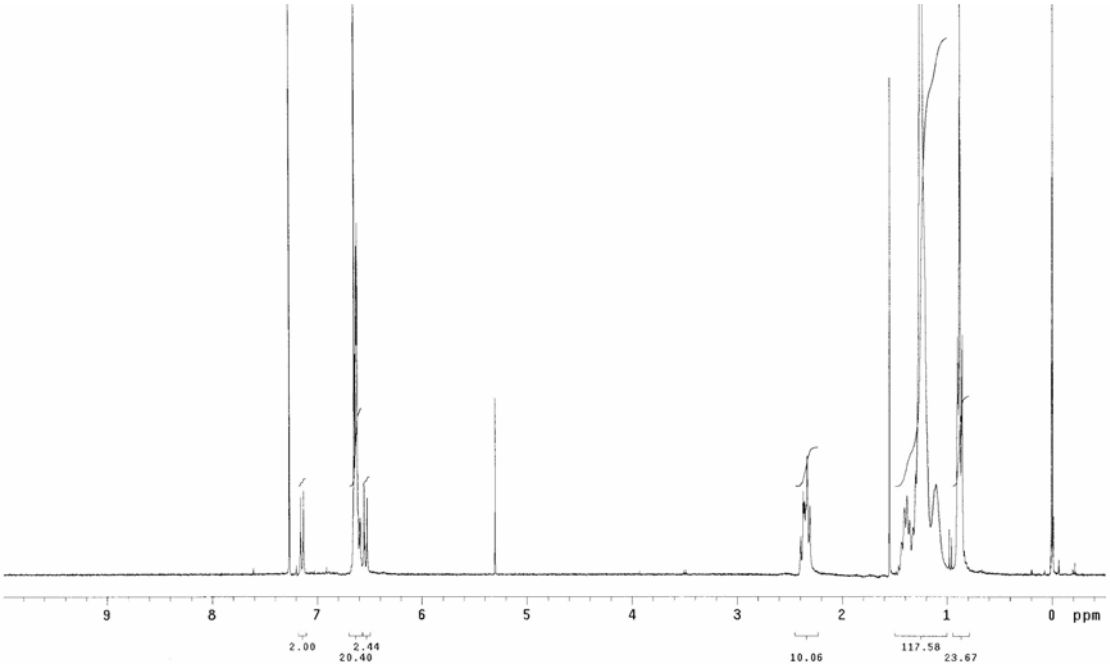


Figure S-7
^{1}H NMR Spectrum of 7 (300 MHz, $CDCl_3$)

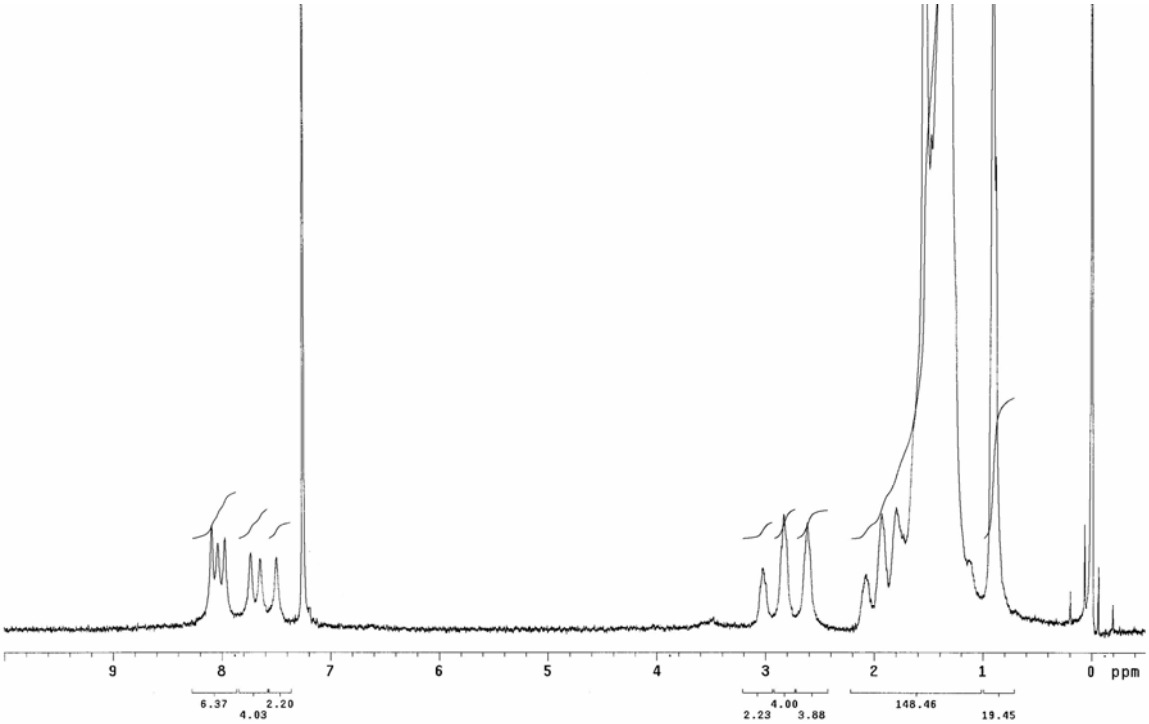
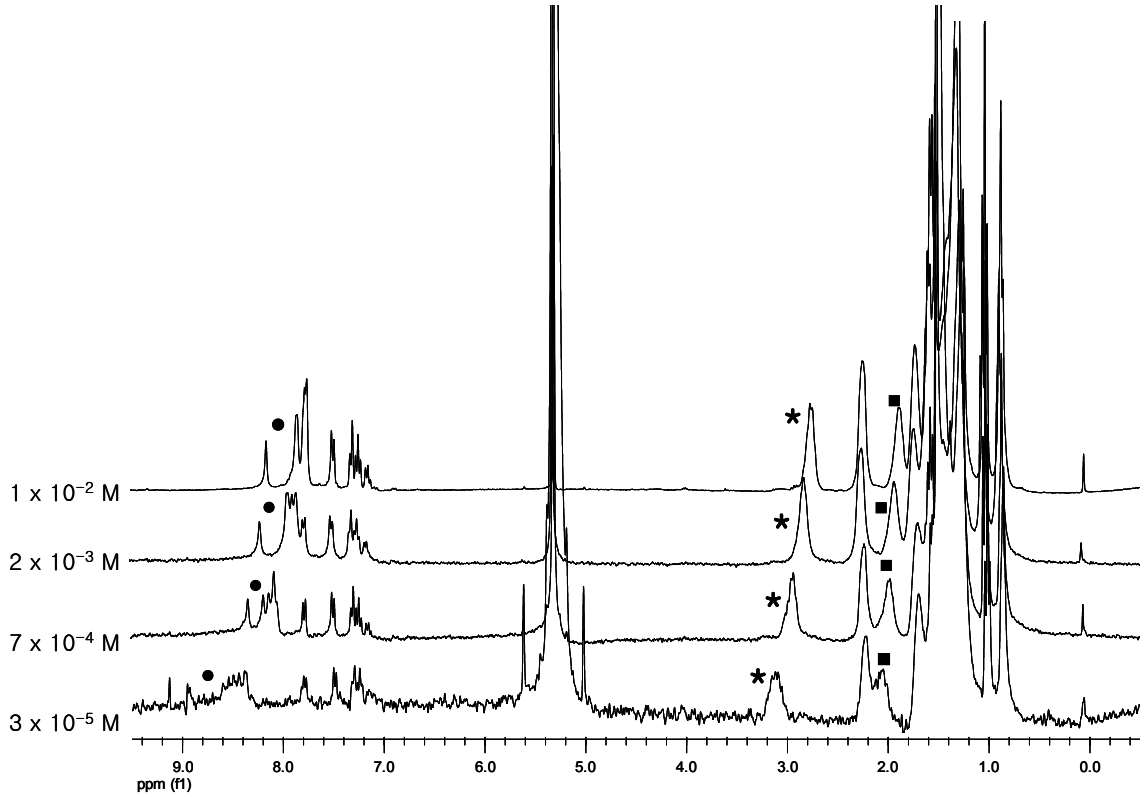
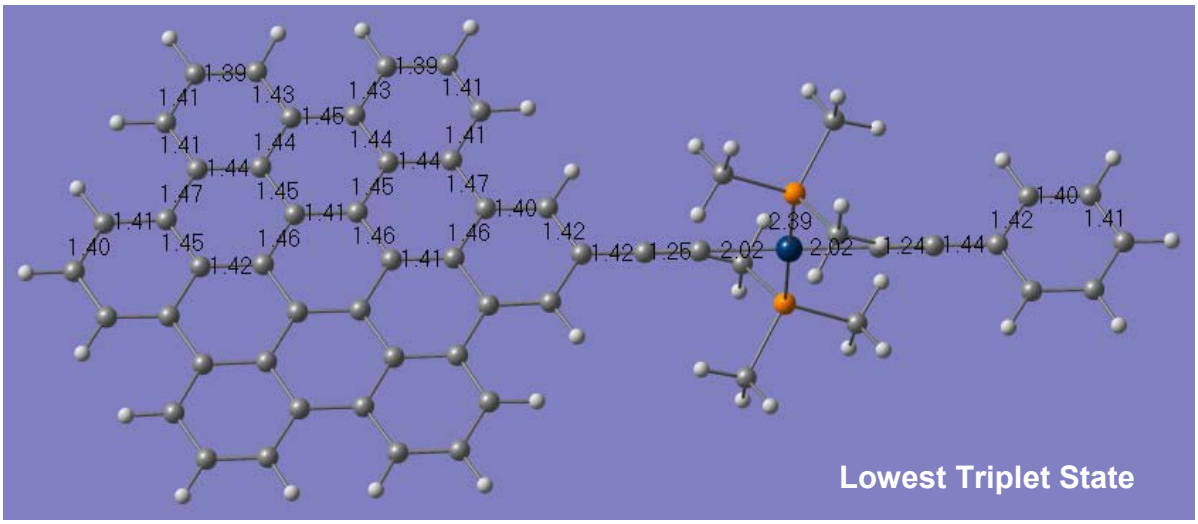


Figure S-8
Concentration dependent ^{1}H NMR Spectra of Complex 2 in CD_2Cl_2 at room temperature (300 MHz)



^{1}H NMR spectra of Pt-HBC **2** in CD_2Cl_2 as a function of concentration. Circles indicate HBC aromatic protons, asterisk and square indicates α- and β-CH_2 protons on HBC alkyl chain, respectively.

Figure S-9. Bond lengths for geometry optimized structures of complex **1** calculated using density functional theory (see text for methods).



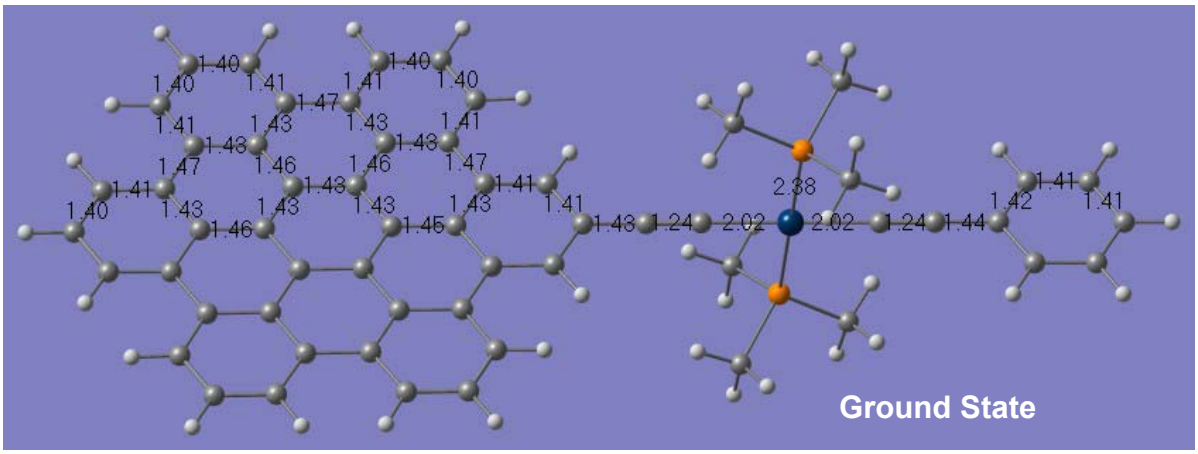


Figure S-10. Frontier orbital plots for optimized ground state geometry of hexa-peri-benzocoronene computed by using DFT.

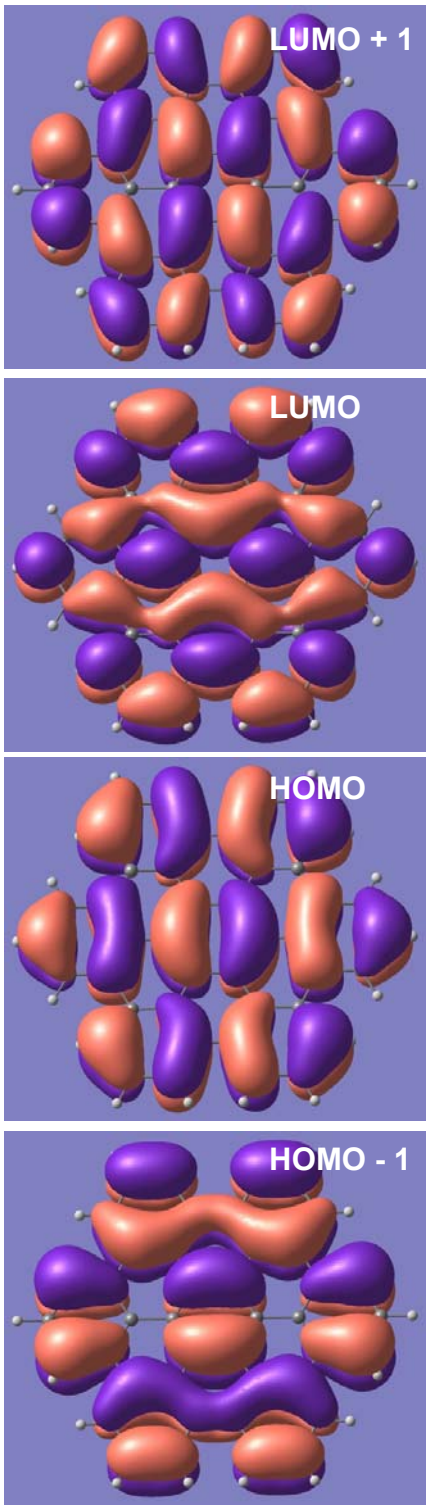
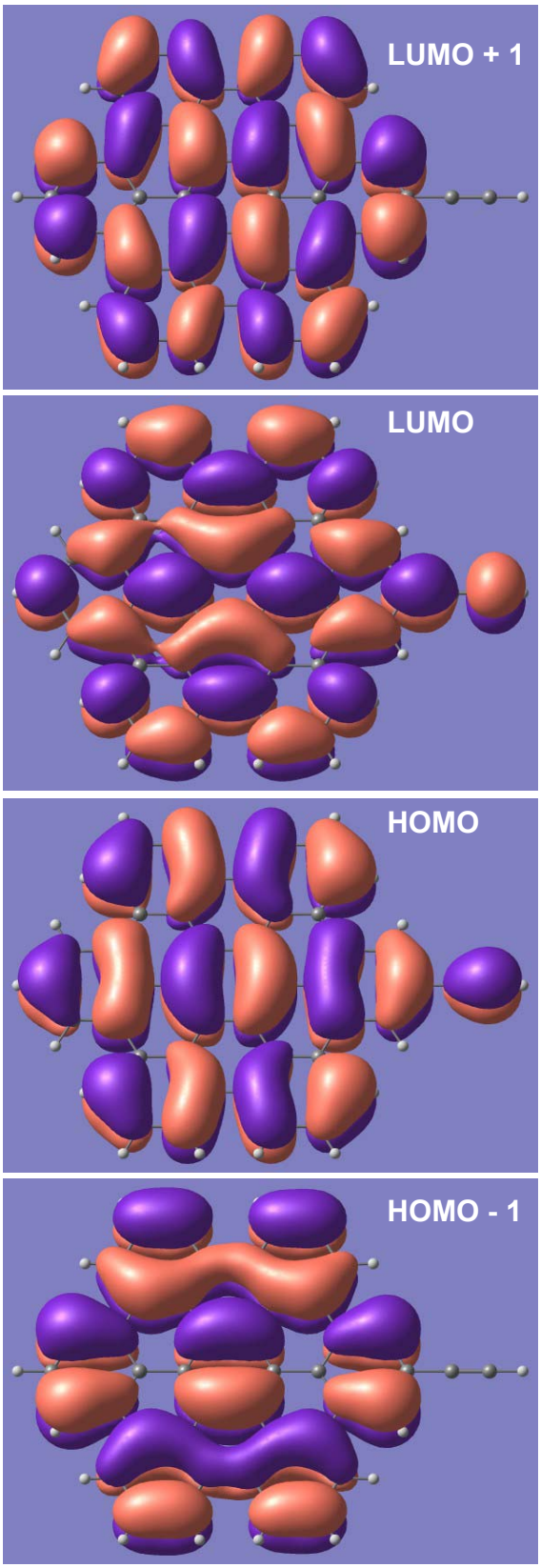



Figure S-11. Frontier orbital plots for optimized ground state geometry of **3** computed by using DFT.