Electronic Supplementary Material (ESI) for Dalton Transactions.

Stabilization of Hexa Coordinated P(V) Corroles by Axial Silyloxy Groups

Tamal Chatterjee[a], Way-Zen Lee[b] and Mangalampalli Ravikanth[*a]

[a]Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400 076, India.

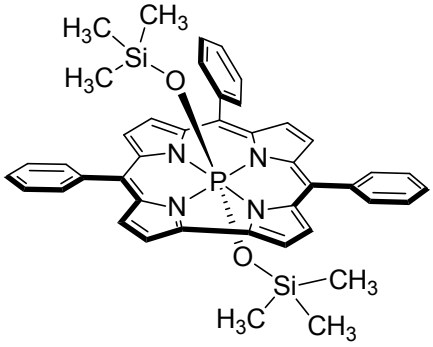
[b]Instrumentation Center, Department of Chemistry, National Taiwan Normal University,88 Sec. 4 Ting-Chow Road, Taipei, 11677, Taiwan

E-mail: ravikanth@chem.iitb.ac.in

Table of Contents

Chemicals: All the solvents such as Chloroform, Toluene, Triethylamine, Dichloromethane, *n*-hexane, Benzene were dried by following available methods and distilled under inert atmosphere prior to use. Deuterated solvents such as $CDCl_3$ and C_6D_6 were obtained from Aldrich and used as received. All the chemicals used for the synthesis were reagent grade. Column chromatography was performed using 60-120 mesh silica gel and basic aluminium oxide obtained from Sisco Research Laboratories, India.

Instrumentation: ^{1}H, ^{13}C and ^{31}P NMR spectra were recorded in C_6D_6 using a Brukar 400 MHz and 500 MHz spectrometer and reported in δ ppm. Absorption spectra were obtained using Cary series UV-VIS NIR spectrophotometer. The fluorescence quantum yields (ϕ_f) were calculated from the emission and absorption spectra by a comparative method at a excitation wavelength of 430 nm using Tetratolyl porphyrin (H_2TTP) (ϕ_f = 0.11) as the standard. The time resolved fluorescence decay measurement were carried out at magic angle (54.60) using a picoseconds diode laser based TCSPC fluorescence spectrometer from IBH, UK. All the decays were fitted to single exponential decay. Cyclic voltammetry (CV) studies are carried out with a BAS electrochemical system by utilizing the three-electrode configuration consisting of glassy carbon (working electrode), platinum wire (auxiliary electrode) and saturated calomel (reference electrode) electrodes. The experiments were carried out in dry dichloromethane using tetrabutylammonium perchlorate as the supporting electrolyte. The high resolution mass spectra (HRMS) were recorded on a Q-Tof micro mass spectrometer.



Compound 2
Mol. Wt. = 732.25

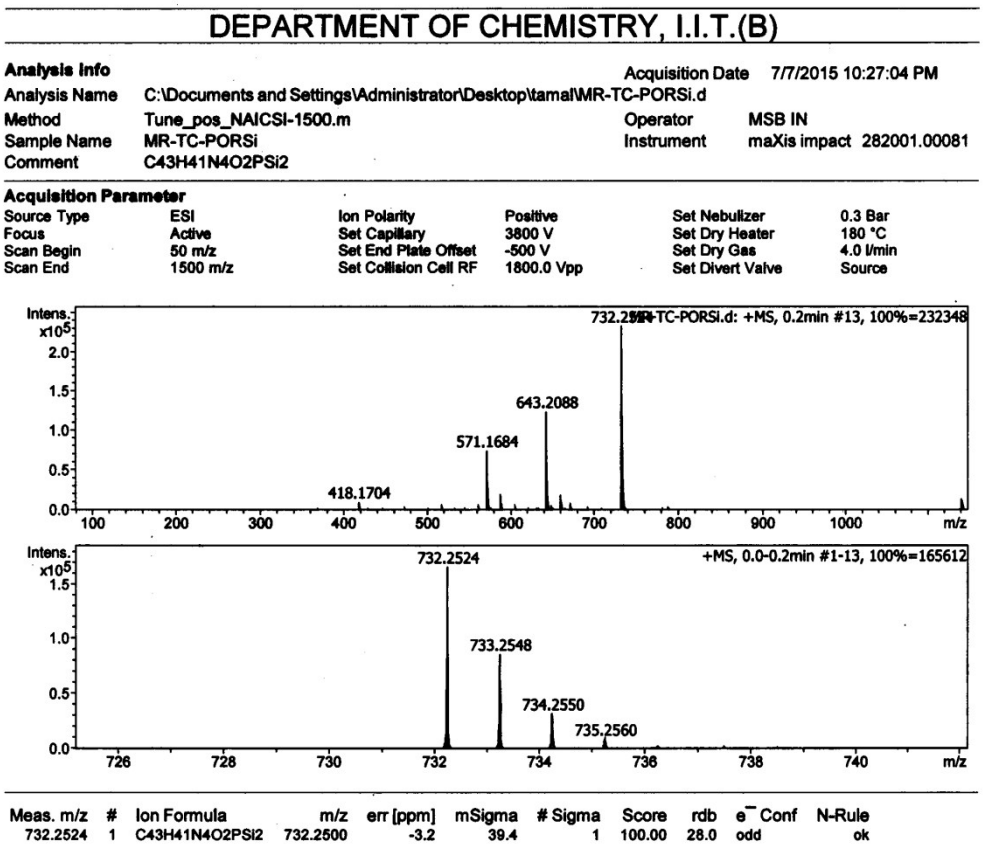
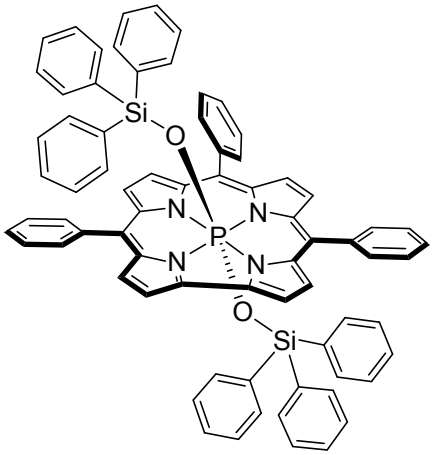


Figure S1: HR-MS mass spectrum of compound **2**.



Compound 3
Mol. Wt. = 1104.34

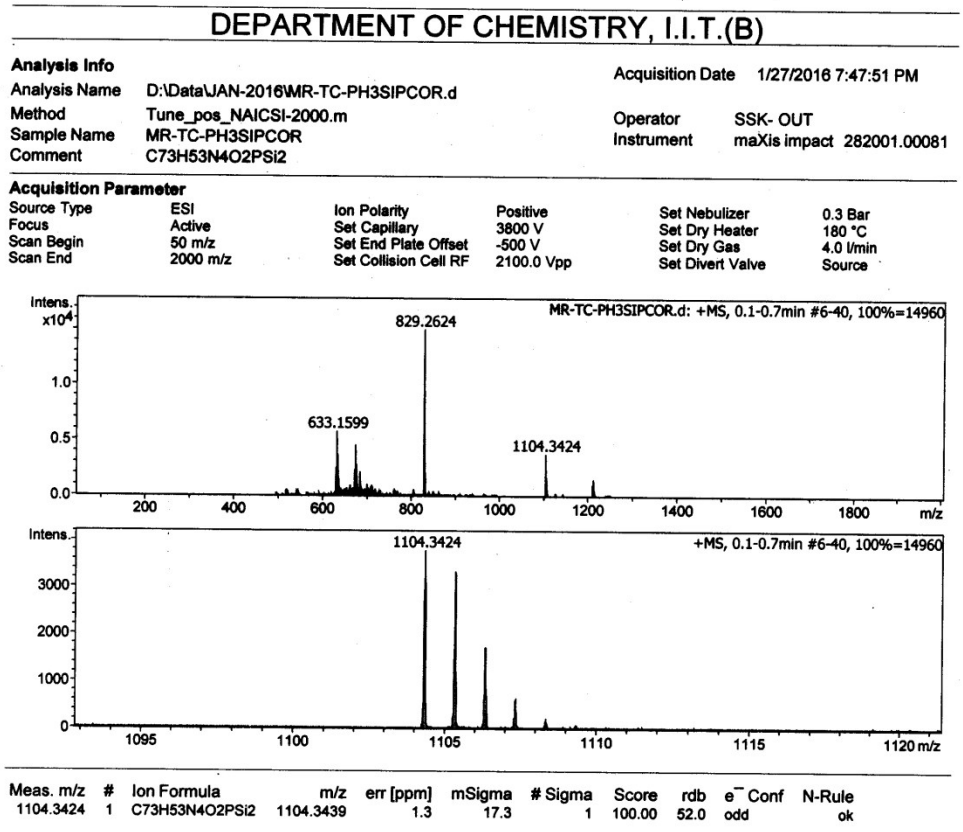
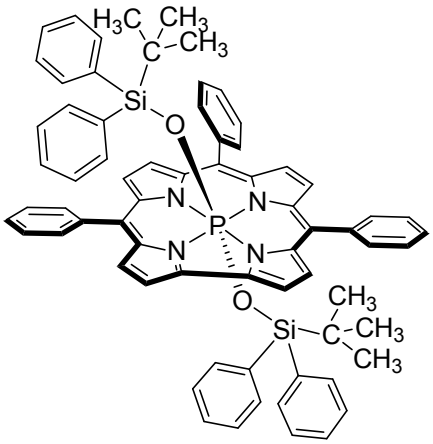


Figure S2: HR-MS mass spectrum of compound **3**.



Compound 4
Mol. Wt. = 1164.40

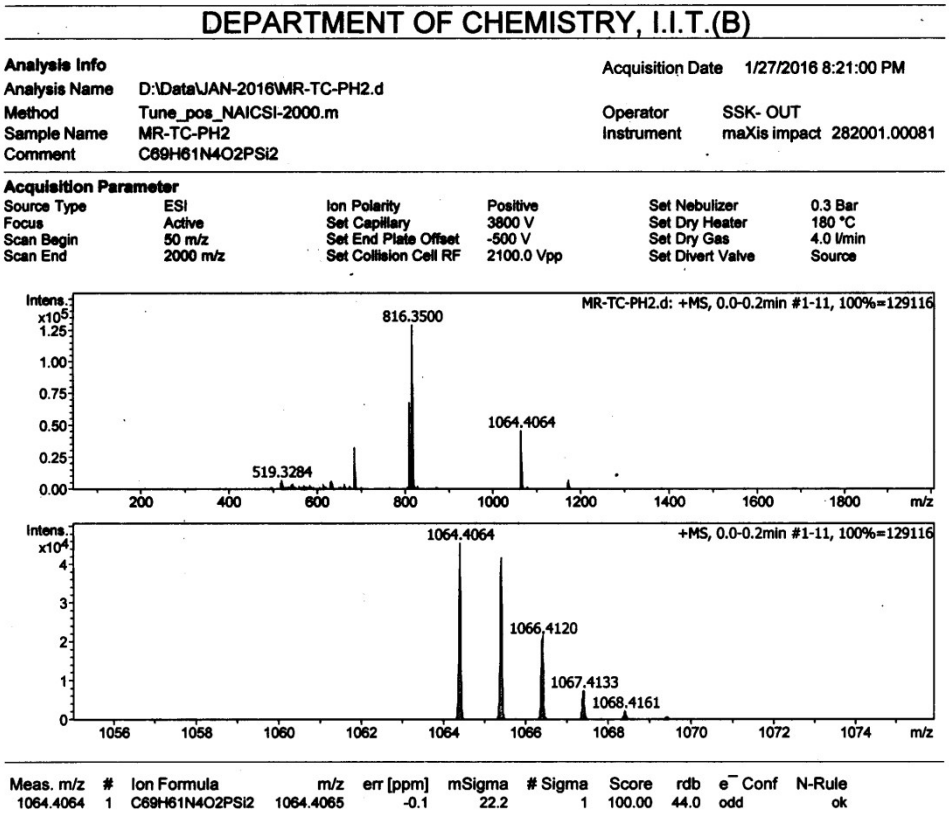
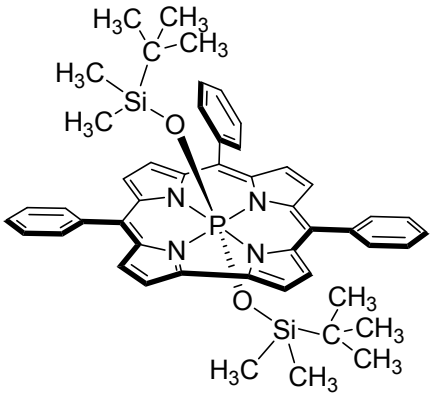


Figure S3: HR-MS mass spectrum of compound **4**.



Compound 5
Mol. Wt. = 816.34

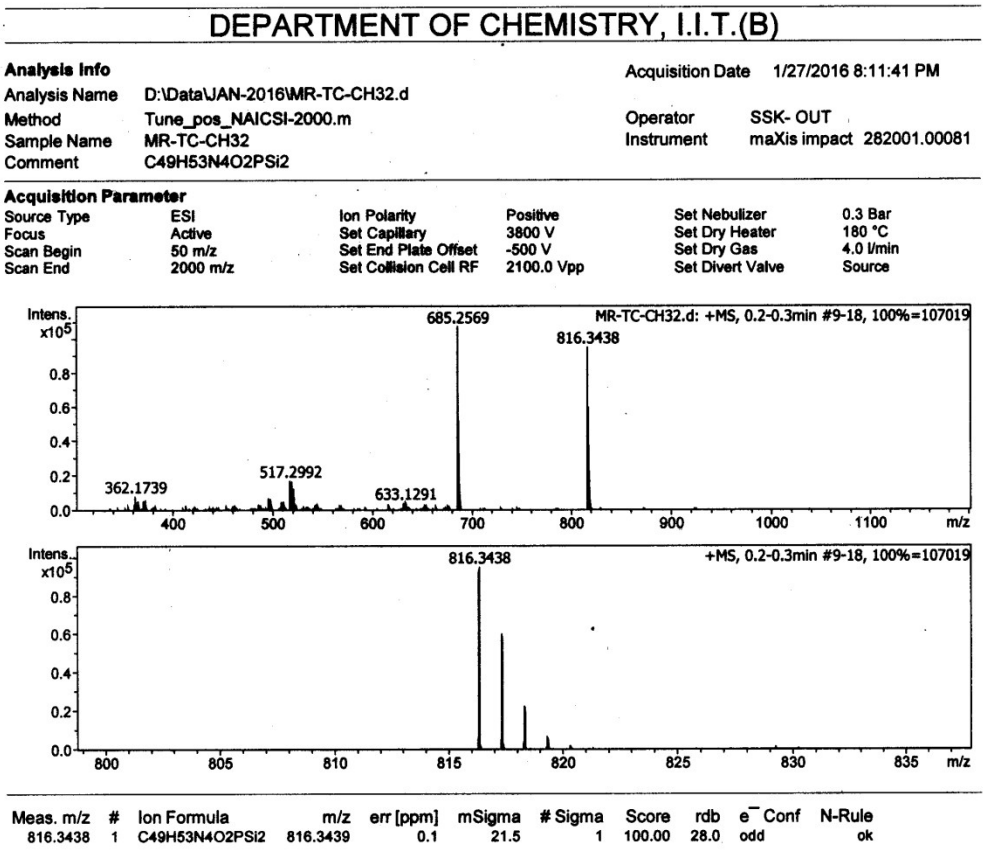


Figure S4: HR-MS mass spectrum of compound **5**.

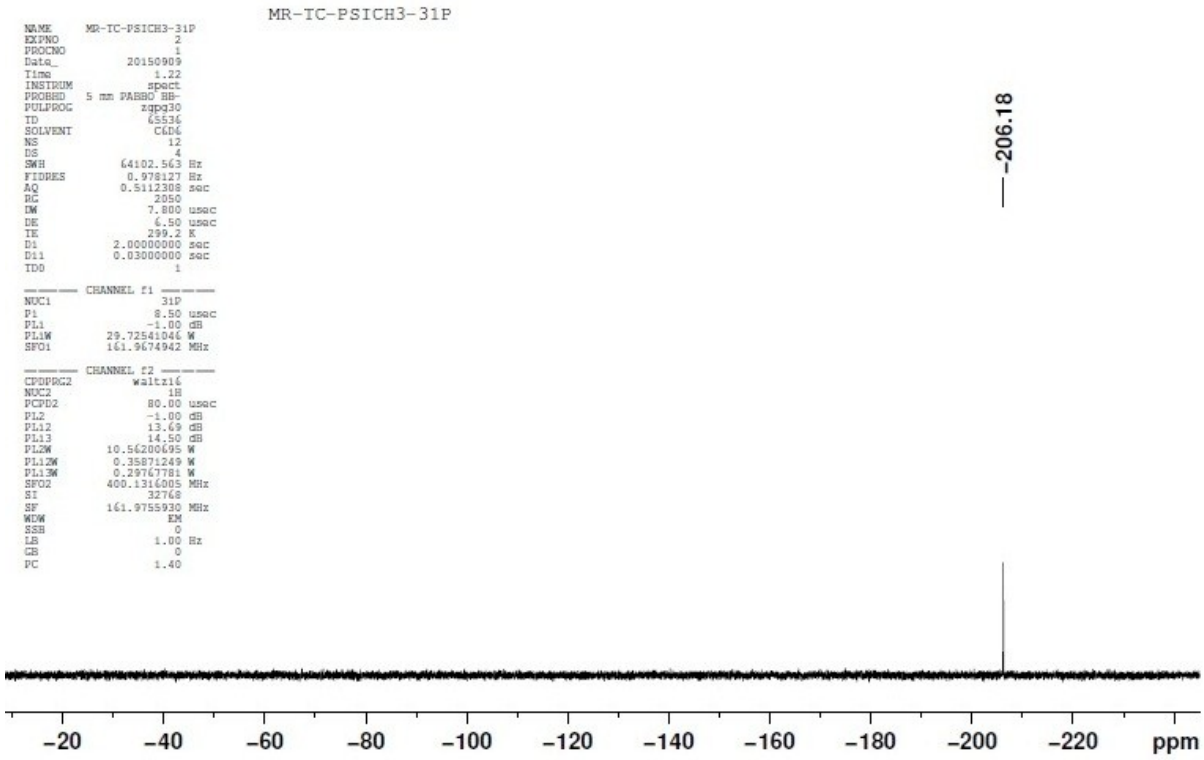


Figure S5. ^{31}P NMR spectrum of compound **2** recorded in C_6D_6 at room temperature.

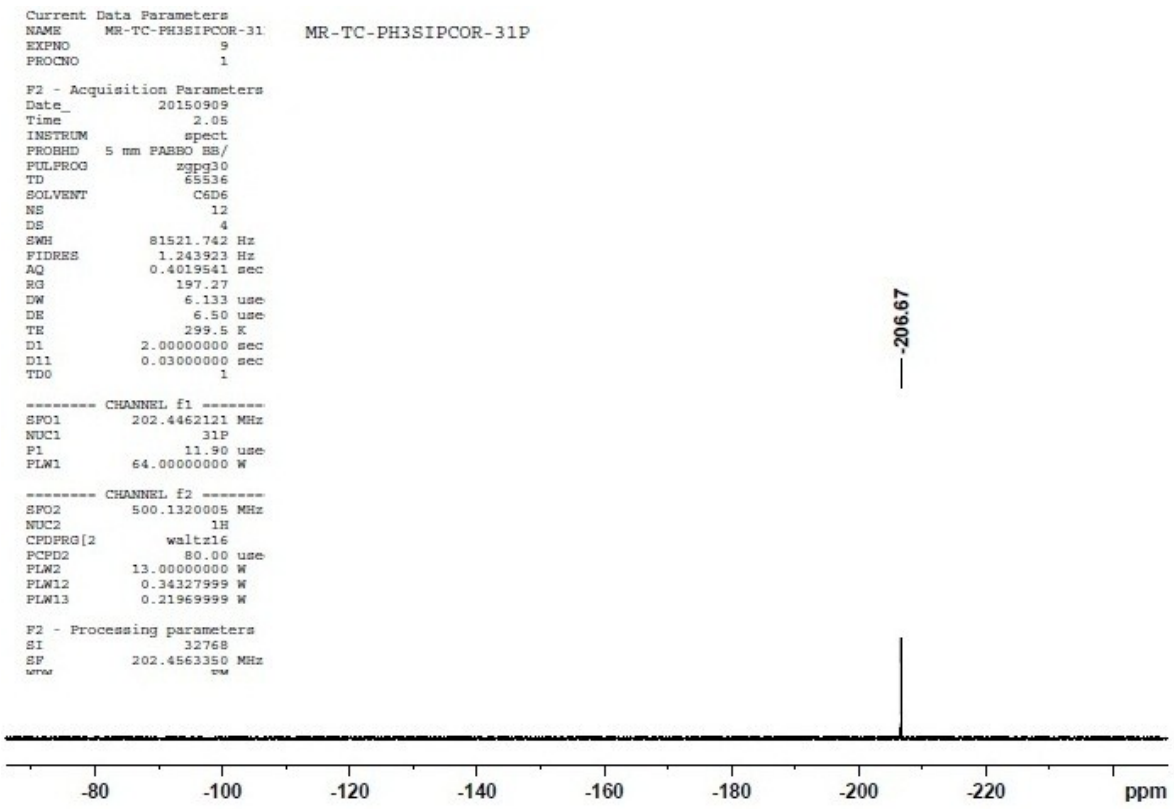


Figure S6. ^{31}P NMR spectrum of compound **3** recorded in C_6D_6 at room temperature.

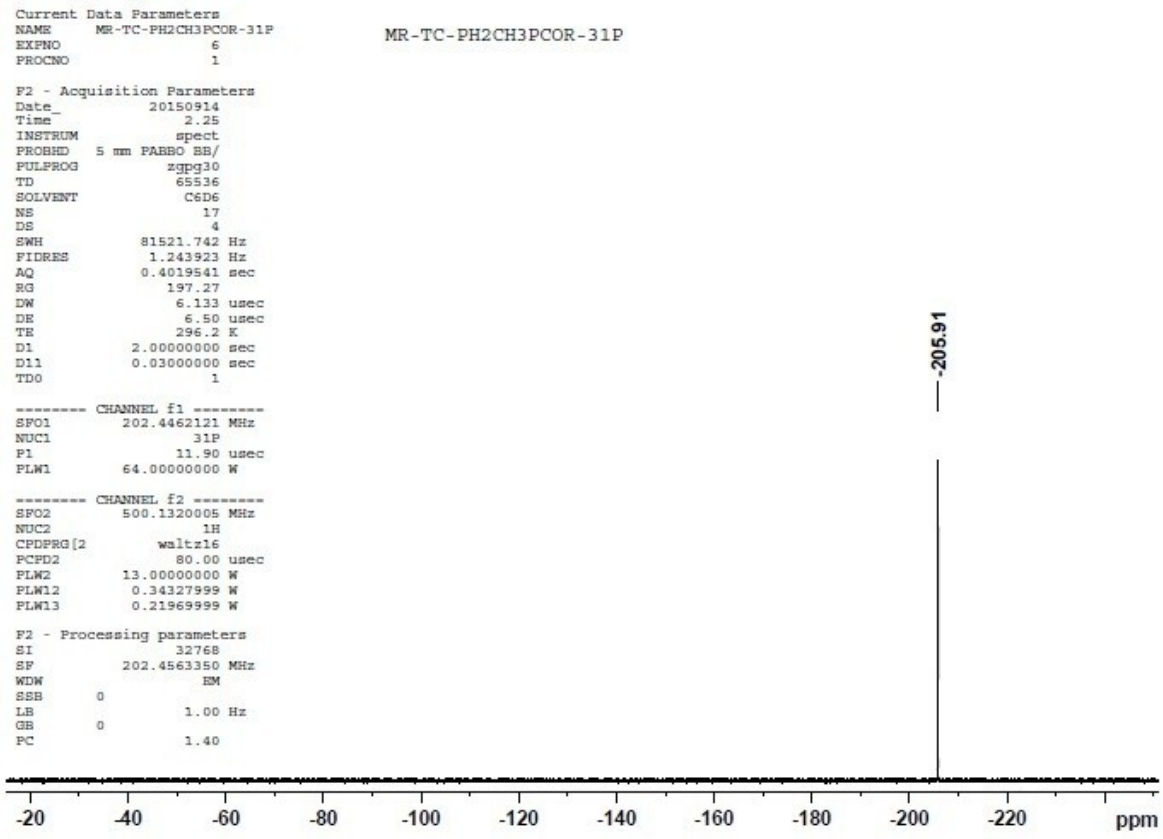


Figure S7. ^{31}P NMR spectrum of compound **4** recorded in C_6D_6 at room temperature.

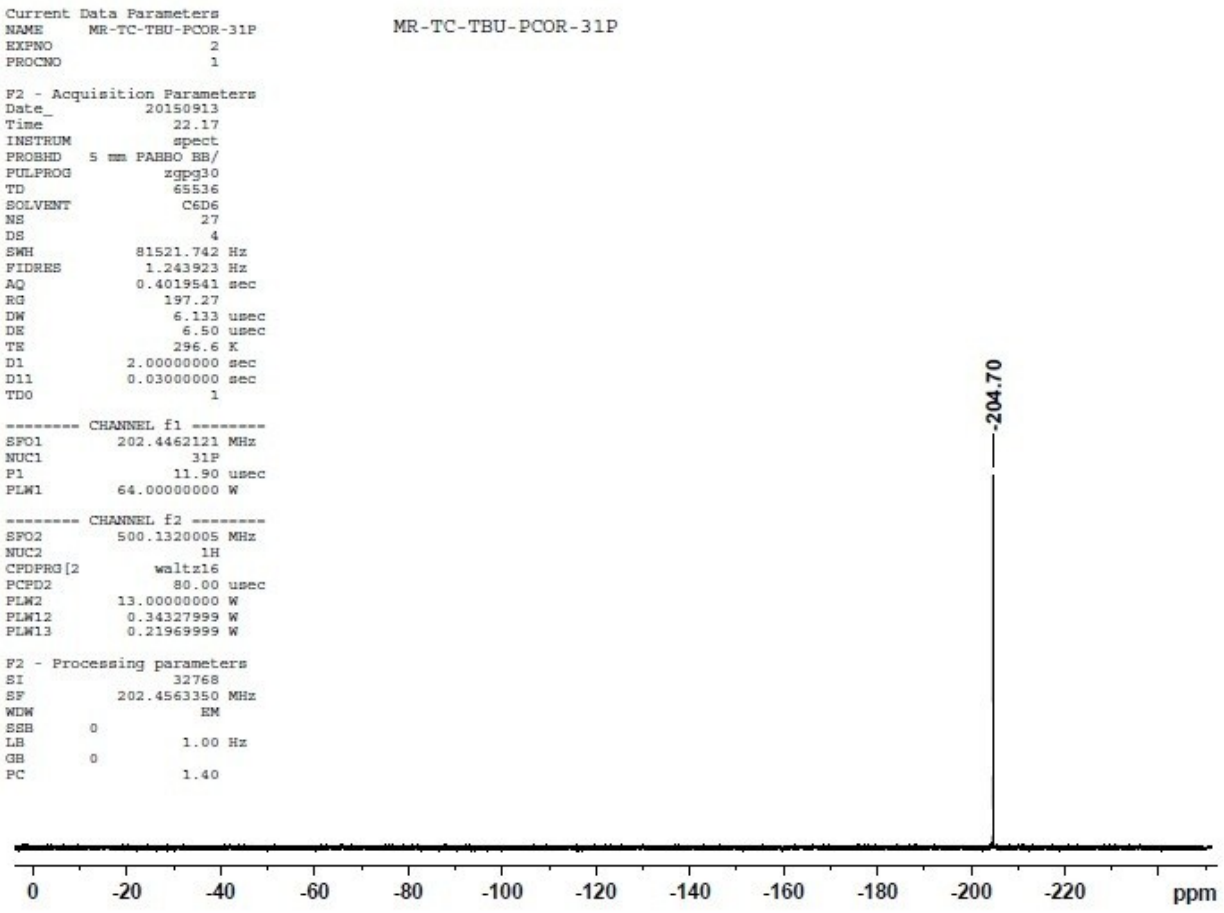


Figure S8. ^{31}P NMR spectrum of compound **5** recorded in C_6D_6 at room temperature.

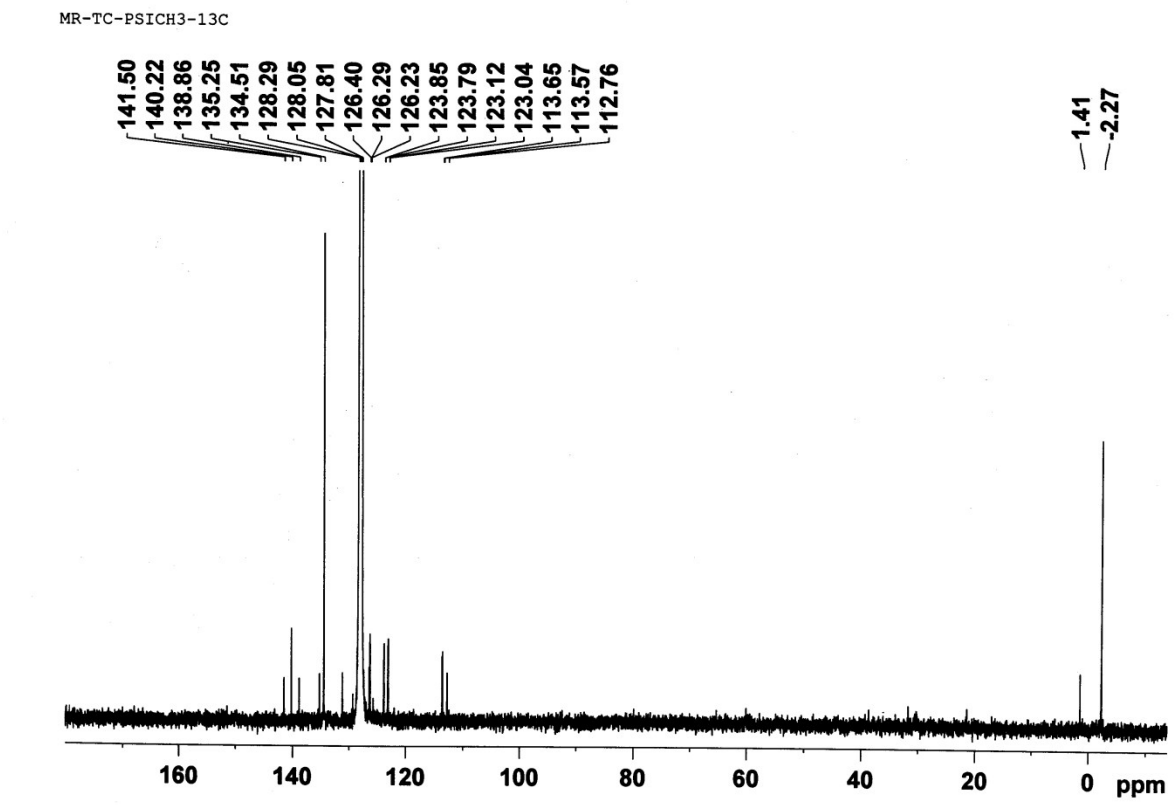


Figure S9. ^{13}C NMR spectrum of compound **2** recorded in C_6D_6 at room temperature.

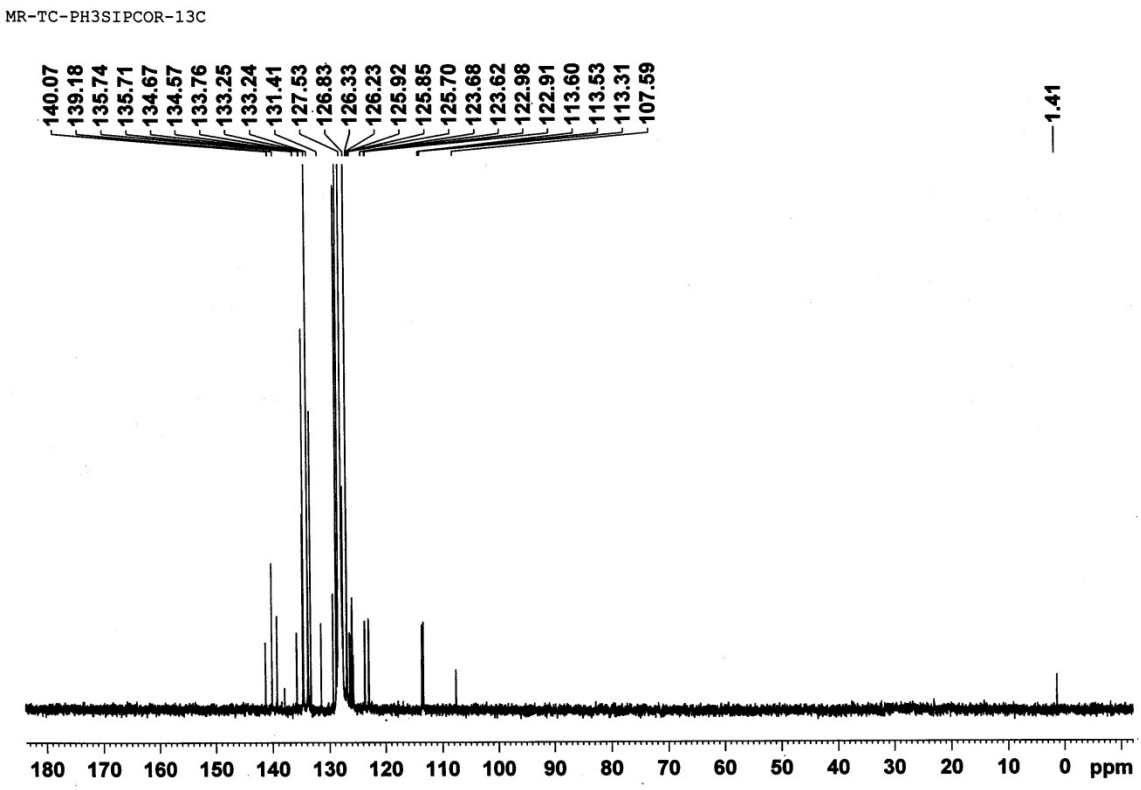


Figure S10. ^{13}C NMR spectrum of compound **3** recorded in C_6D_6 at room temperature.

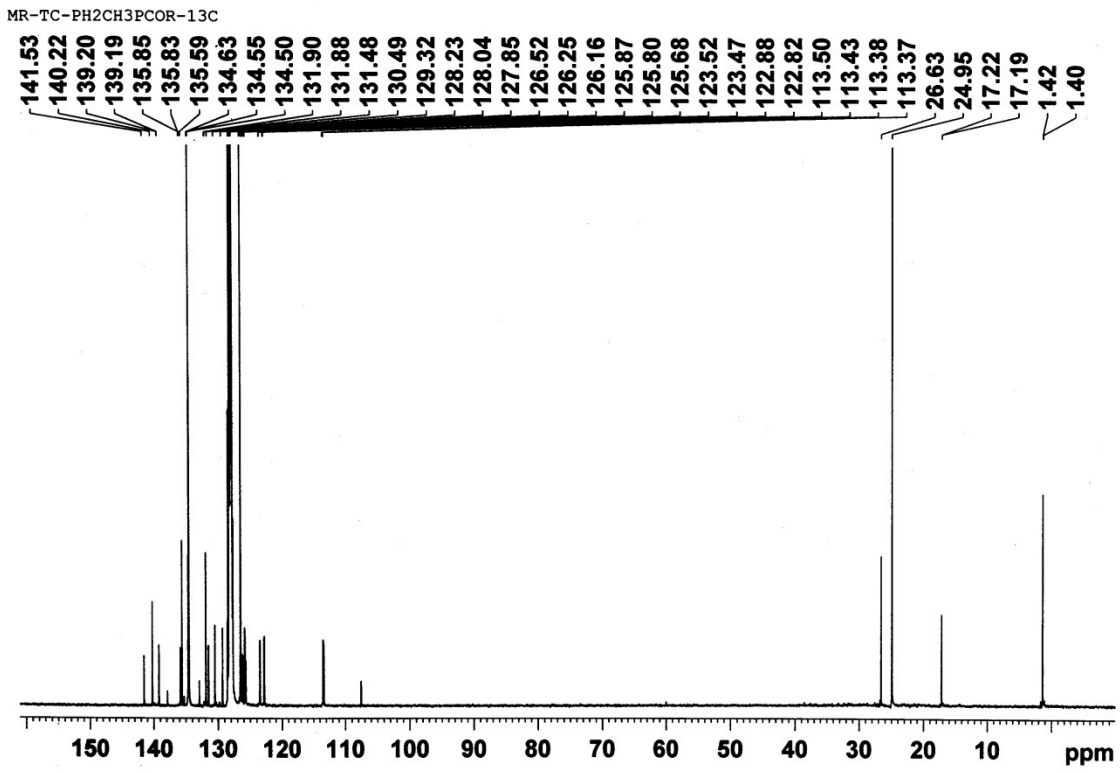


Figure S11. ^{13}C NMR spectrum of compound **4** recorded in C_6D_6 at room temperature.

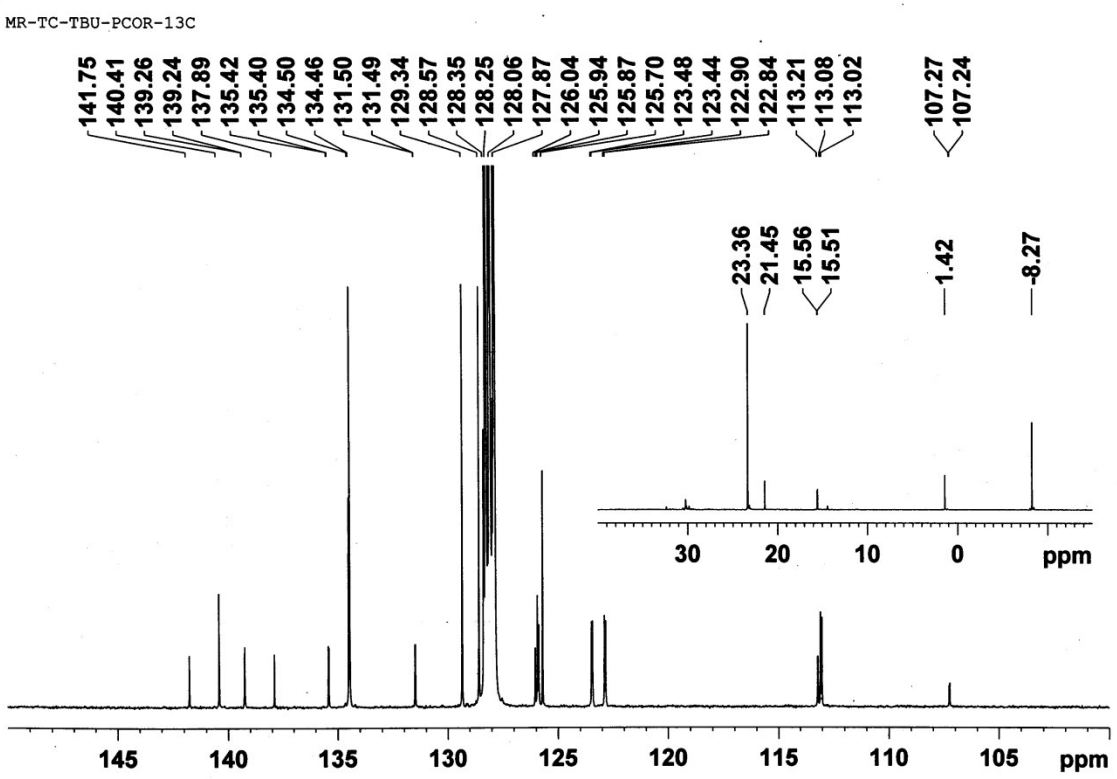


Figure S12. ^{13}C NMR spectrum of compound **5** recorded in C_6D_6 at room temperature.

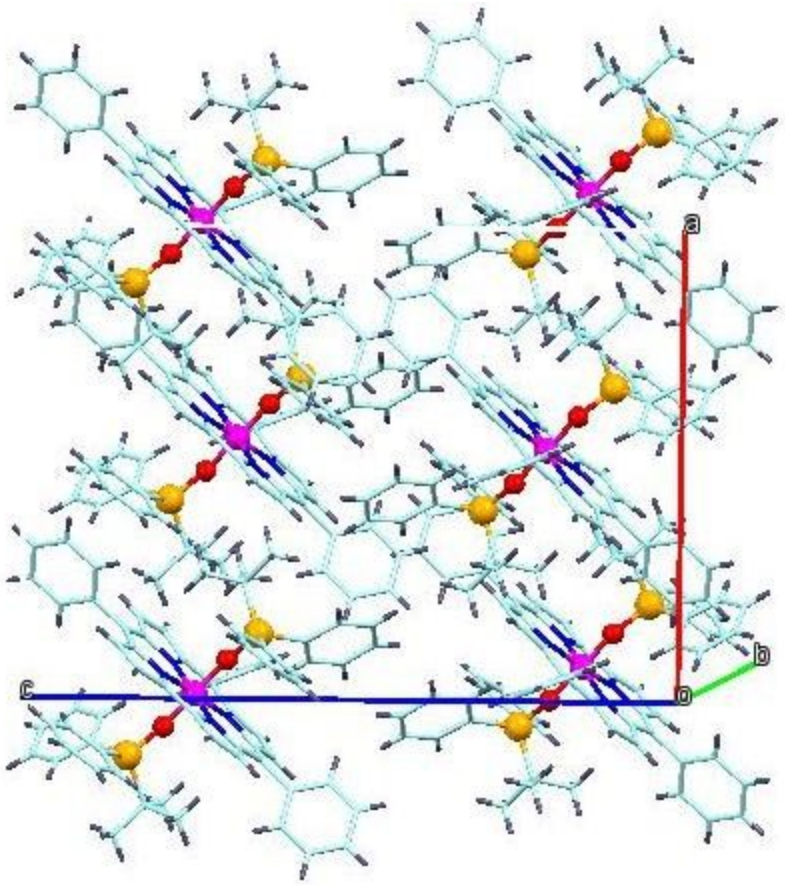


Figure S13. Unit cell packing diagram for **4** as determined from the single crystal structural analysis.