Electronic Supplementary Information for Dalton Transactions
This journal is © The Royal Society of Chemistry 2009

Supplementary Information

for

Pt(II) N-confused porphyrin: An expanded pyrrole that affords stable π-anion

Dong-Hoon Won, Motoki Toganoh, Hidemitsu Uno, and Hiroyuki Furuta*

Table of Contents

Figure S1. ^{1}H NMR spectrum of **1-Pt** in $CDCl_3$ ---------- S2

Figure S2. ^{1}H NMR spectrum of **2-Pt** in $CDCl_3$ ---------- S2

Figure S3. ^{1}H NMR spectrum of **3** in $CDCl_3$ ---------- S3

Figure S4. ^{1}H NMR spectrum of **3-Pt** in $CDCl_3$ ---------- S3

Figure S5. pH titration curves for **1-Pt** and **1-Cu** ----------S4

Figure S6. Packing diagram of $\mathbf{Bu_4N^+ \bullet (1\text{-}Pt^-)}$ ----------S5

Figure S7. Calculated charge density for **1-Pt** and $\mathbf{1\text{-}Pt^-}$ ----------S6

This journal is © The Royal Society of Chemistry 2009

Figure S1. ^{1}H NMR spectrum of **1-Pt** in $CDCl_3$.

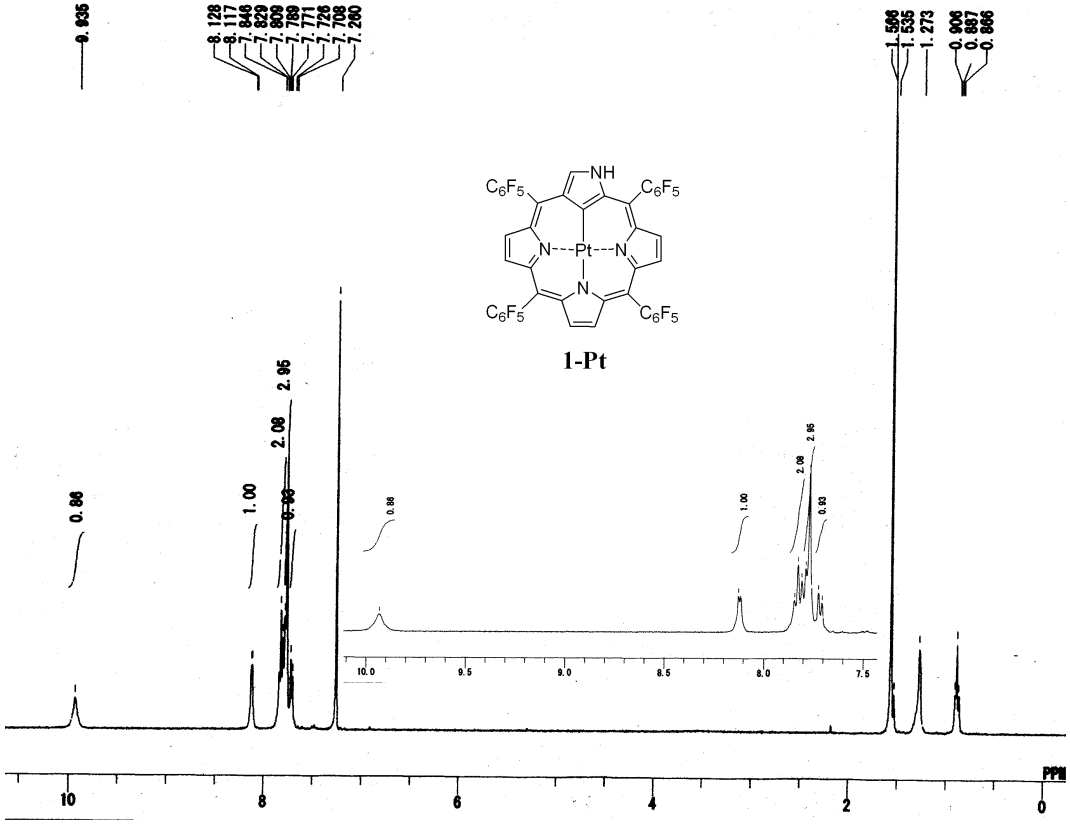


Figure S2. ^{1}H NMR spectrum of **2-Pt** in $CDCl_3$.

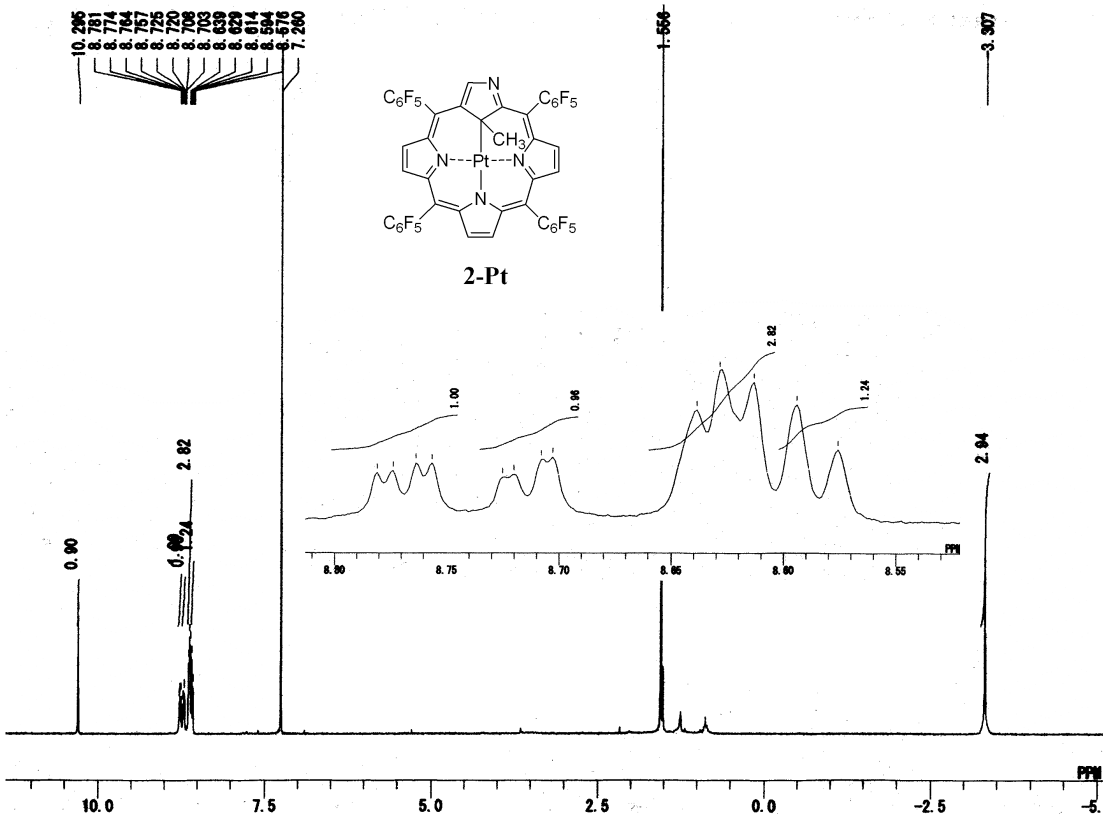


Figure S3. ^{1}H NMR spectrum of **3** in $CDCl_3$.

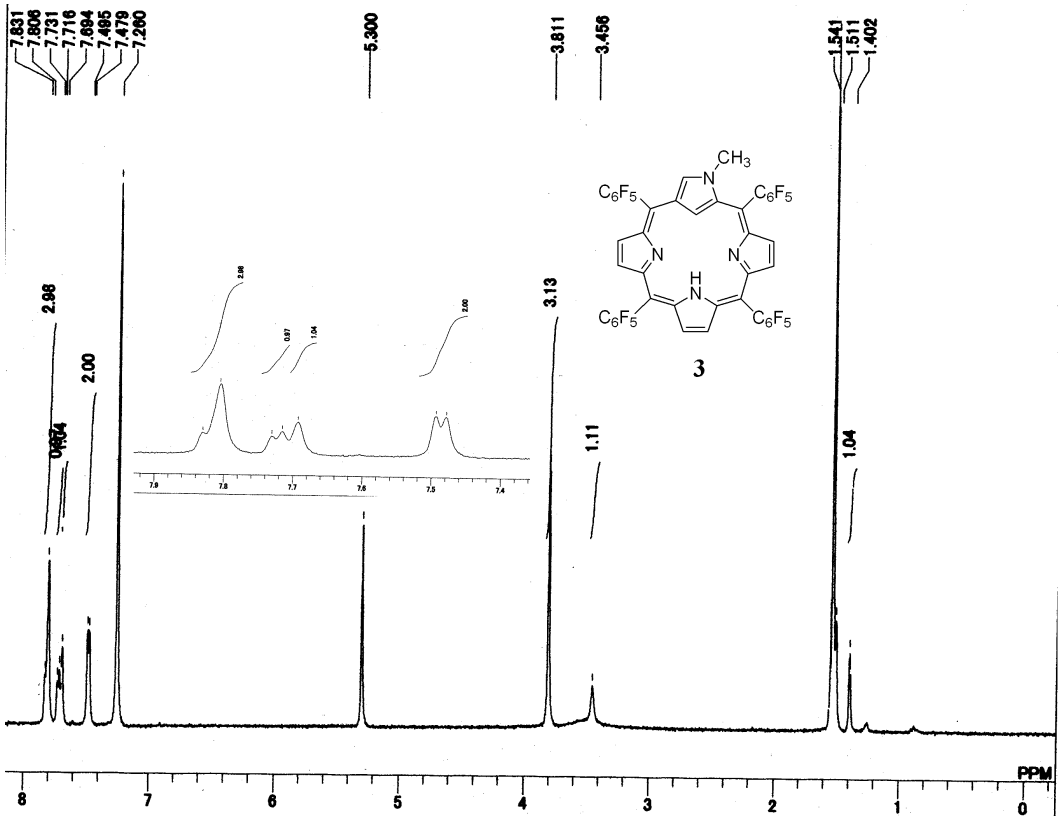
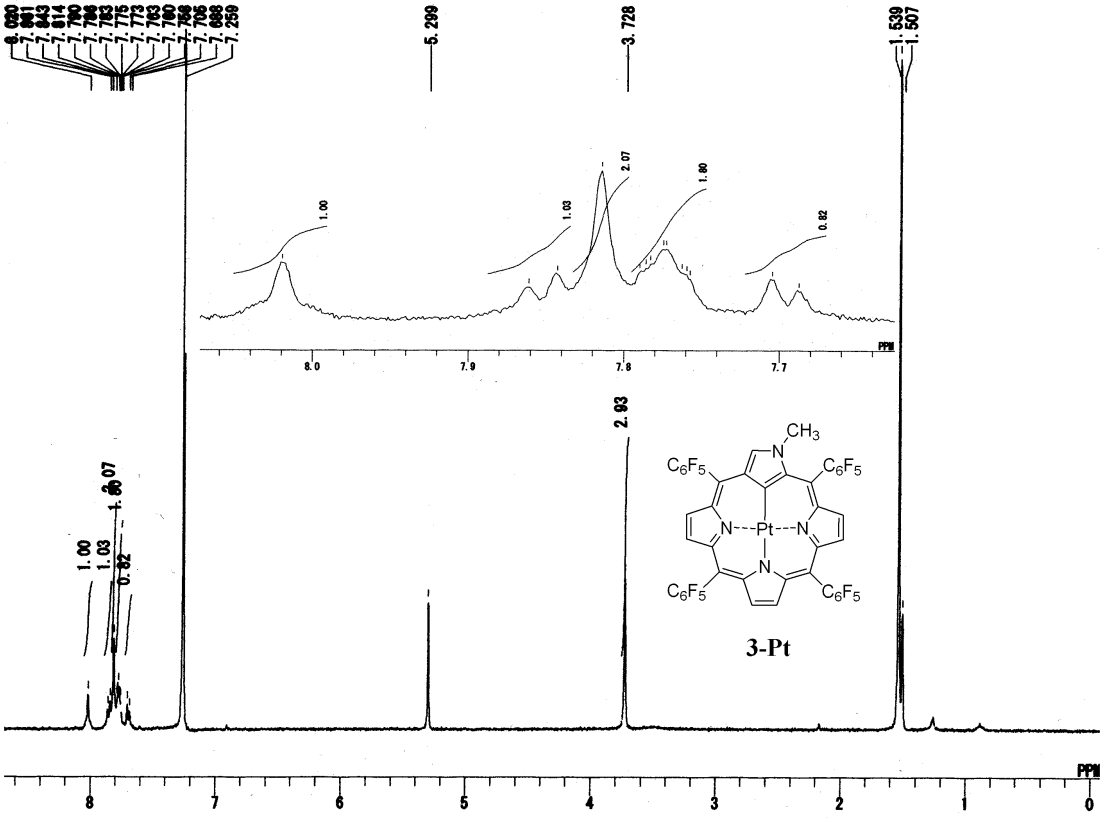
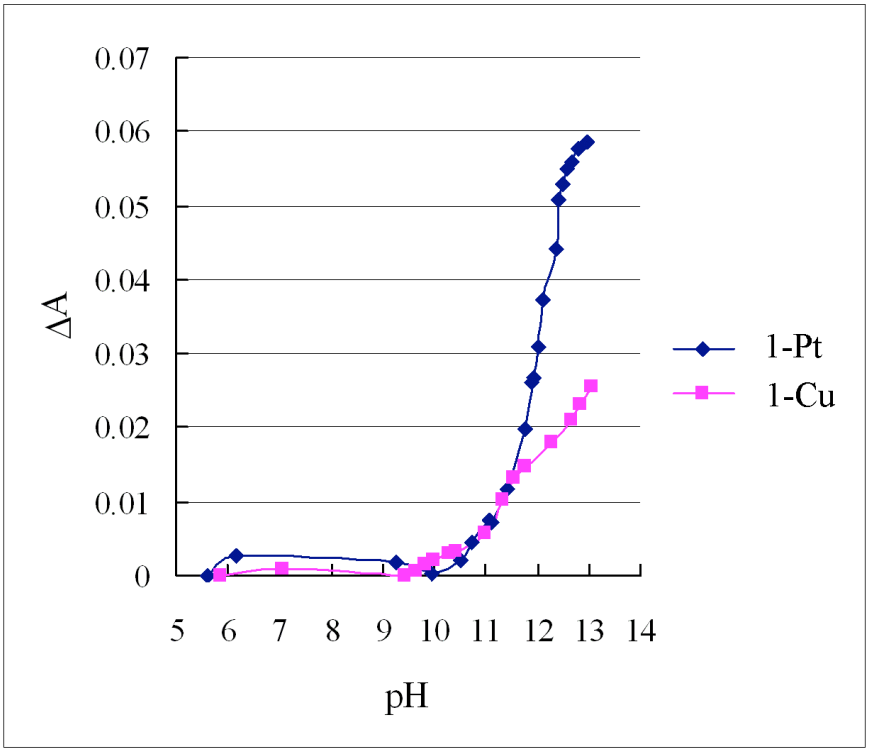


Figure S4. ^{1}H NMR spectrum of **3-Pt** in $CDCl_3$.



This journal is © The Royal Society of Chemistry 2009

Figure S5. pH titration curves for **1-Pt** and **1-Cu**. Titration was performed in 3.5% sodium dodecyl sulfate by adjusting the pH with HCl-NaOH; [**1-Pt**] = ~2 x 10^{-5} M, [**1-Cu**] = ~1 x 10^{-5} M.



This journal is © The Royal Society of Chemistry 2009

Figure S6. Packing diagram of **Bu_4N^+•(1-Pt^-).**

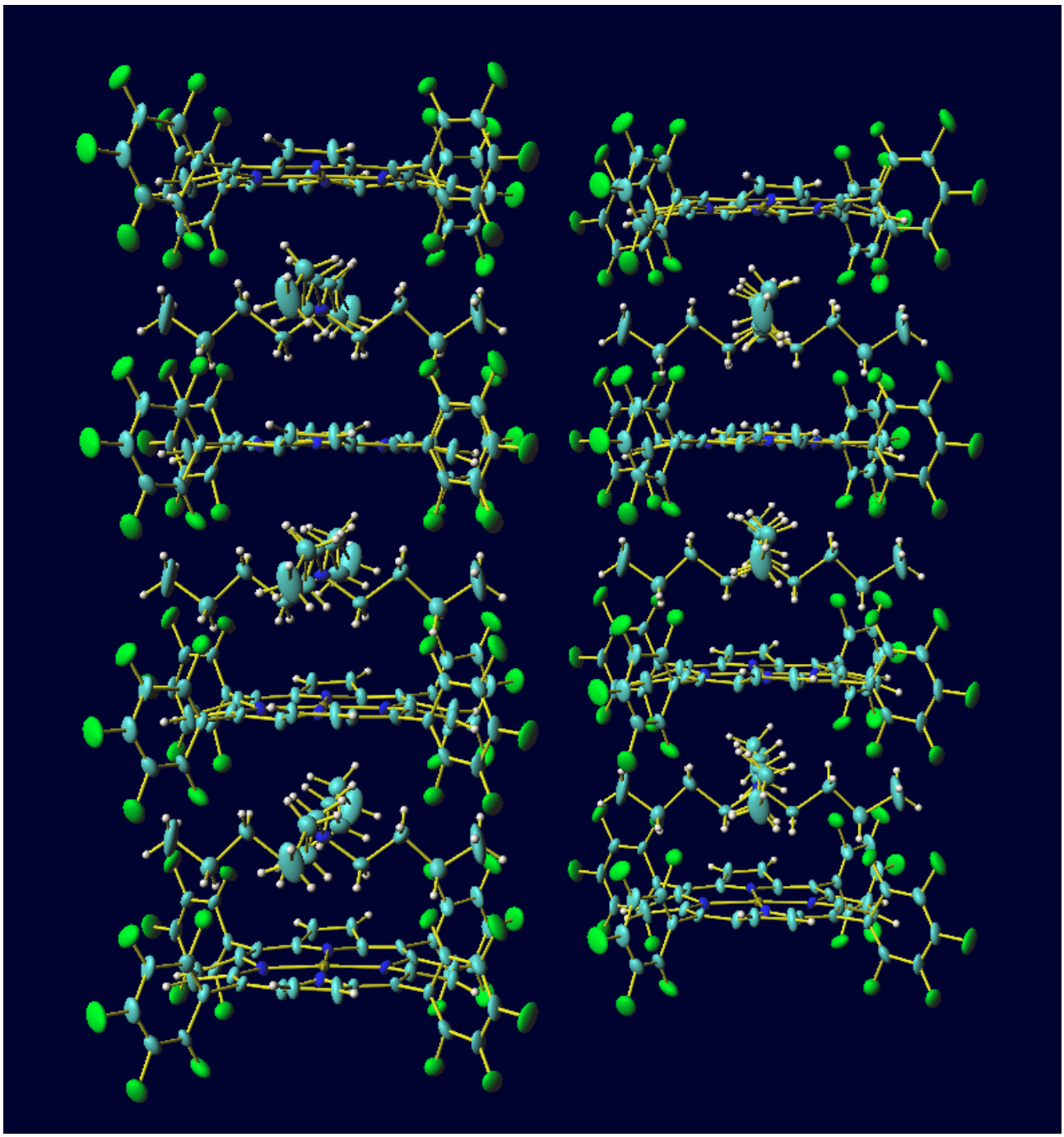
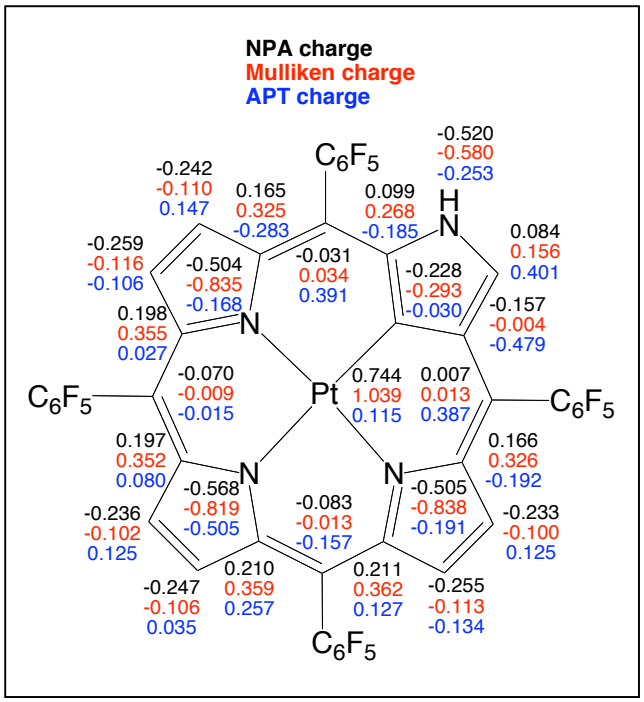
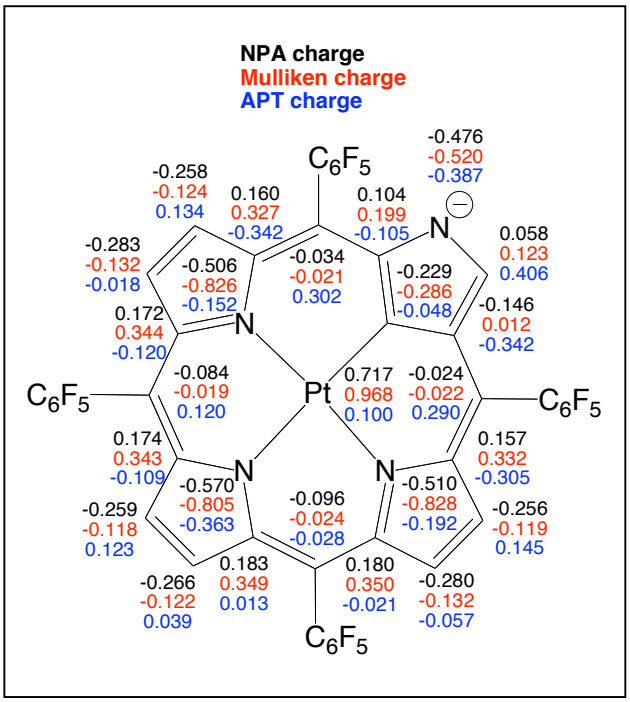
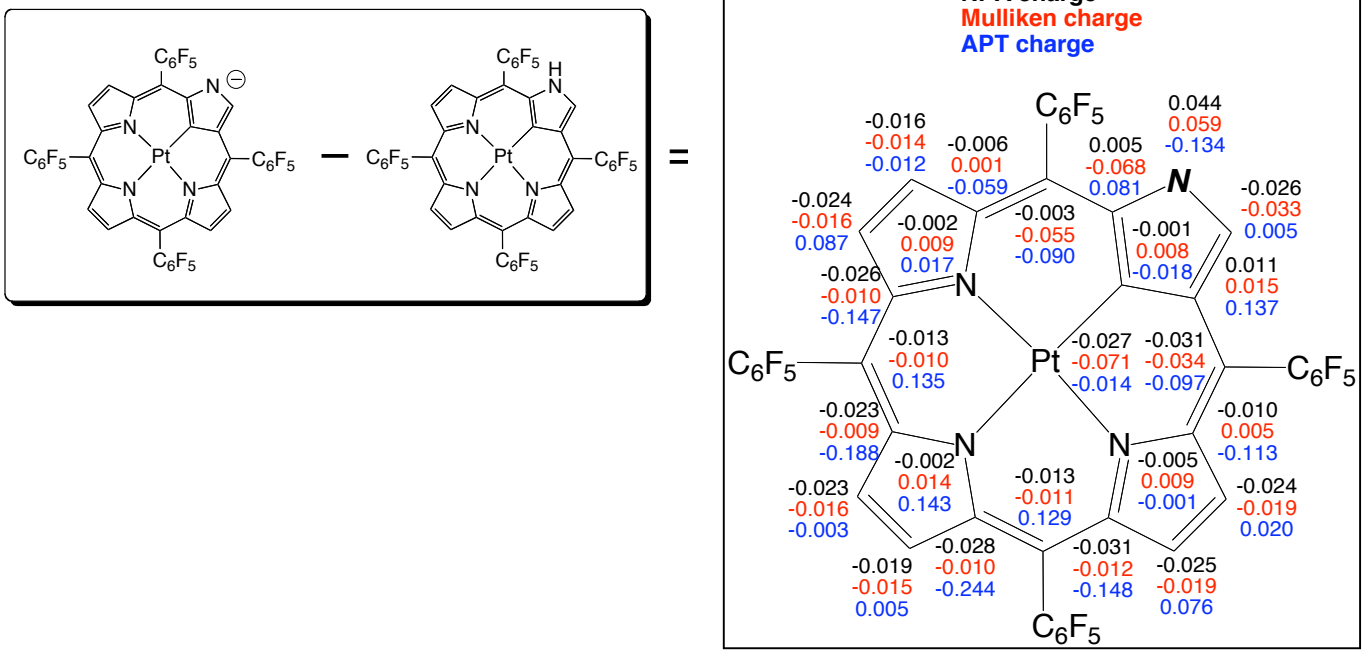


Figure S7. Calculated charge density for a) **1-Pt**, b) **1-Pt$^-$**, and c) their difference.

(a) **1-Pt**



(b) 1-Pt$^-$



(c) [**1-Pt$^-$**] – [**1-Pt**]