Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

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New Red-Emitting Schiff Base Chelates: Promising Molecular Thermometers for Sensing and Imaging via Phosphorescence Decay Time

Sergey M. Borisov,*[1] Reinhold Pommer,[1] Jan Svec,[2] Sven Peters,[3] Veronika Novakova,[2] Ingo Klimant[1]

[1] Institute of Analytical Chemistry and Food Chemistry, Graz University of Technology, Stremayrgasse 9, 8010, Graz, Austria. E-mai: sergey.borisov@tugraz.at

[2] Department of Pharmaceutical Chemistry and Pharmaceutical Analysis, Faculty of Pharmacy in Hradec Kralove, Charles University, Akademika Heyrovskeho 1203, Hradec Kralove, Czech Republic

[3] Department of Ophthalmology, University Hospital Jena, Jena, Germany

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*Attempted synthesis of (4E,5E)-4,5-bis(4-(dibutylamino)-2-hydroxybenzylideneamino)benzene-1,2-dinitrile (**1**)*

4-(dibutylamino)-2-hydroxybenzaldehyde (70.1 mg, 0.28 mmol, 3.4 eq.) and 4,5-diaminobenzene-1,2-dinitrile (13 mg, 0.082 mmol, 1 eq.) were dissolved in 5 mL of anhydrous ethanol and the dispersion was deoxygenated with argon in a Schlenk flask. The solution was heated to 50 °C and 12 μL of methanesulfonic acid (18 mg, 0.19 mmol, 2.3 eq.) were added as a catalyst. A brown precipitate was formed after 90 min, the reaction was stopped and the product was precipitated in methanol. The precipitate was washed several times with cyclohexane to remove the excess of the aldehyde. The monosubstituted product, (E)-4-(4-(dibutylamino)-2-hydroxybenzylideneamino)-5-aminobenzene-1,2-dinitrile was isolated as a yellow solid.

Yield: 30 mg (93 %). UV-Vis (toluene), $\lambda_{max}/\varepsilon$ (nm/$M^{-1}cm^{-1}$): 381/41100.

^{1}H-NMR: (300 MHz, DMSO-d6): 8.30 (s, 1H), 7.89 (s, 1H), 7.9 – 7.75 (m, 3H), 6.46 (s, 1H), 6.25 (s, 1H), 3.44 – 3.19 (m, 4H), 2.39 (s, 2H), 1.53 (d, 4H), 1.36 (d, 4H), 0.94 (t, 6H).

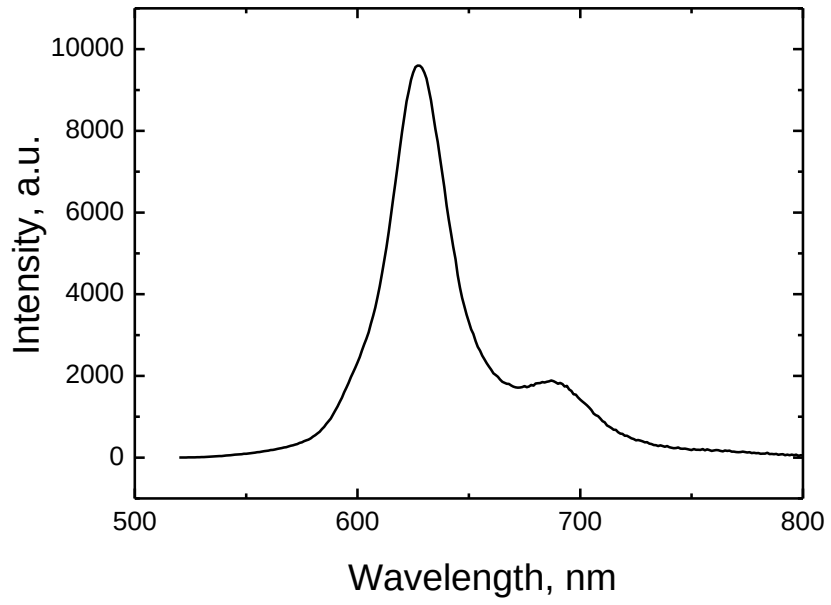

Figure S1. Emission spectrum of **Pt-1** in anoxic toluene at 20 °C. λ_{exc} = 502 nm.

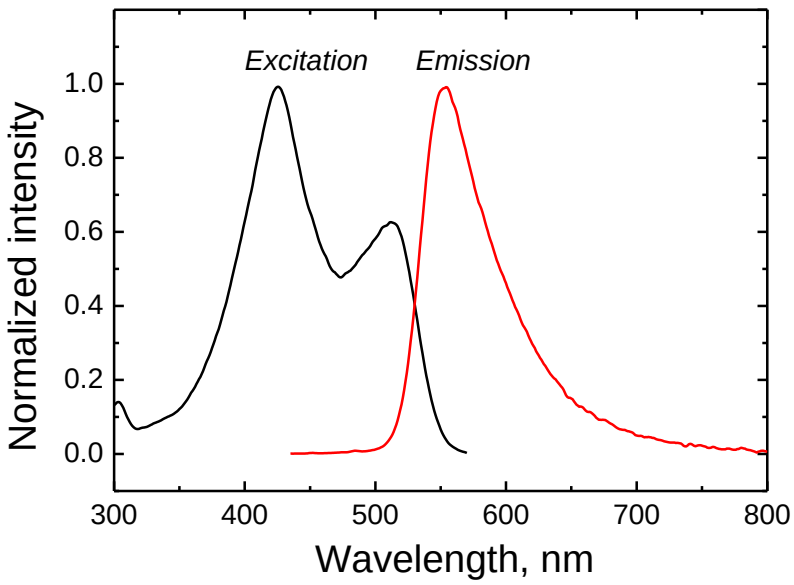

Figure S2. Excitation (λ_{em} = 600 nm) and emission (λ_{exc} = 400 nm) spectra **Zn-1** in dimethylformamide at 20 °C.

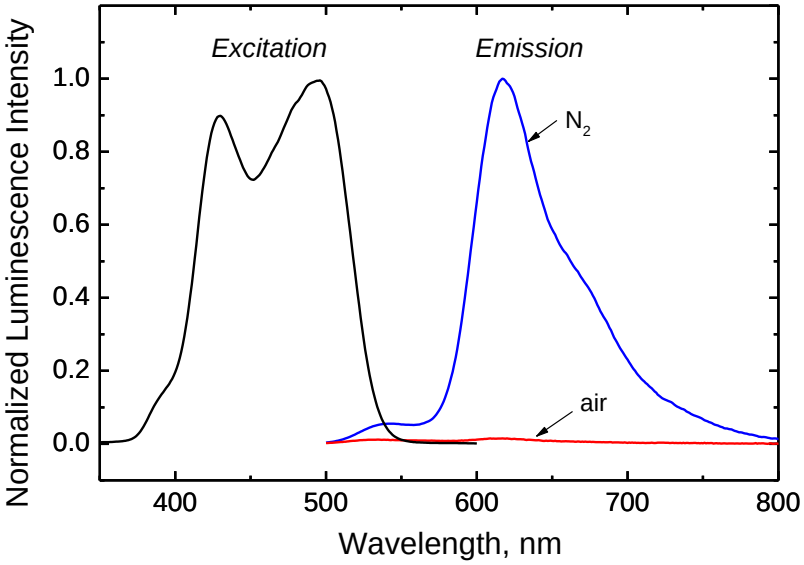

Figure S3. Excitation (λ_{em} = 620 nm) and emission (λ_{exc} = 480 nm) spectra **Gd-1** in ethanol. The complex was obtained via reaction of **1** with gadolinium(III) nitrate in ethanol in presence of KPF_6 and under basic conditions (addition of NaOH) and was not isolated.

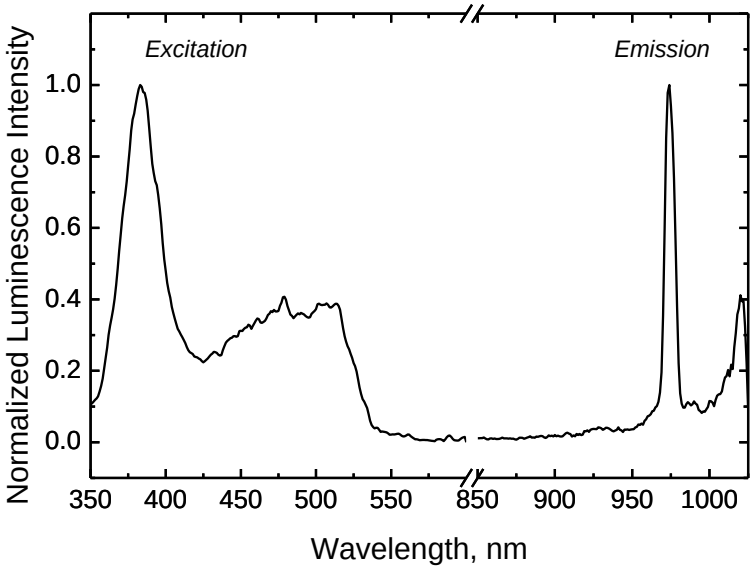

Figure S4. Excitation (λ_{em} = 975 nm) and emission (λ_{exc} = 505 nm) spectra **Yb-1** in ethanol. The complex was obtained via reaction of **1** with ytterbium(III) nitrate in ethanol in presence of KPF_6 and under basic conditions (addition of NaOH) and was not isolated.

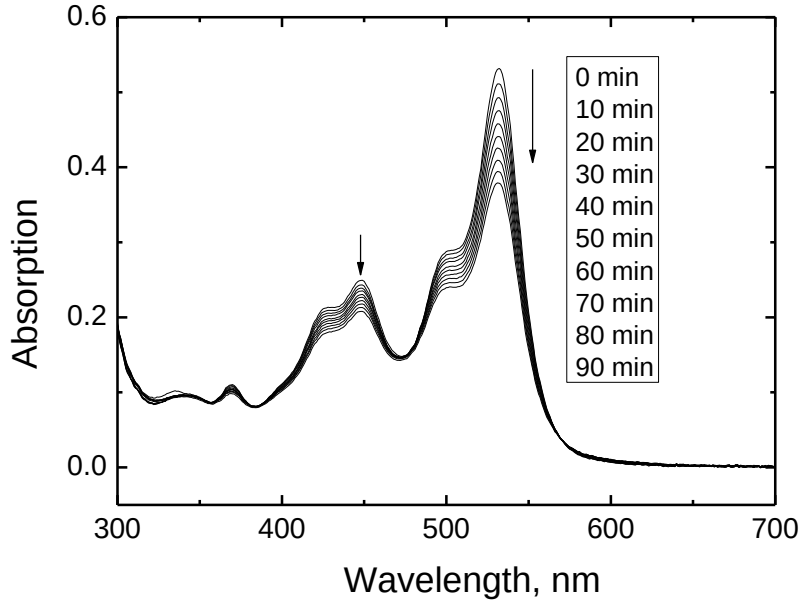

Figure S5. Absorption spectra of **Pt-1** in air-saturated toluene upon irradiation with a high power 470 nm LED array (photon flux 5600 μmol s^{-1} m^{-2} μA).

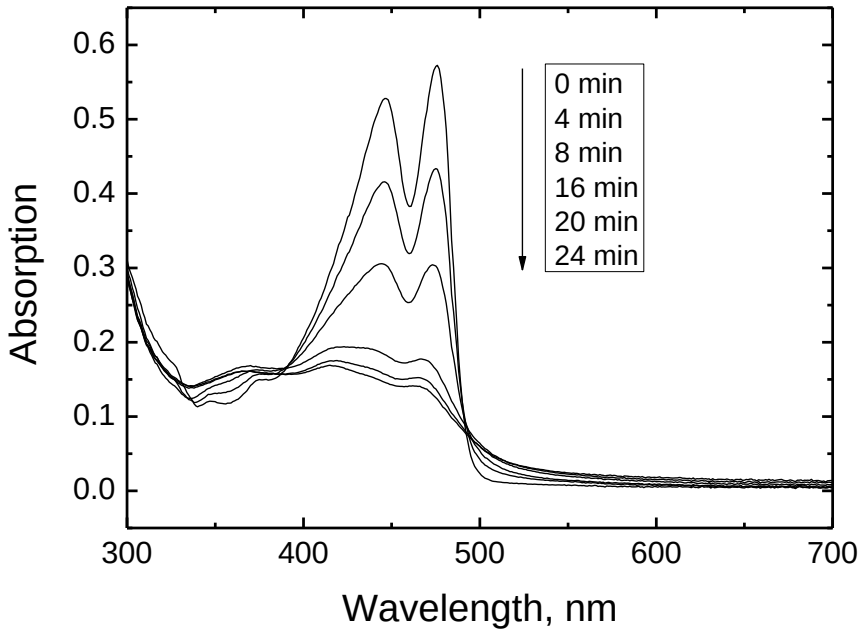

Figure S6. Absorption spectra of $Ir(C_S)_2acac$ in air-saturated toluene upon irradiation with a high power 470 nm LED array (photon flux 5600 µmol s^{-1} m^{-2} µA).

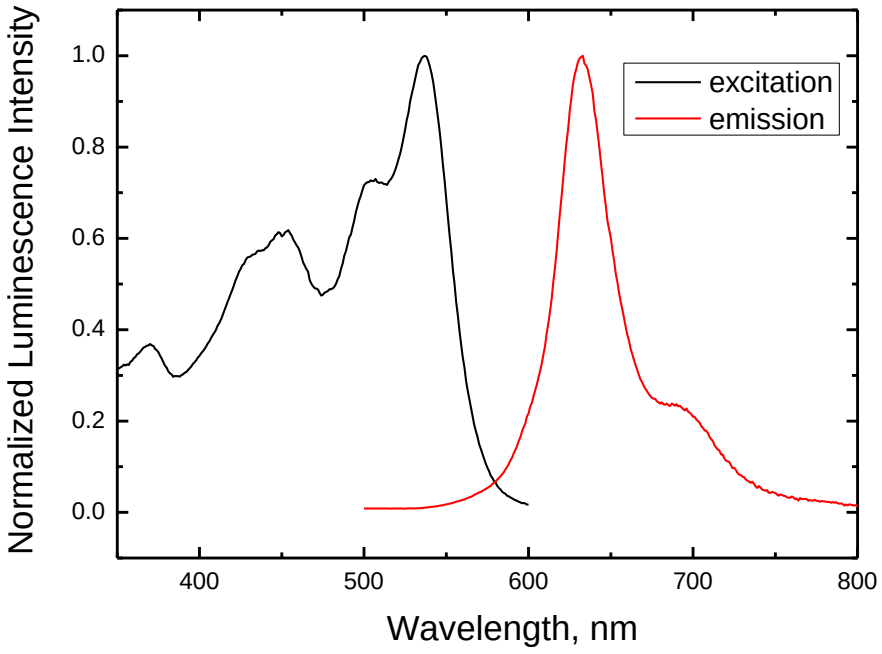

Figure S7. Excitation (λ_{em} = 640 nm) and emission (λ_{exc} = 480 nm) spectra **Pt-1** in polystyrene.

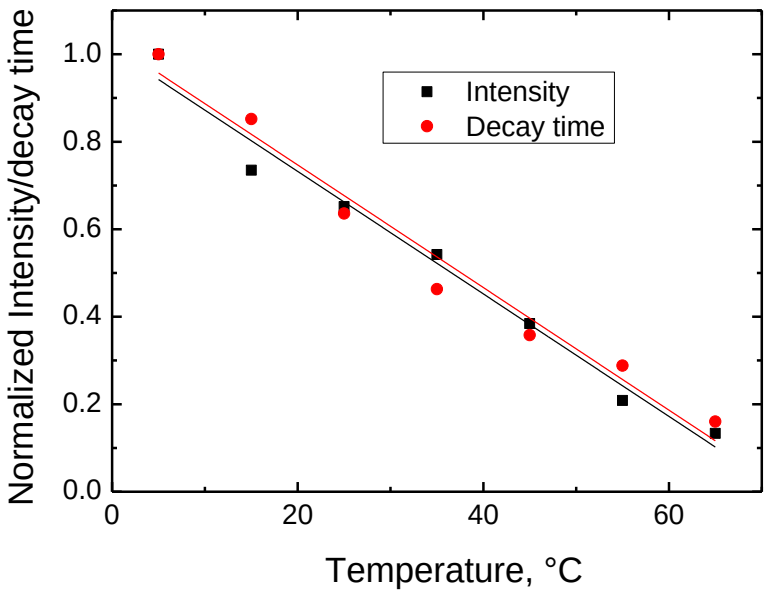

Figure S8. Comparison of the response of luminescence intensity and decay time to temperature for **Pd-1** immobilized into PViCl-PAN.

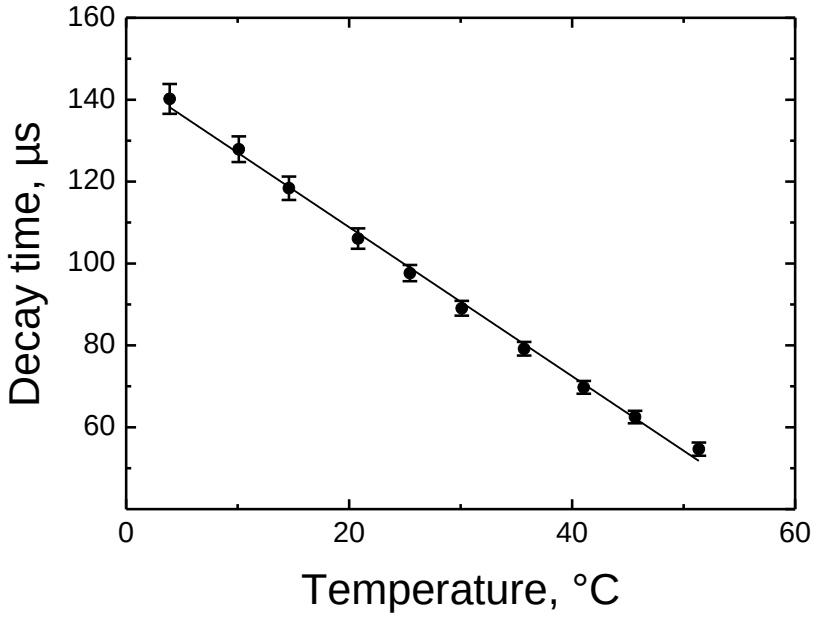

Figure S9. Temperature dependency of the decay time of **Pd-1**/PViCl-PAN sensor obtained from time-resolved imaging experiments.

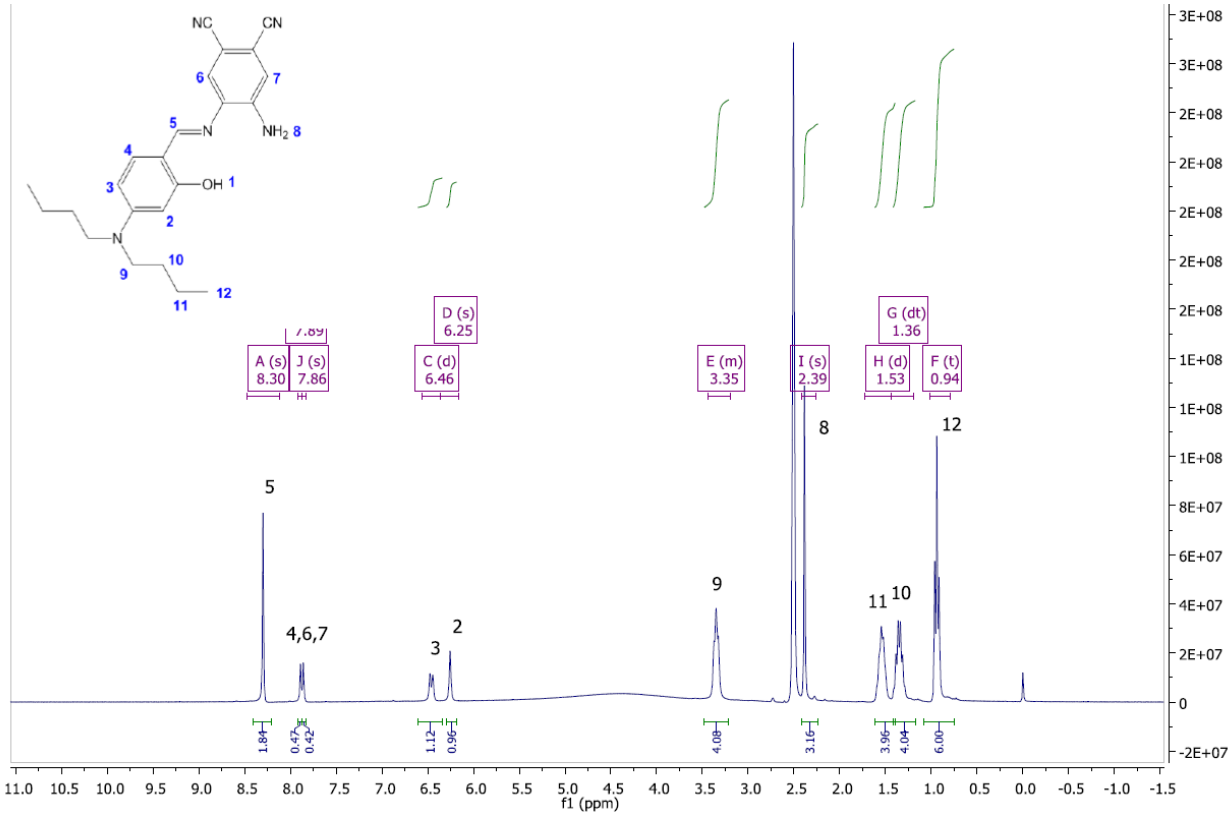

Figure S10. [1]H NMR spectrum (300 MHz, DMSO-d6) of (E)-4-(4-(dibutylamino)-2-hydroxybenzylideneamino)-5-aminobenzene-1,2-dinitrile.

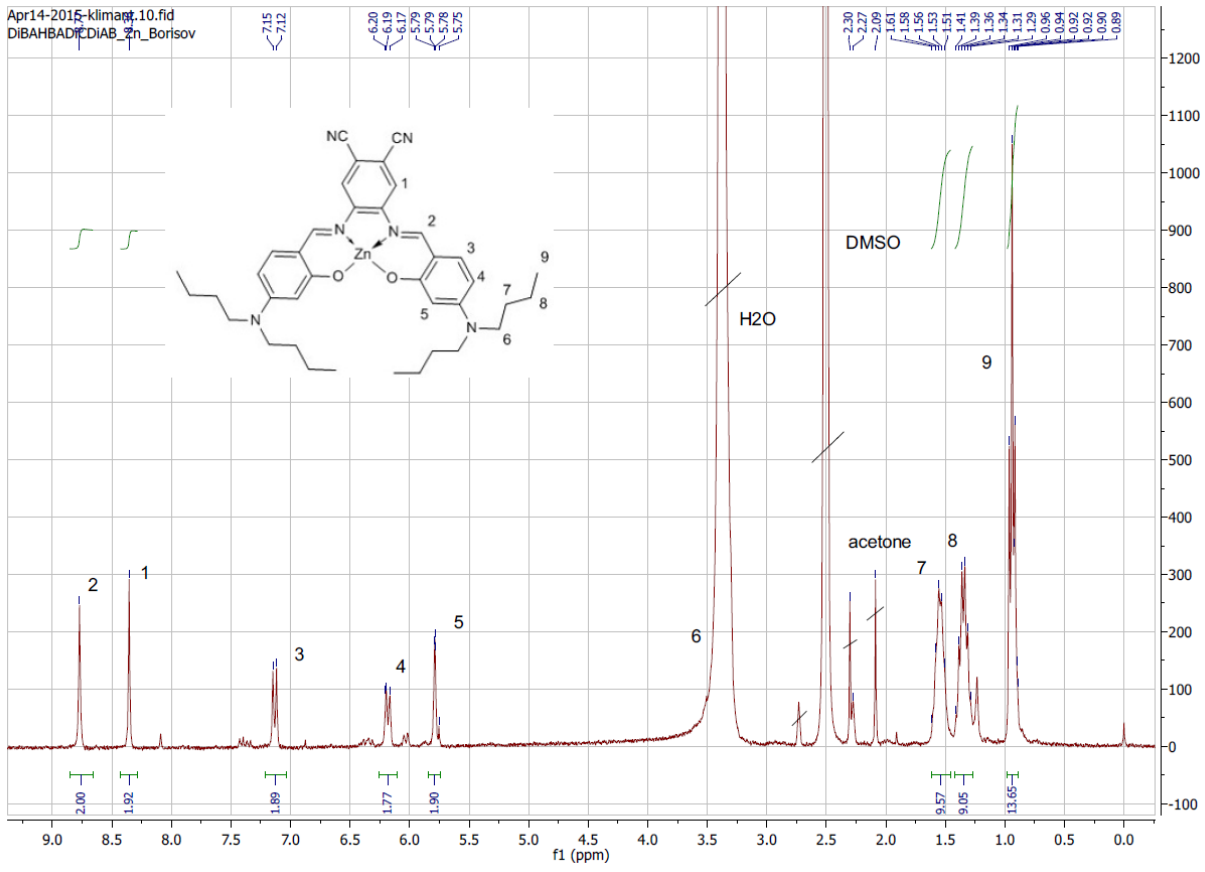

Figure S11. [1]H NMR spectrum (300 MHz, DMSO-d6) of **Zn-1.**

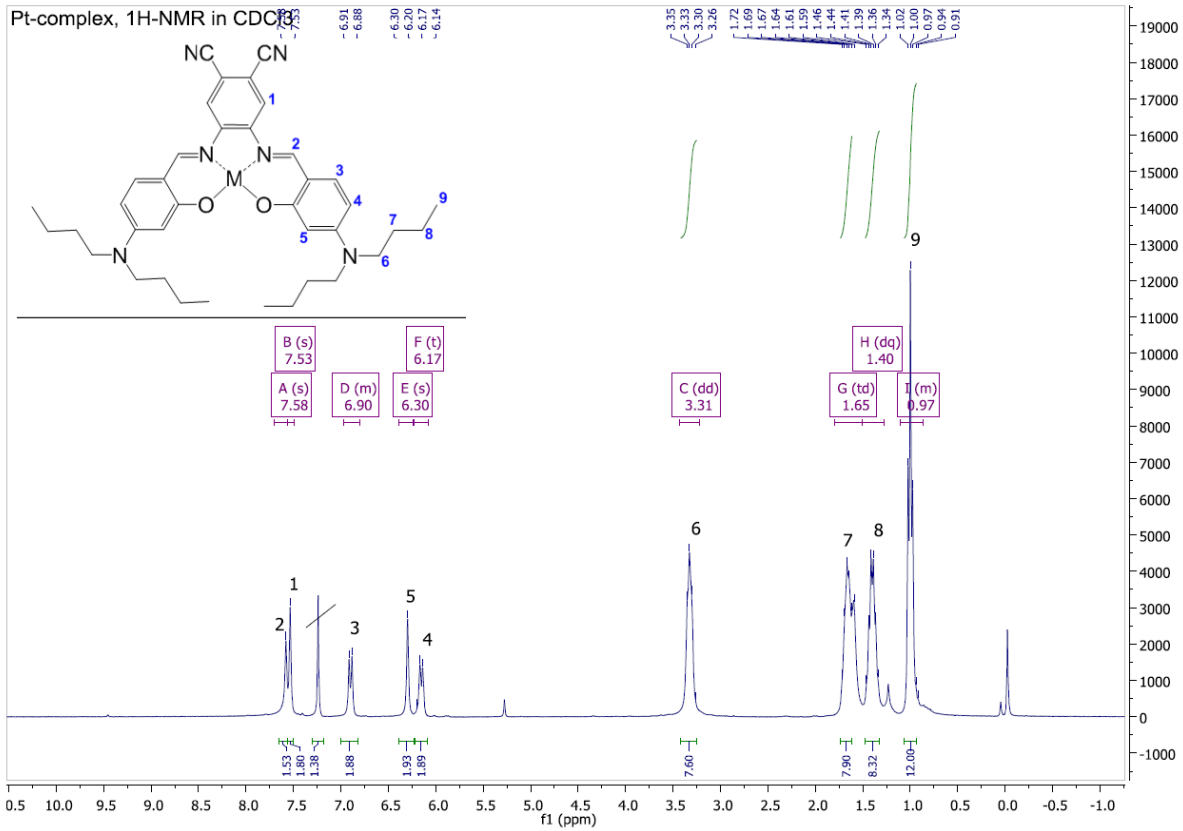

Figure S12. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **Pt-1**.

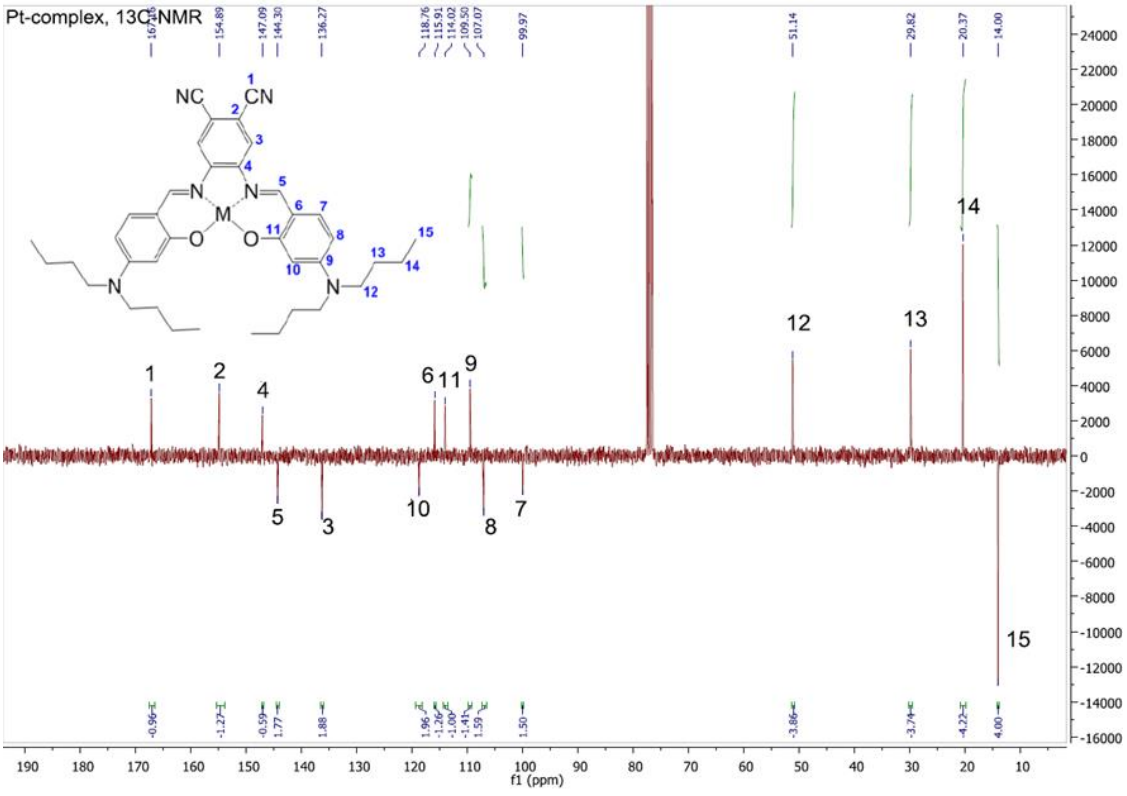

Figure S13. ^{13}C APT-NMR spectrum (300 MHz, $CDCl_3$) of **Pt-1**.

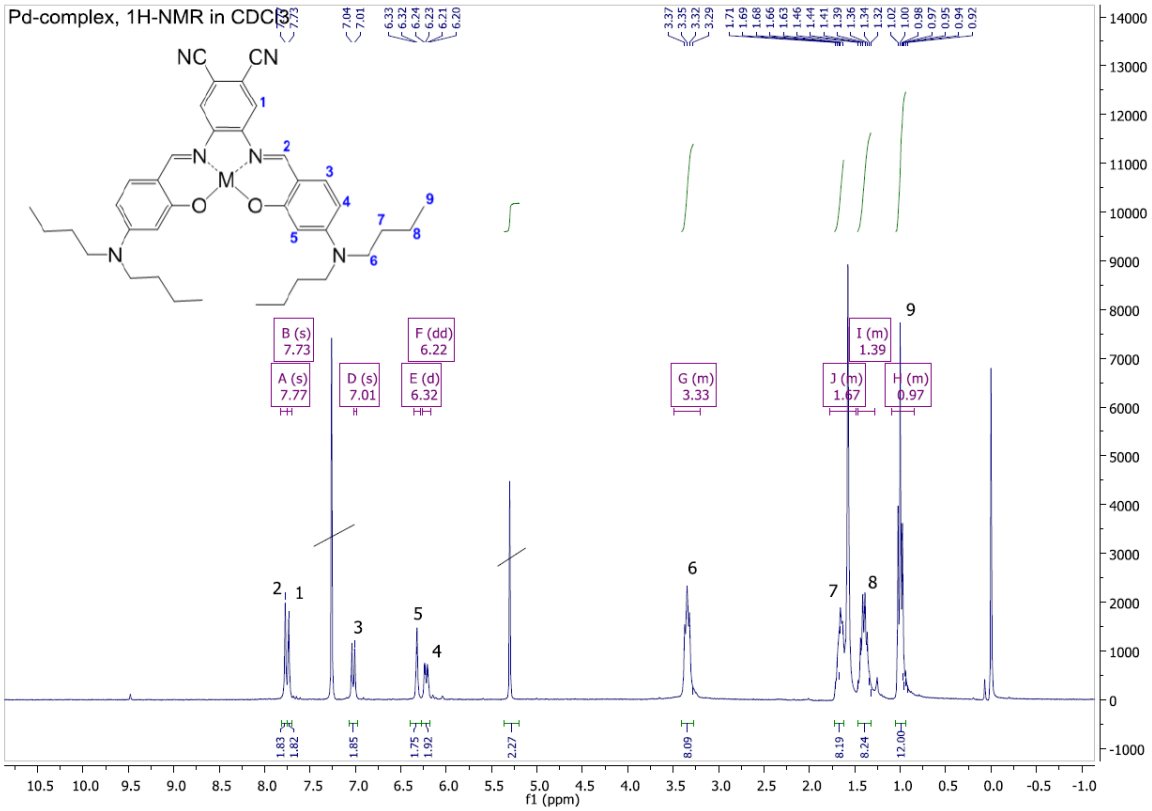

Figure S14. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of **Pd-1**.

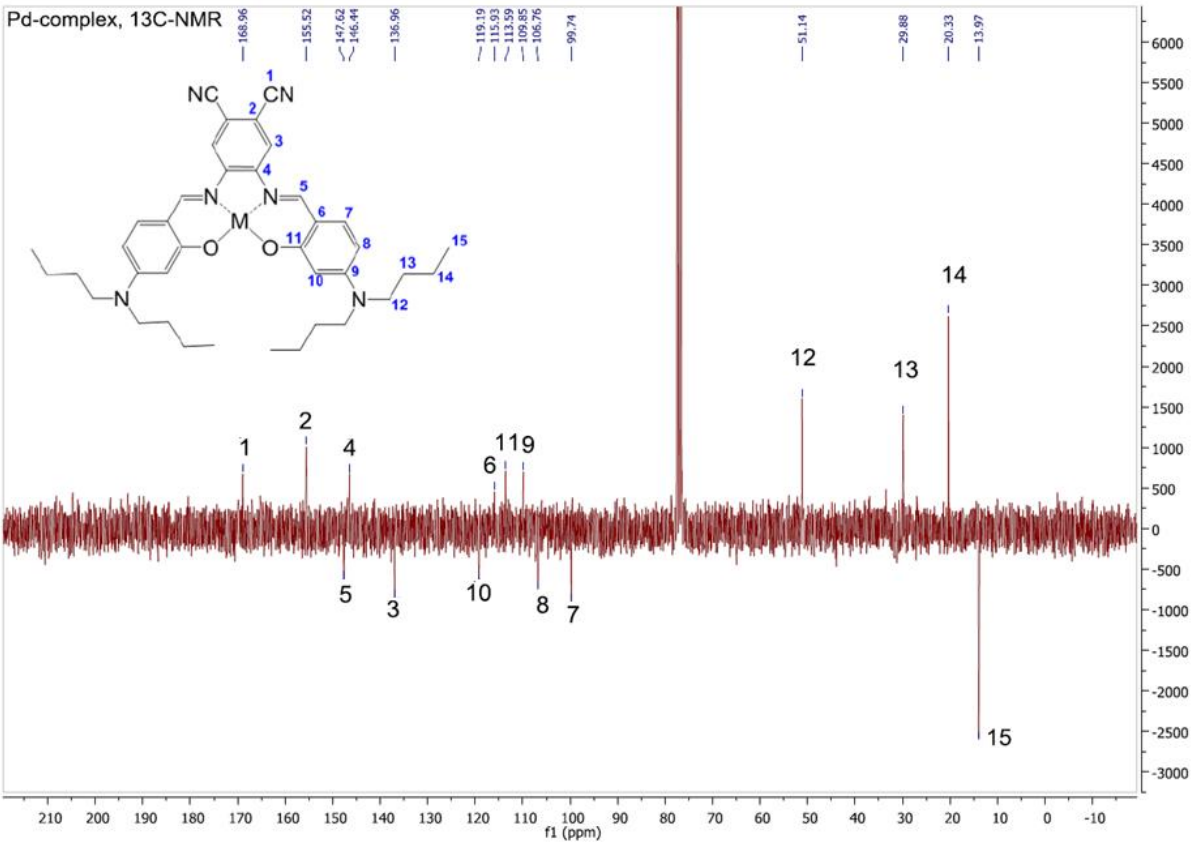

Figure S15. ^{13}C APT-NMR spectrum (300 MHz, $CDCl_3$) of **Pd-1**.

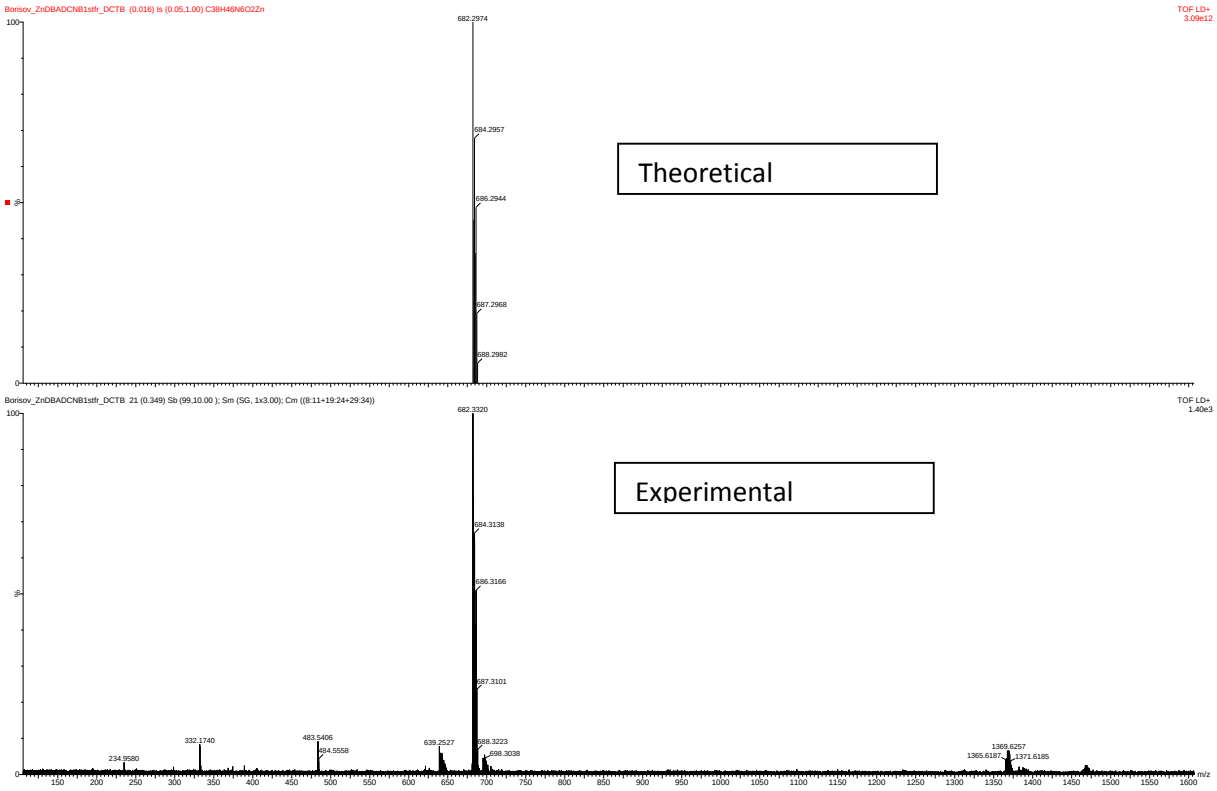

Figure S16. Mass-Spectrum (MALDI-TOF) of **Zn-1**.

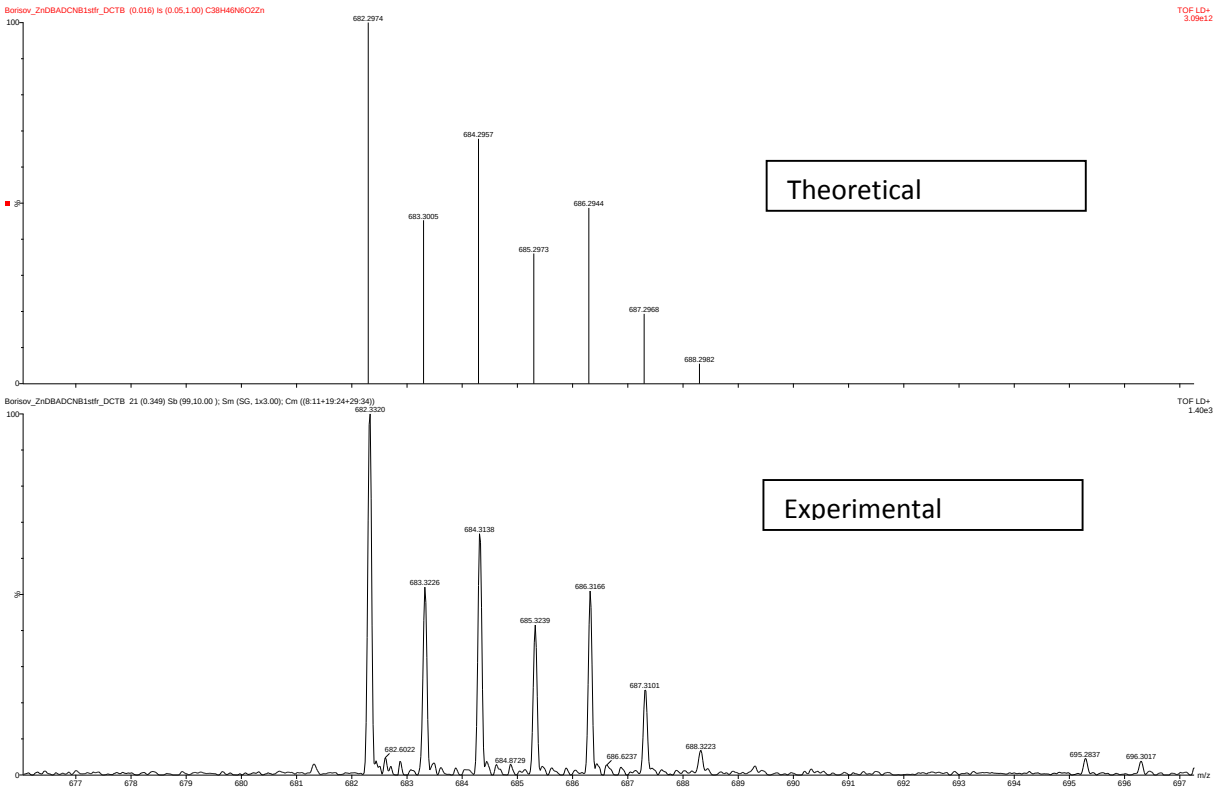

Figure S17. Isotope pattern of **Zn-1**.

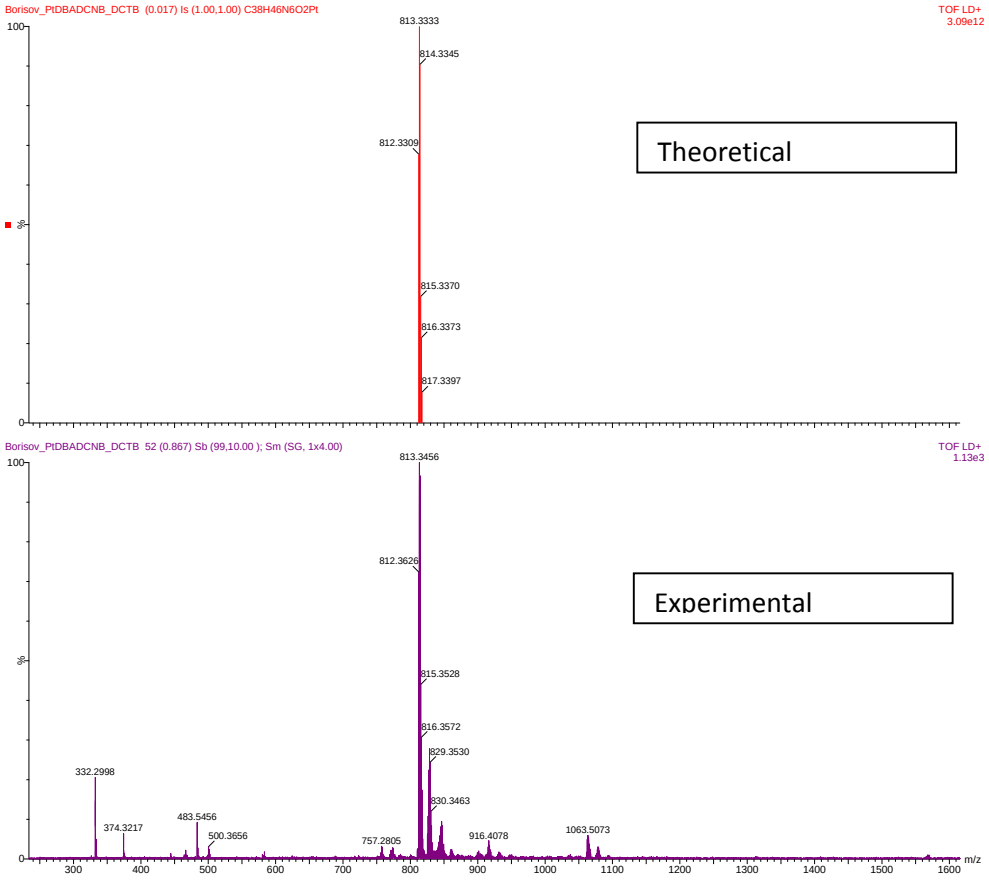

Figure S18. Mass-Spectrum (MALDI-TOF) of **Pt-1**.

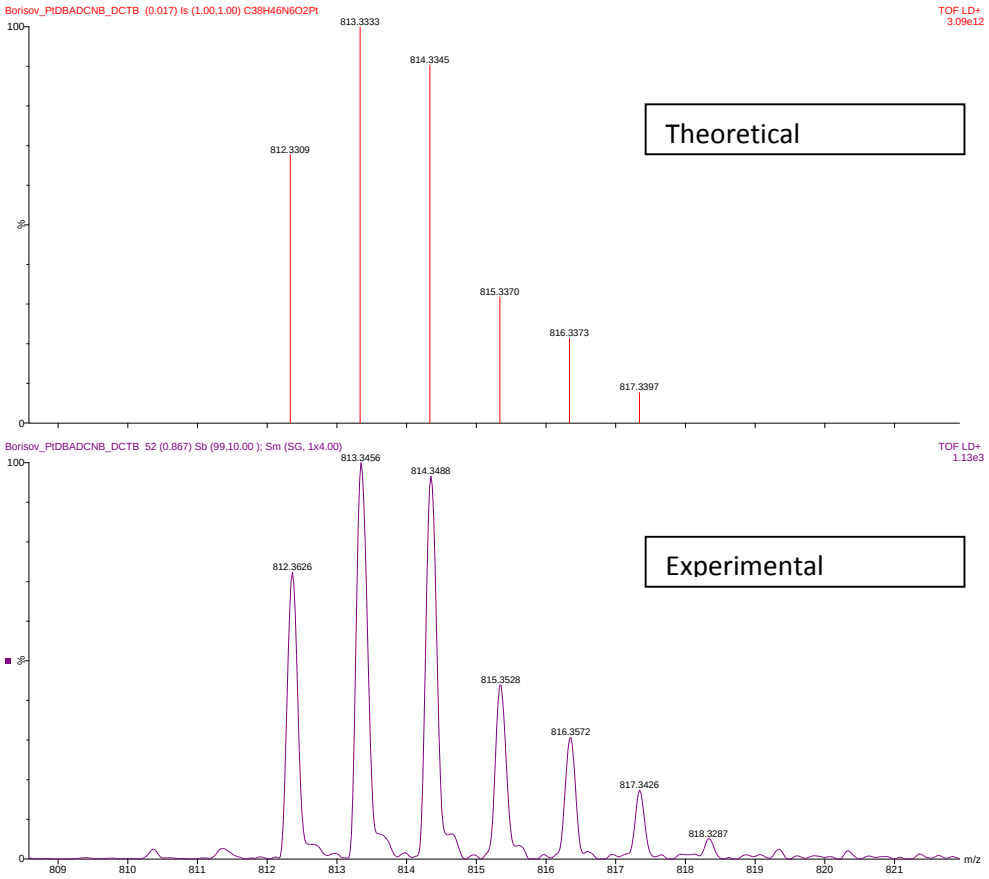

Figure S19. Isotope pattern of **Pt-1**.

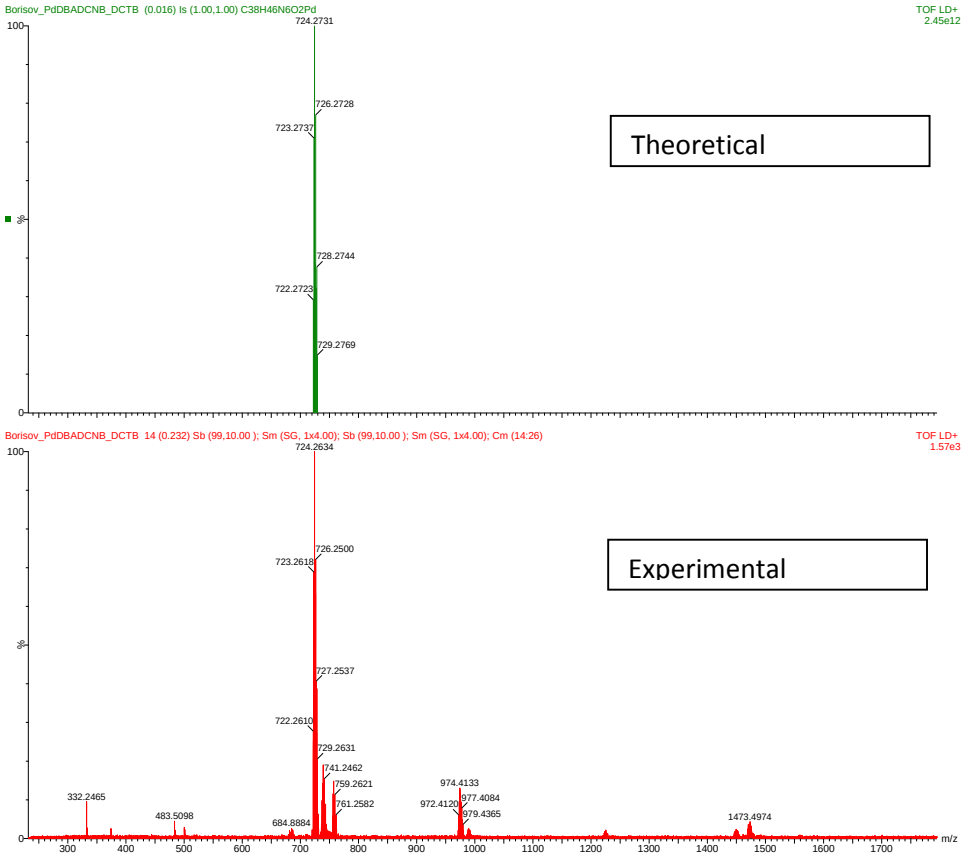

Figure S20. Mass-Spectrum (MALDI-TOF) of **Pd-1**.

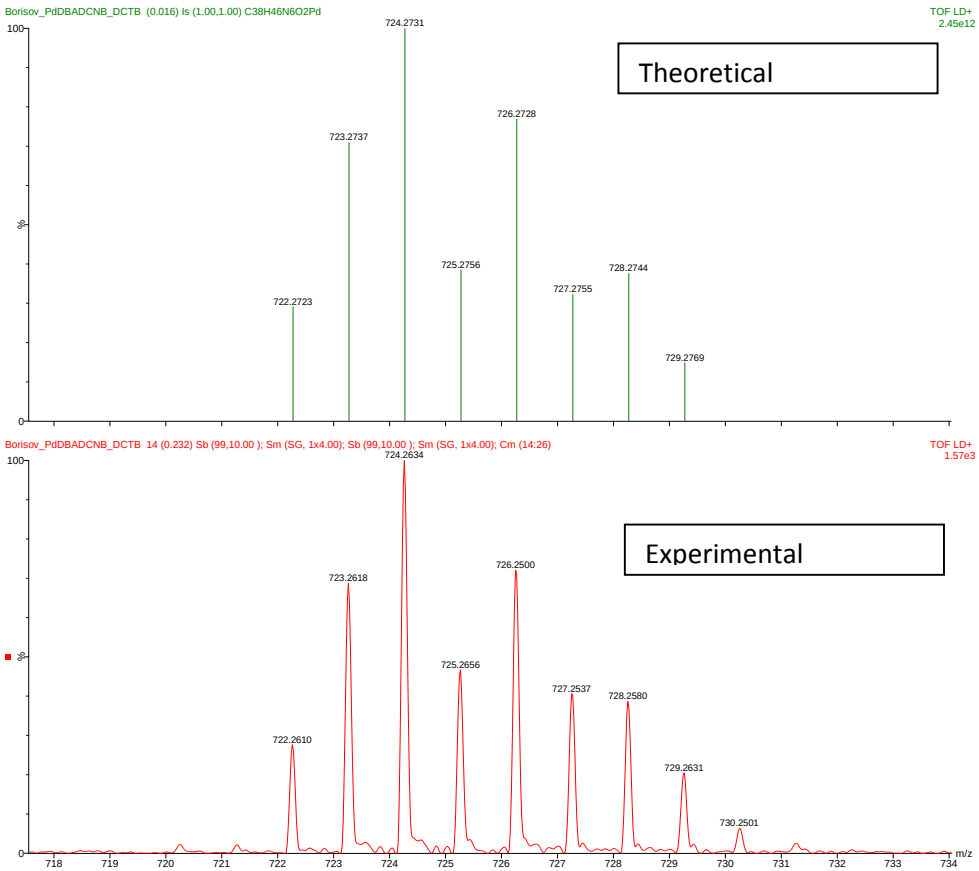

Figure S21. Isotope pattern of **Pd-1**.

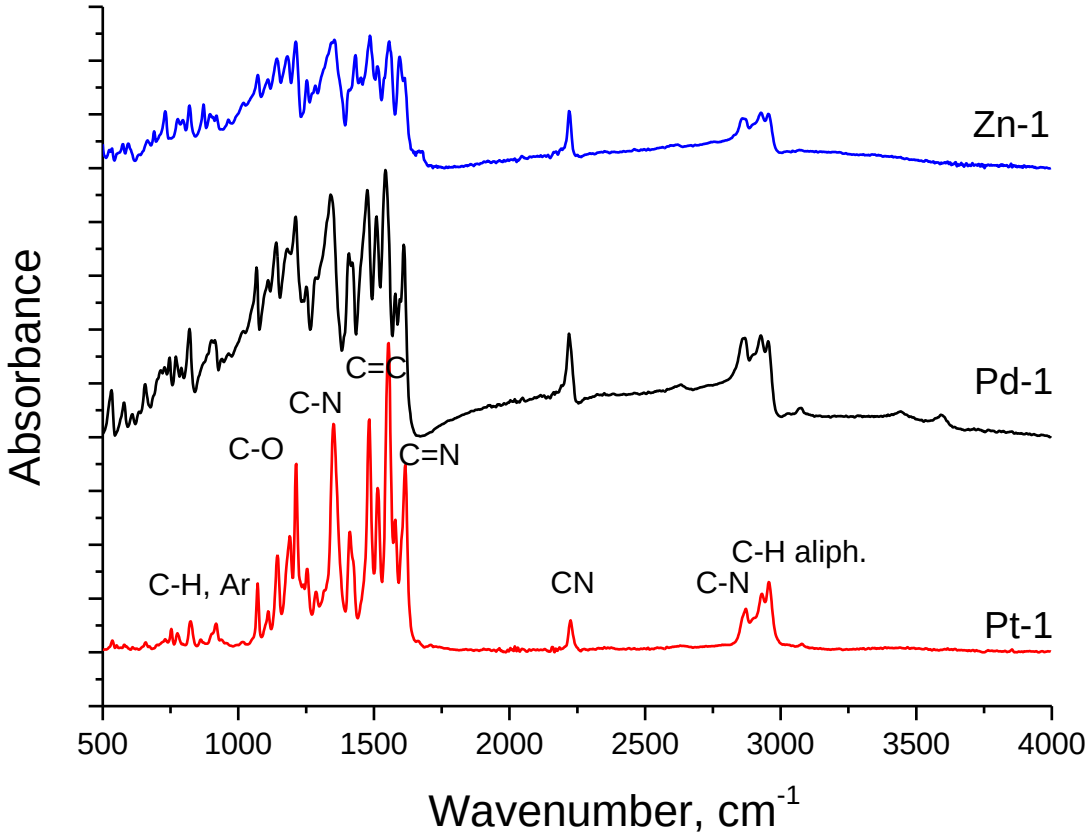

Figure S22. IR spectra of the Schiff base complexes.