Supplementary information of

Cubane Copper(I) Iodide Clusters with Remotely Functionalized Phosphine Ligands: Synthesis, Structural Characterization and Optical Properties

Damien Bissessar [1], Thibault Thierry [1], Julien Egly [1], Valerio Giuso, [1] Thierry Achard [1], Pascal Steffanut [2], Matteo Mauro [1,*] and Stéphane Bellemin-Laponnaz [1,*]

[1] Institut de Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg-CNRS UMR7504, 23 Rue du Loess, BP 43, CEDEX 2, 67034 Strasbourg, France
[2] CLARIANT Plastics and Coatings AG, Rothausstrasse 61, 4132 Muttenz, Switzerland
* Correspondence: bellemin@unistra.fr; mauro@unistra.fr

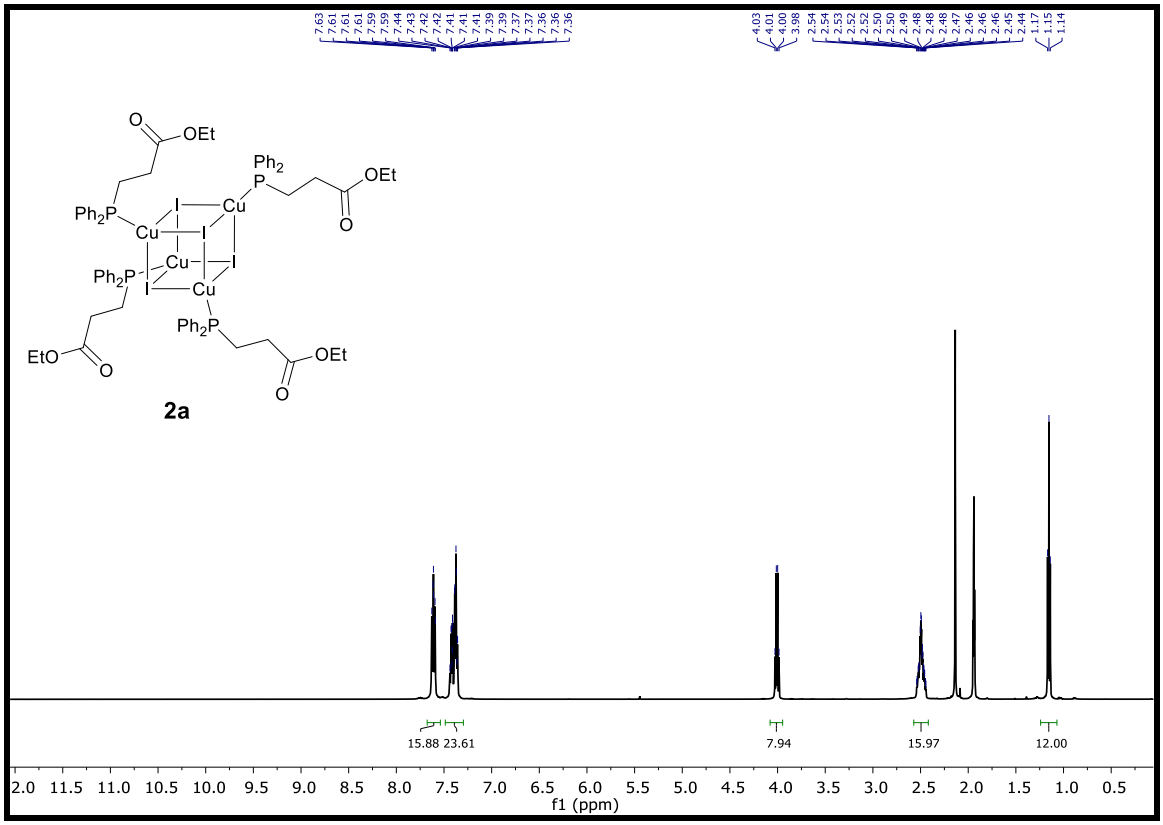
General remarks

All the manipulations of the air- and moisture-sensitive compounds were done using standard Schlenk techniques -or alternatively a dry box- under argon or nitrogen atmosphere. Solvents were purified and degassed following standard procedures or obtained from M-Braun SPS drying system. All the reagents were purchased from commercial chemical suppliers and used without further purification. ^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectra were recorded on a Bruker AVANCE 300 or Bruker AVANCE 500 spectrometer (Bruker, Wissembourg, France) using the residual solvent peak as a reference ($CDCl_3$: δ_H = 7.26 ppm; δ_C = 77.16 ppm) at 295 K. Positive mode electrospray ionization mass spectra (ESI-HRMS) analyses were carried out on a microTOF Bruker Daltonics (Bruker, Wissembourg, France).

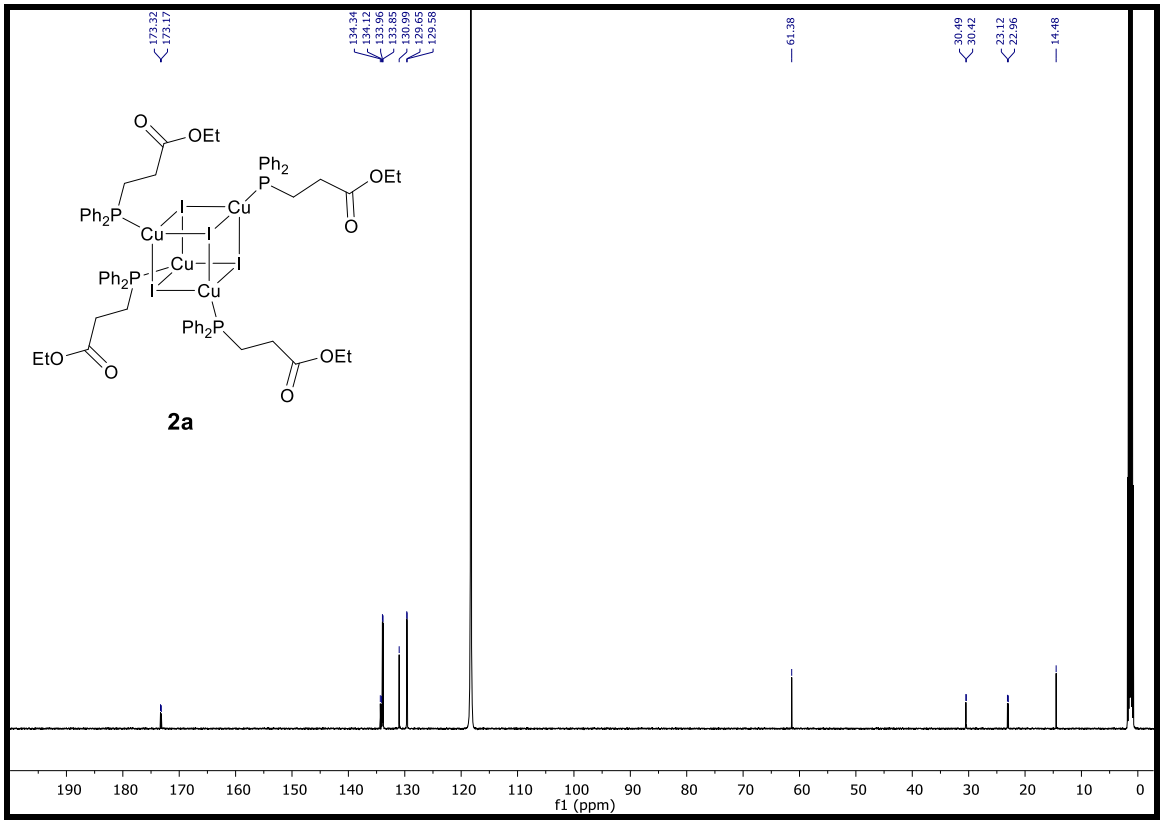
Steady-state emission spectra were recorded on a Horiba Jobin−Yvon IBH FL-322 Fluorolog 3 spectrometer equipped with a 450 W xenon arc lamp, double-grating excitation, and emission monochromators (2.1 nm mm^{-1} of dispersion; 1200 grooves mm^{-1}) and a Hamamatsu R13456 red sensitive Peltier-cooled PMT detector. Emission and excitation spectra were corrected for source intensity (lamp and grating) and emission spectral response (detector and grating) by standard correction curves. Time-resolved measurements were performed using the time-correlated single-photon counting (TCSPC) electronics option of the TimeHarp 260 board installed on a PicoQuant FluoTime 300 fluorimeter (PicoQuant GmbH, Germany), equipped with a PDL 820 laser pulse driver. A pulsed laser diode LDH-P-C-375 (λ = 375 nm, pulse full width at half maximum FWHM <50 ps, repetition rate 200 kHz–40 MHz) was used to excite the sample and mounted directly on the sample chamber at 90°. The photons were collected by a PMA Hybrid-07 single photon counting detector. The data were acquired by using the commercially available software EasyTau II (PicoQuant GmbH, Germany), while data analysis was performed using the built-in software FluoFit (PicoQuant GmbH, Germany).

For time resolved measurements, data fitting was performed by employing the maximum likelihood estimation (MLE) methods and the quality of the fit was assessed by inspection of the reduced χ^2 function and of the weighted residuals. The absolute photoluminescence quantum yields (PLQY) were measured on a Hamamatsu Quantaurus-QY C11347-11 integrating sphere in air-equilibrated condition using an empty quartz tube as the reference upon excitation at λ_{exc} = 320 nm.

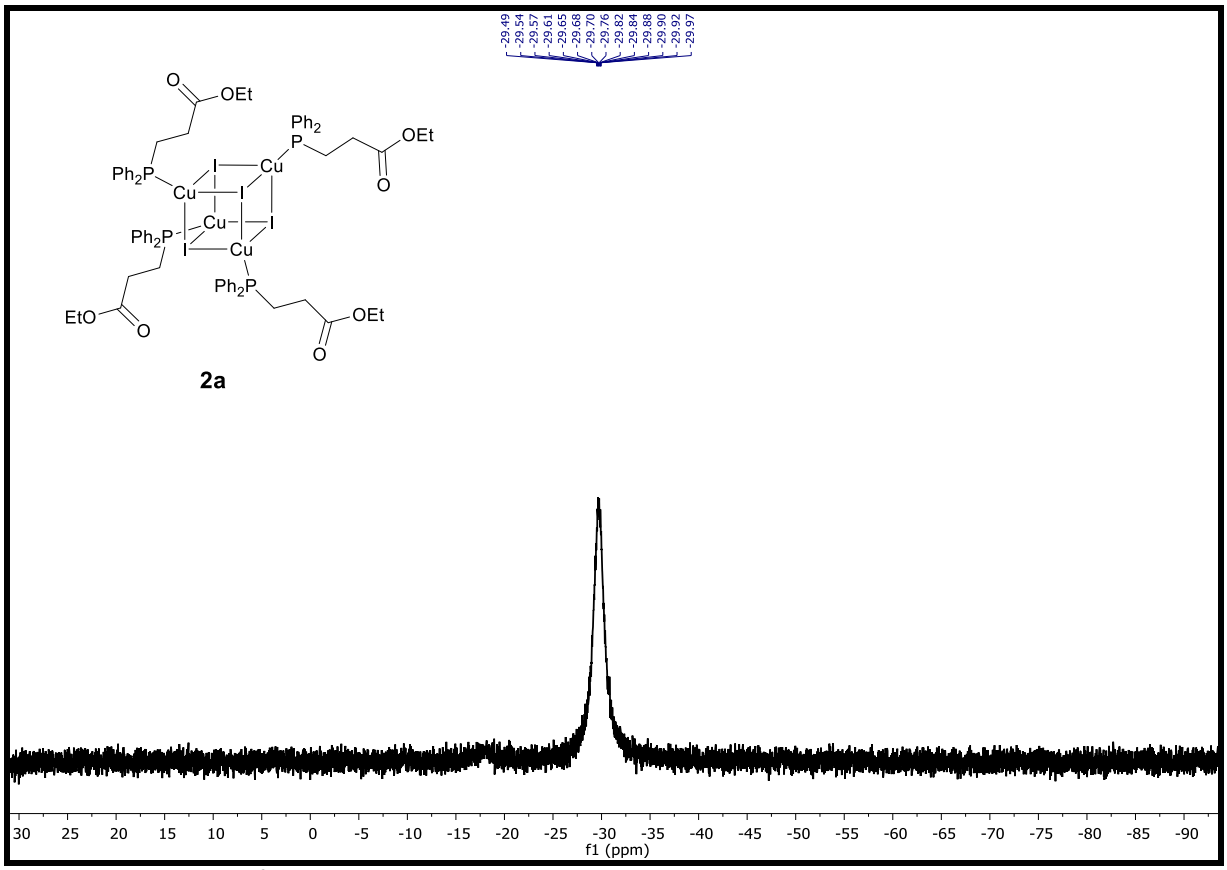
NMR spectra



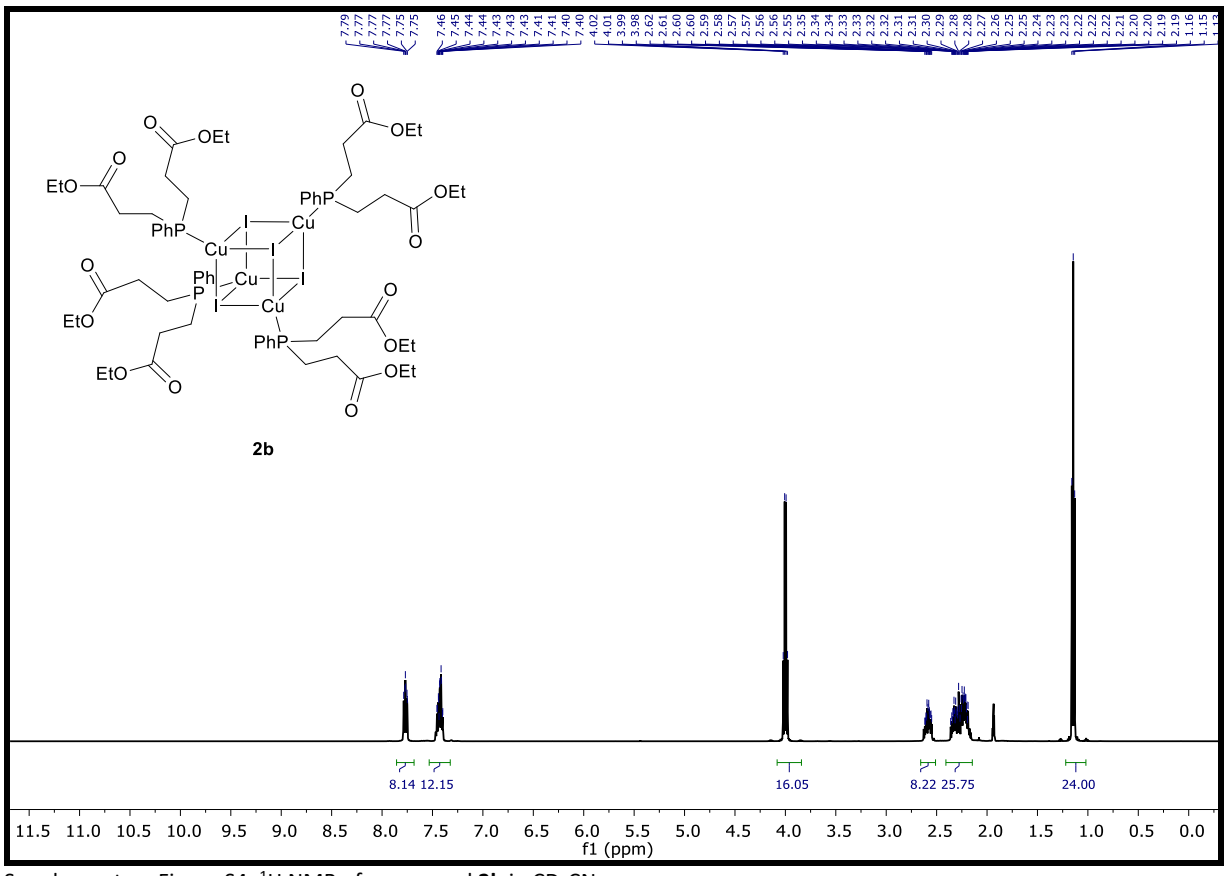
Supplementary Figure S1. ^{1}H NMR of compound **2a** in CD_3CN.



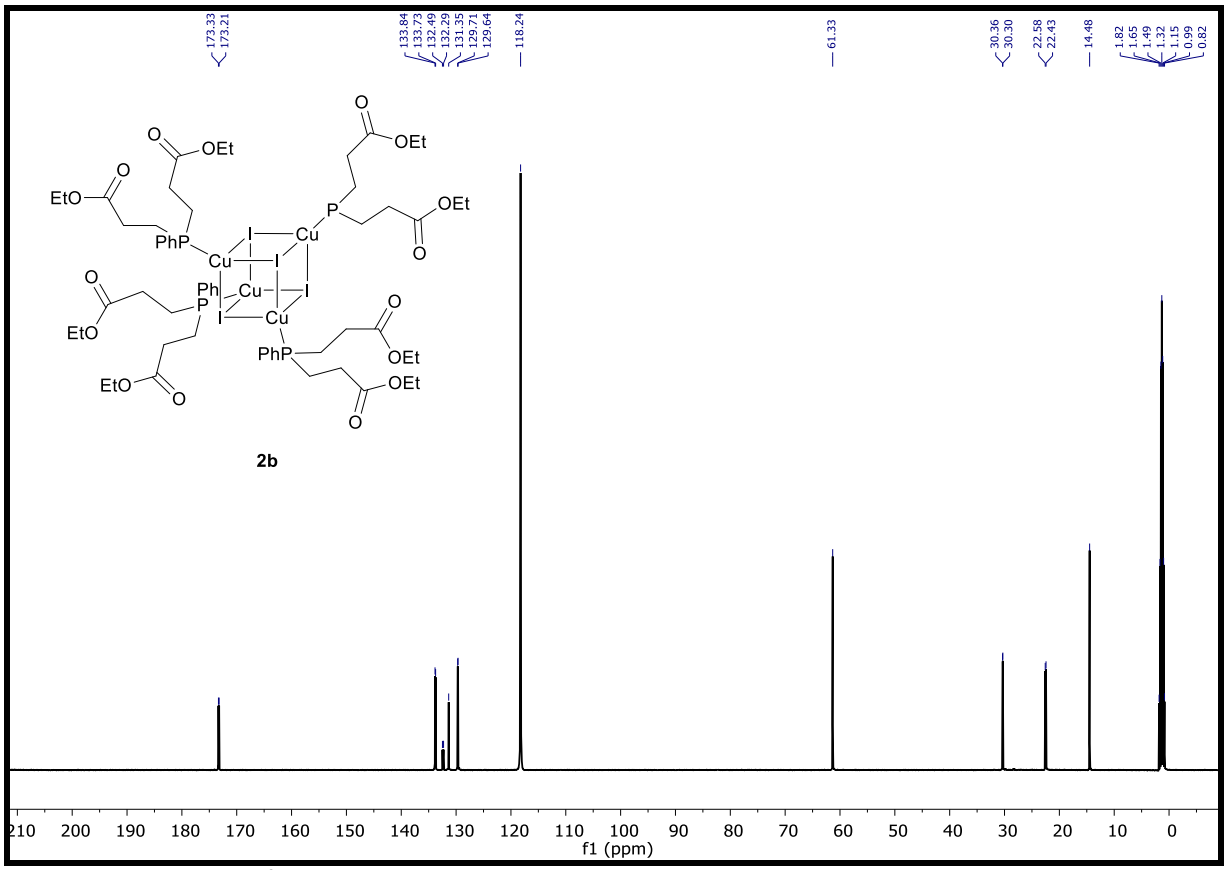
Supplementary Figure S2. ^{13}C NMR of compound **2a** in CD_3CN.



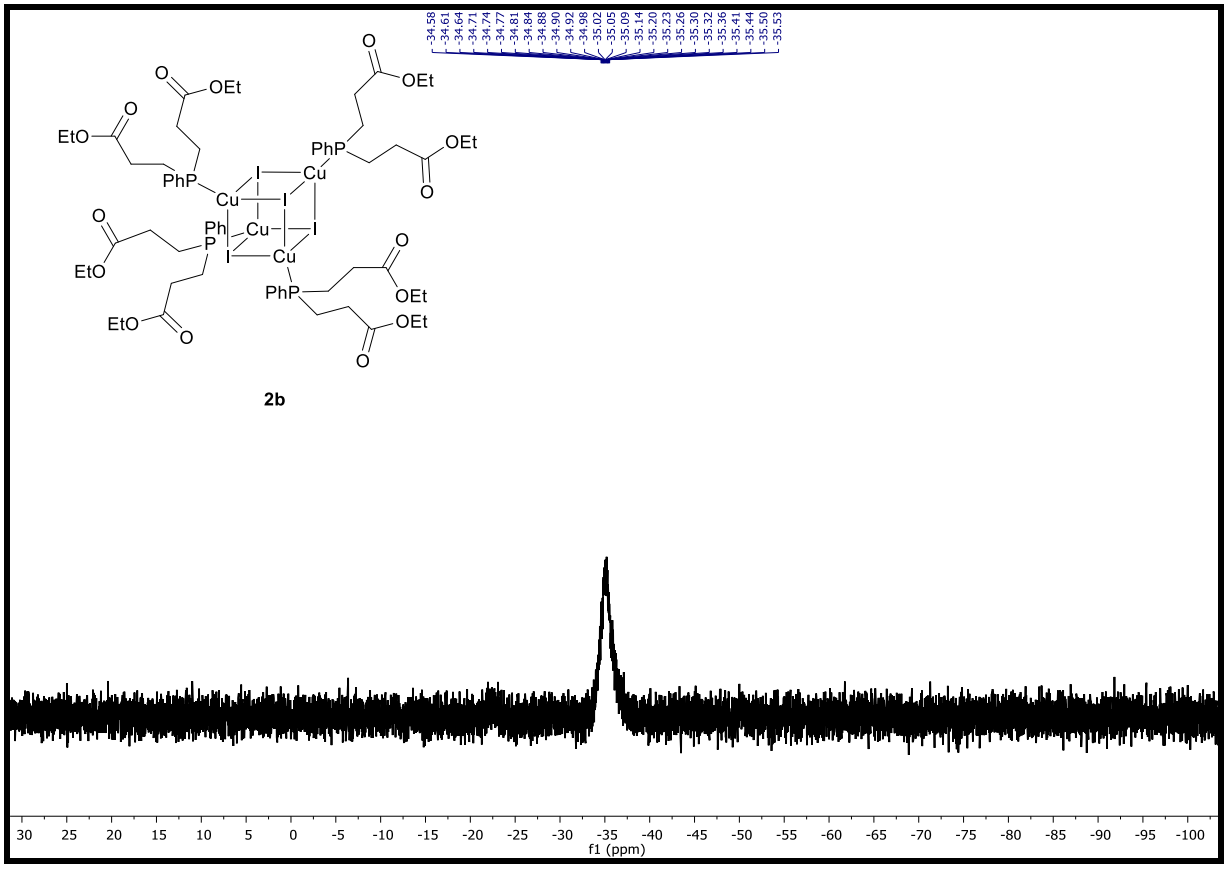
Supplementary Figure S3. ^{31}P NMR of compound **2a** in CD_3CN.



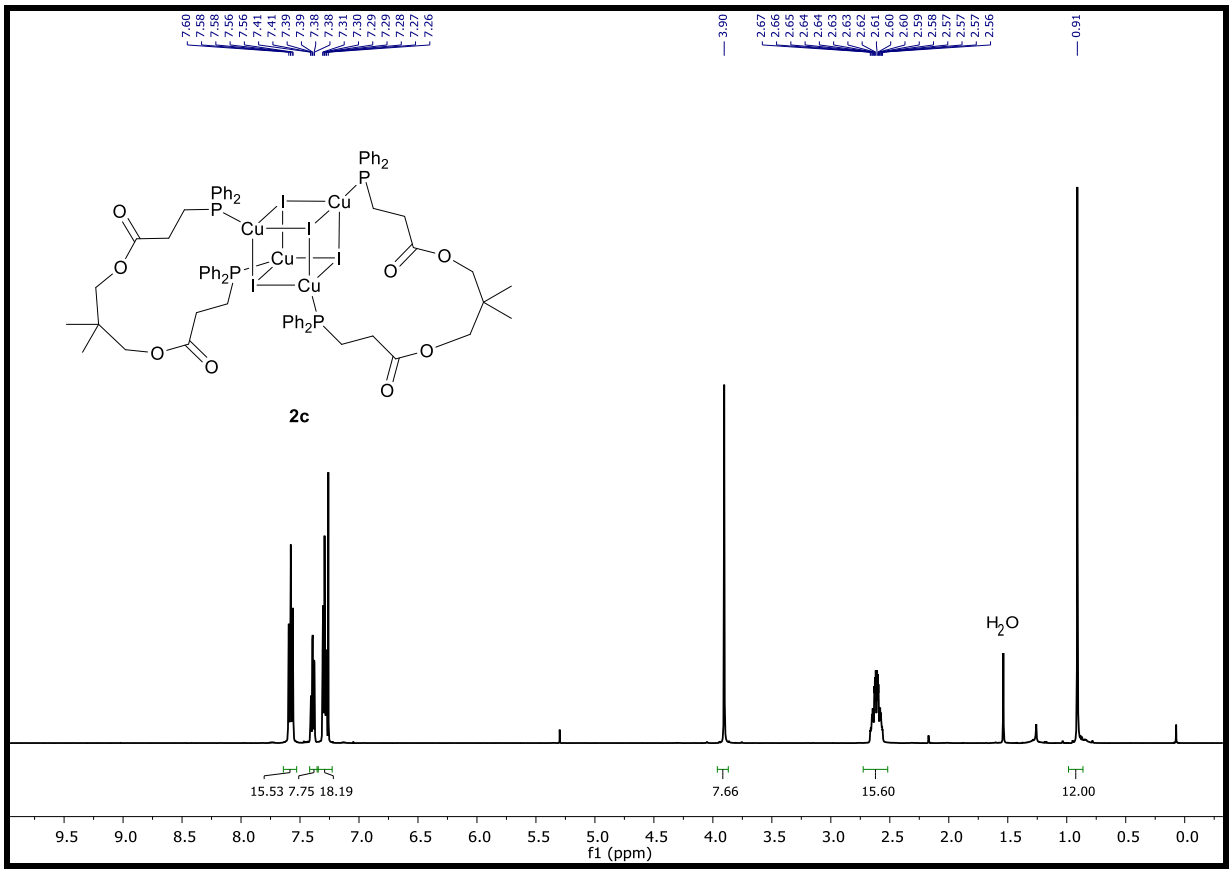
Supplementary Figure S4. ^{1}H NMR of compound **2b** in CD_3CN.



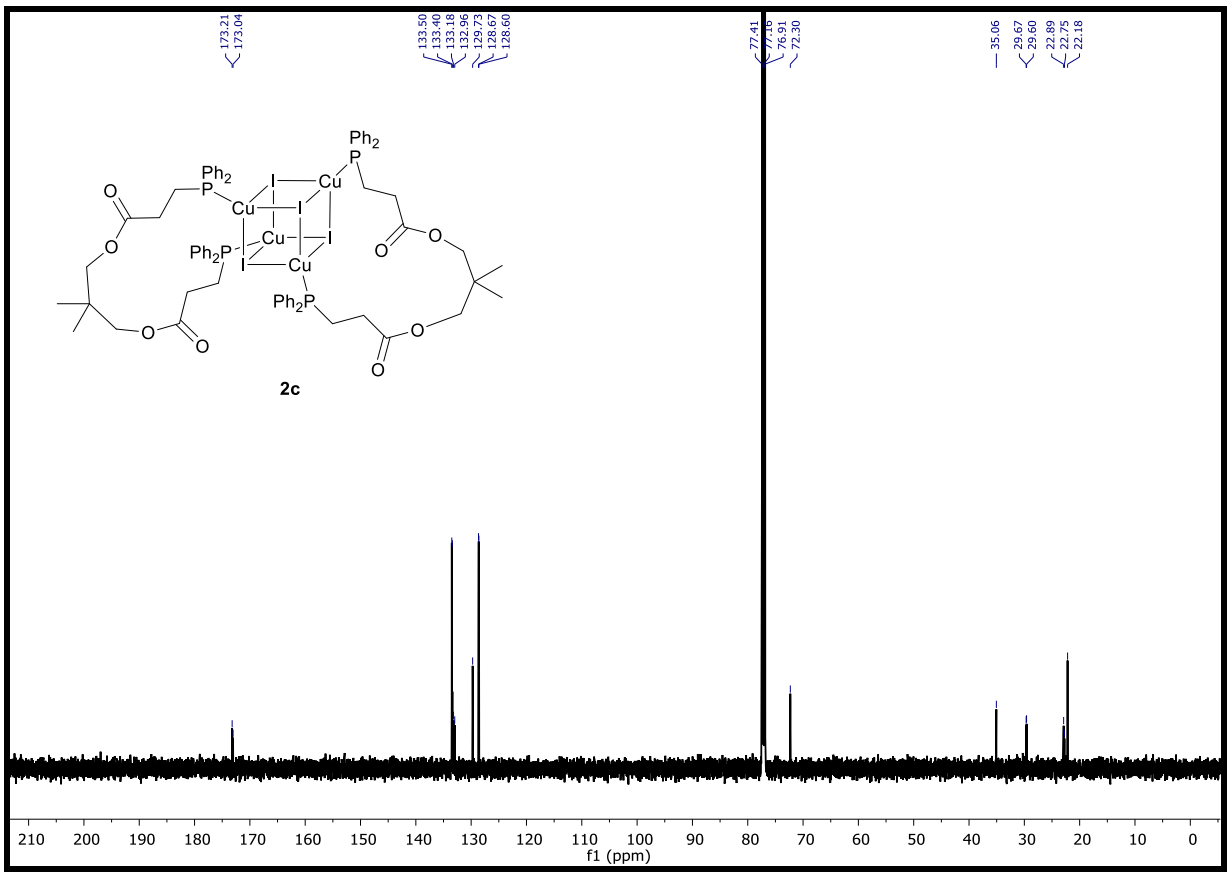
Supplementary Figure S5. ^{13}C NMR of compound **2b** in CD_3CN.



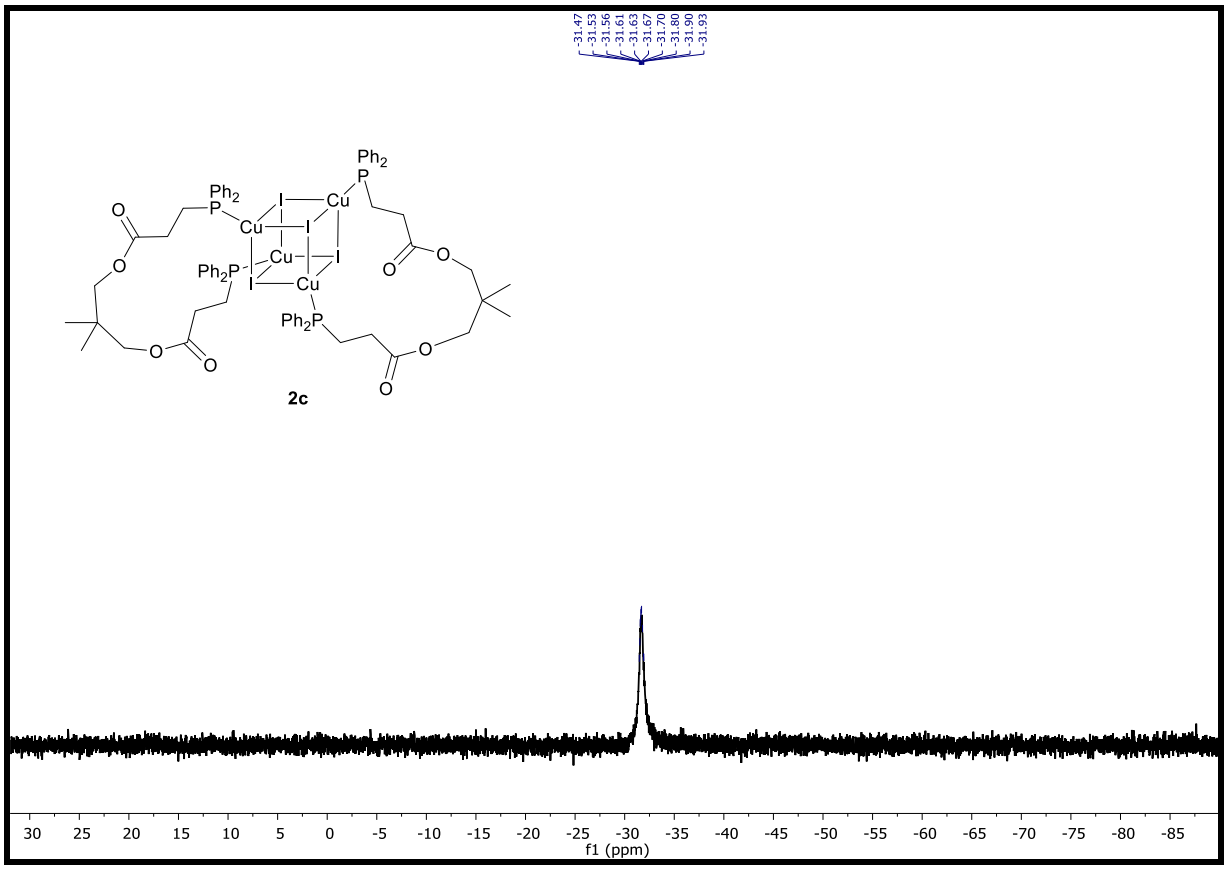
Supplementary Figure S6. ^{31}P NMR of compound **2b** in CD_3CN.



Supplementary Figure S7. ^{1}H NMR of compound **2c** in $CDCl_3$.

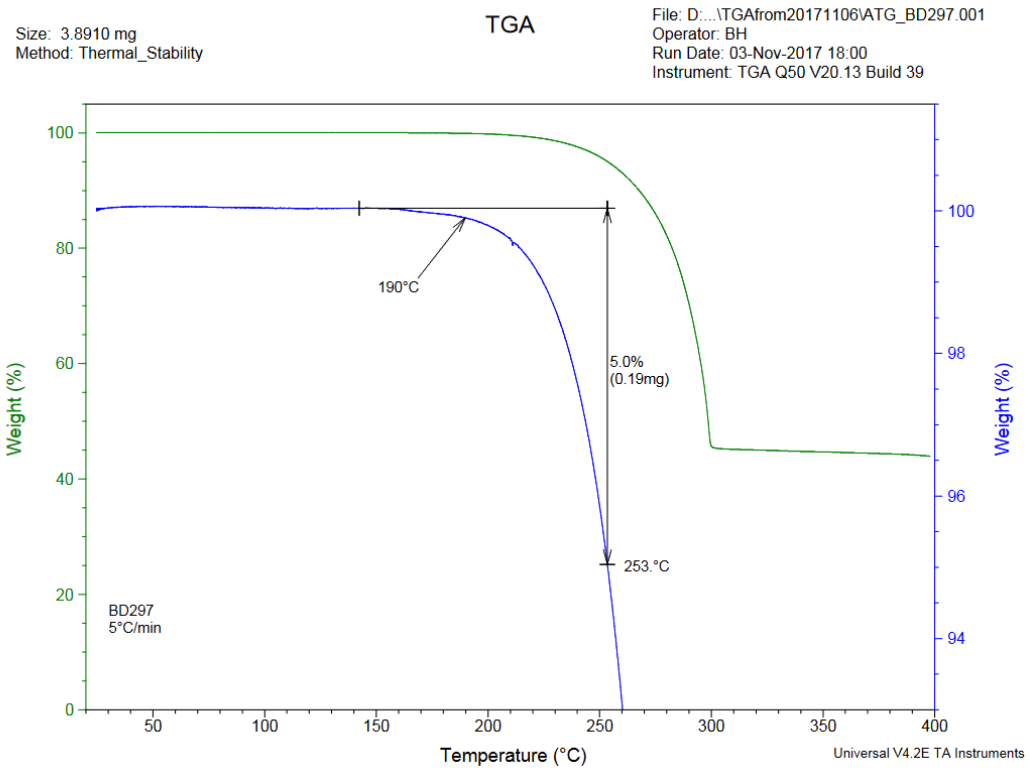


Supplementary Figure S8. ^{13}C NMR of compound **2c** in $CDCl_3$.

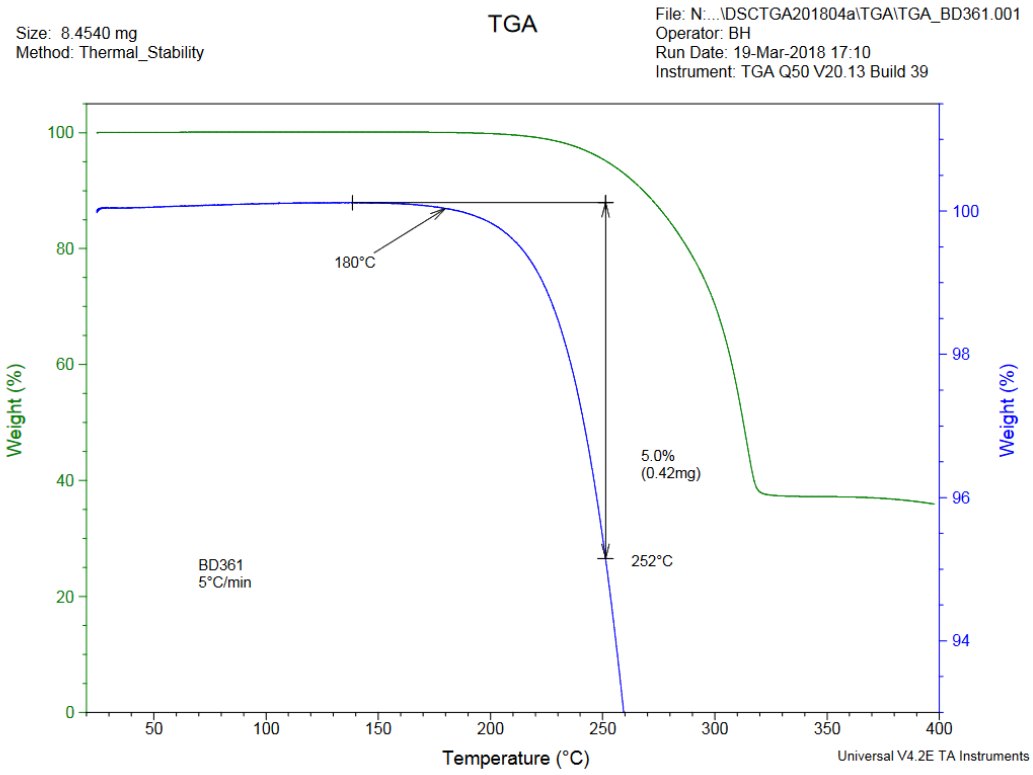


Supplementary Figure S9. ^{31}P NMR of compound **2c** in $CDCl_3$.

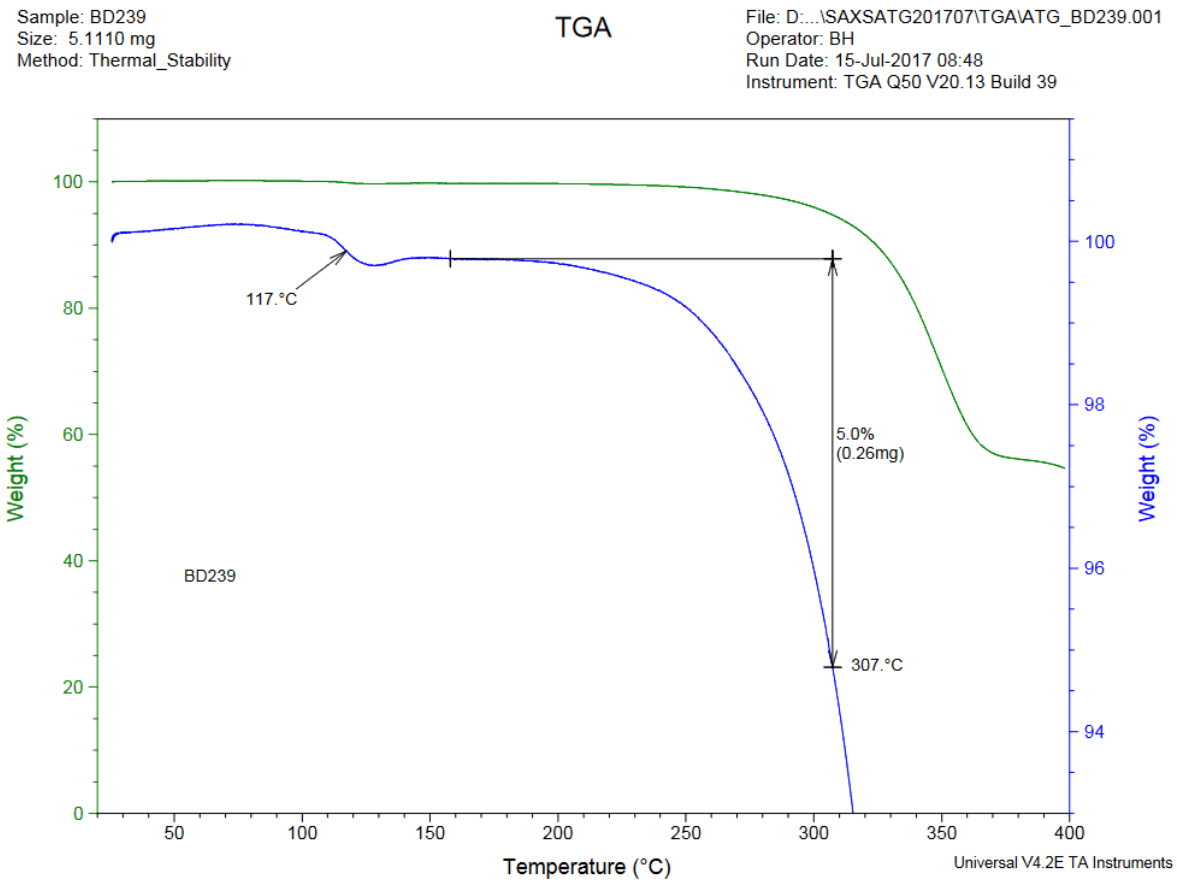
TGA analysis



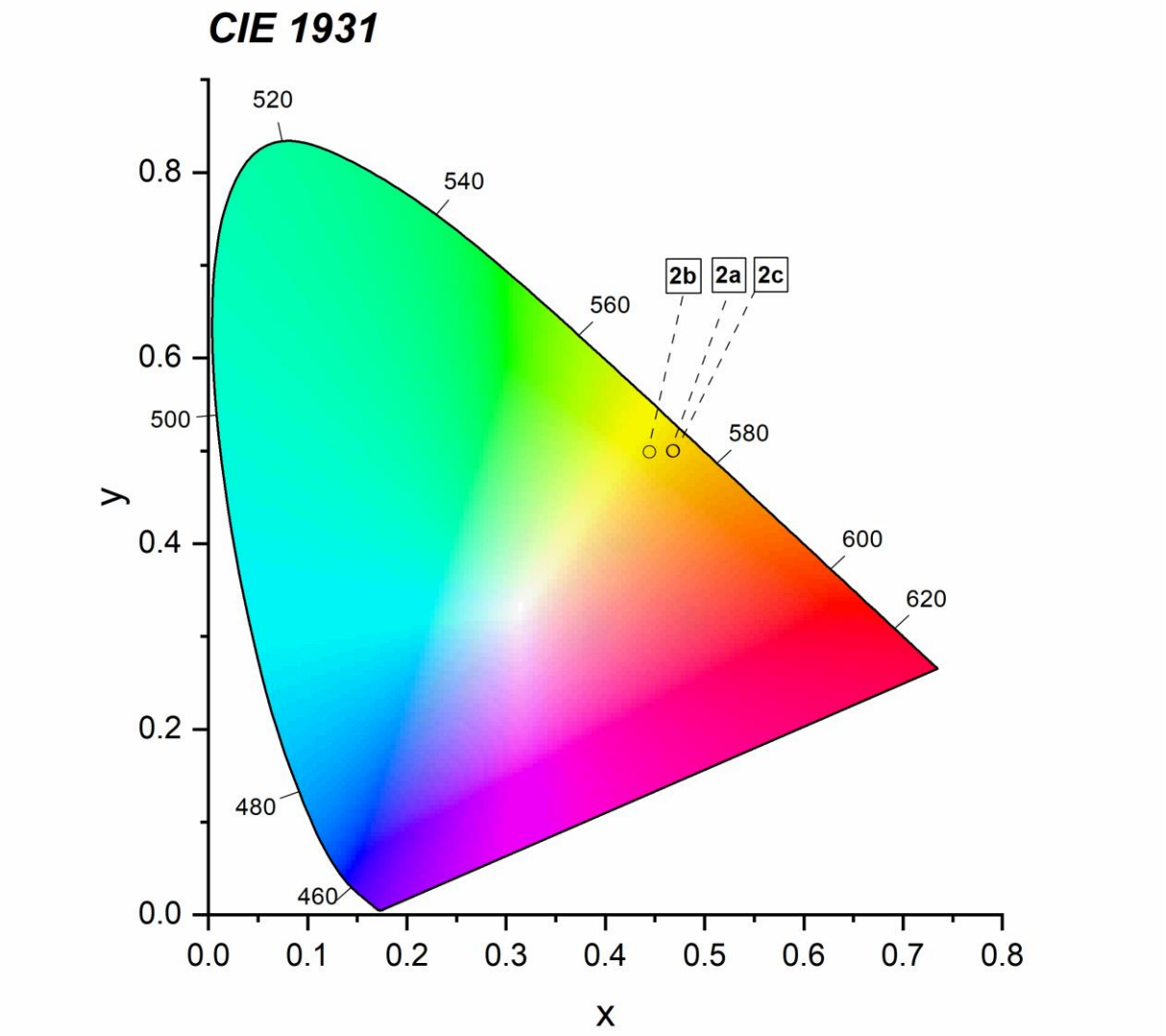
Supplementary Figure S10. TGA of compound **2a**



Supplementary Figure S11. TGA of compound **2b**



Supplementary Figure 12. TGA of compound **2c**



Supplementary Figure S13. CIE coordinates for compound **2a**-**2c.**