

Multifunctional Organometallic Compounds: An Interesting Luminescent NLO-Active Alkynylplatinum (II) Complex

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European Journal of Inorganic Chemistry

Supporting Information

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I. General Information

Solvents and all commercially available chemicals were used without further purification. Air- and water-sensitive reactions were performed in flame-dried glassware under argon atmosphere.

NMR spectra were recorded on a Bruker AC 400 spectrometer. Chemical shifts δ are given in ppm and coupling constants J in Hz. Multiplicities are presented as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet.

Electronic absorption spectra were recorded at room temperature using a Shimadzu UV3600 spectrophotometer and quartz cuvettes with 1 cm optical path length.

The absolute photoluminescence quantum yield (Φ) was measured using a C11347 Quantaaurus Hamamatsu Photonics K.K spectrometer; steady state and time-resolved fluorescence data were obtained using a FLS980 spectrofluorimeter (Edinburgh Instrument Ltd). Emission spectra were corrected for background intensity and quantum efficiency of the photomultiplier tube, while excitation spectra were corrected for the intensity fluctuation of a 450 W Xenon arc lamp. Quartz cuvettes with 1 cm optical path length were used for the measurements.

The structure's parameters were determined performing the X-ray analysis using a D8 VENTURE Bruker AXS diffractometer, Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$), $T = 150 \text{ K}$.

II. NMR spectra

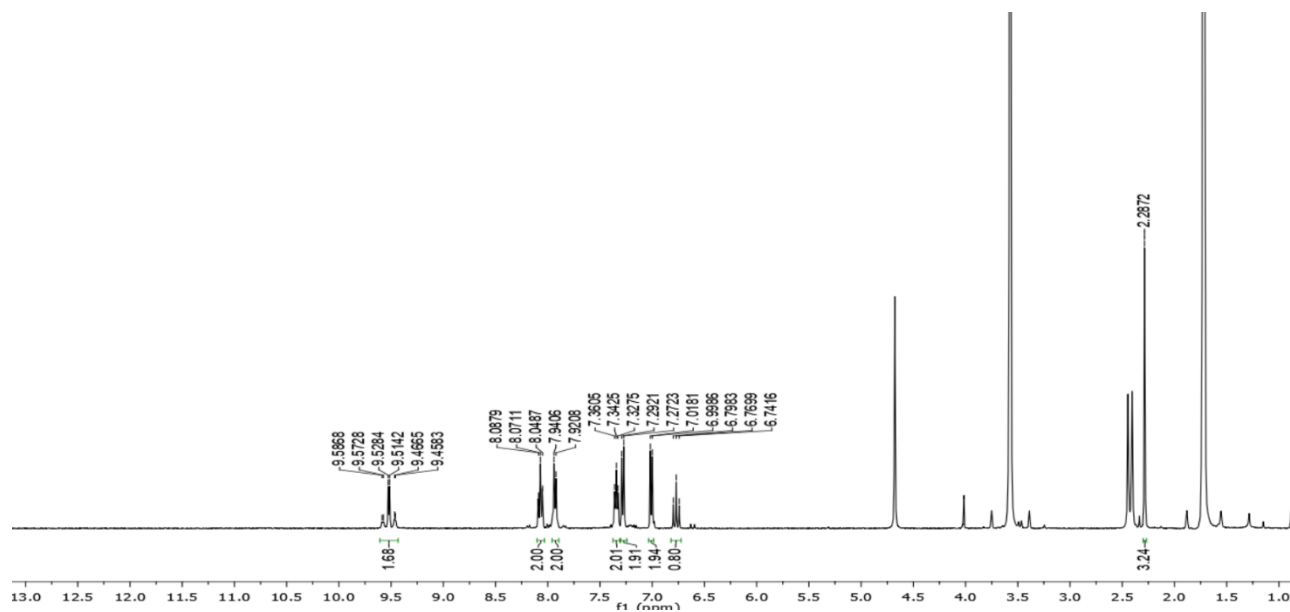


Figure S1. ^1H NMR spectrum ($\text{THF-}d_8$, 400 MHz) of complex **1**.

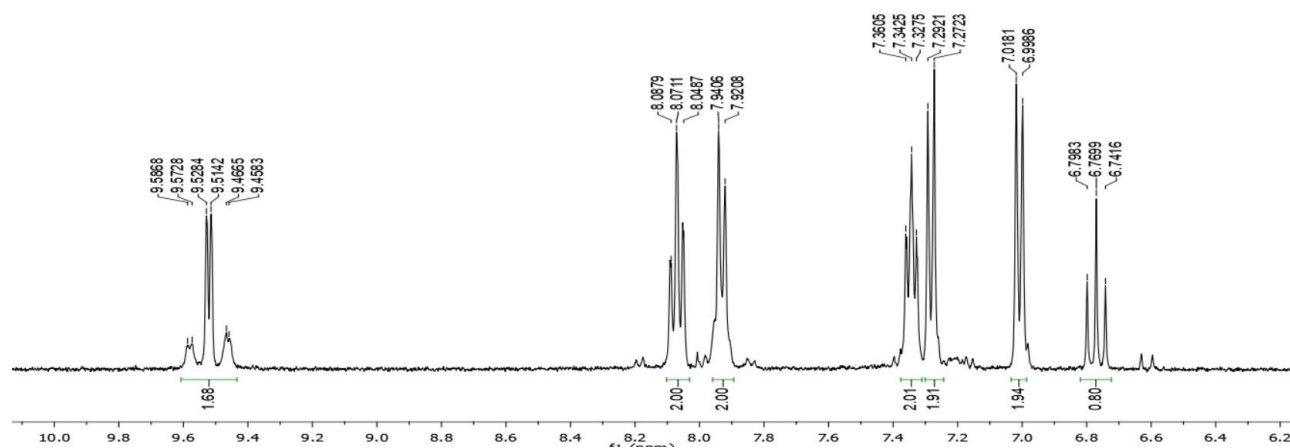


Figure S2. ^1H NMR spectrum ($\text{THF-}d_8$, 400 MHz) of complex **1**, aromatic region.

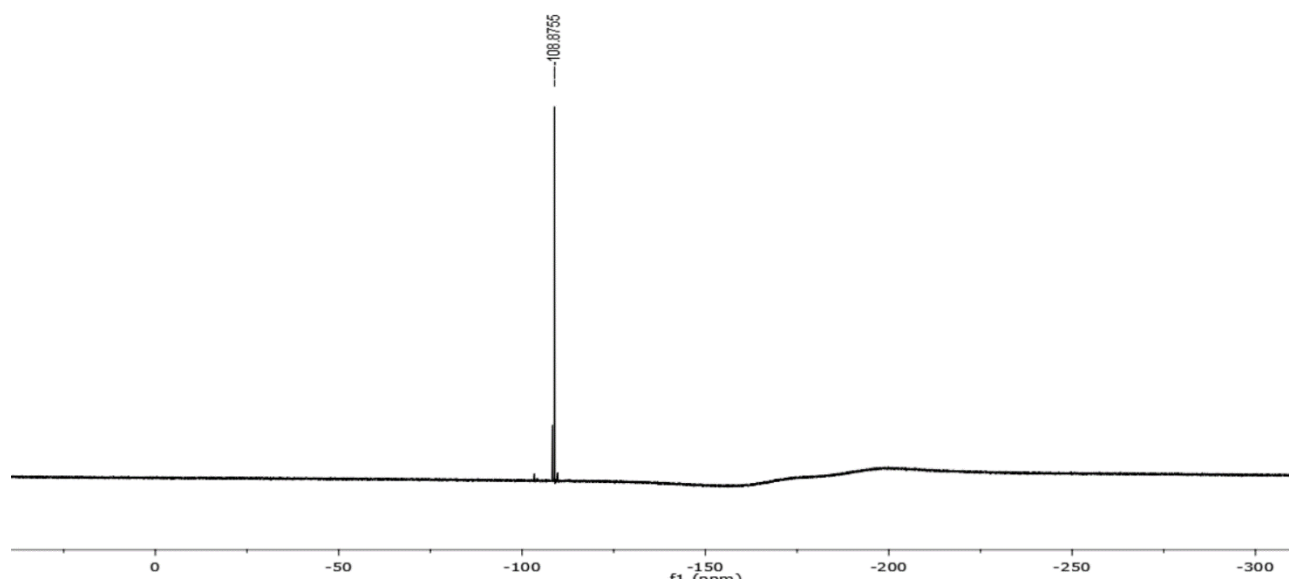


Figure S3. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum (THF- d_8 , 282.36 MHz) of complex **1**.

III. Photophysical data in solution

Luminescence measurements

Luminescence measurements were carried out in CH₂Cl₂ solution after three cycles of the Freeze-Pump-Thaw (FPT) procedure, required to remove dissolved oxygen.

The absolute photoluminescence quantum yield (Φ) in solution was calculated through Equation:

$$\Phi = \frac{PN(Em)}{PN(Abs)}$$

where PN(Em) is the number of emitted photons, PN(Abs) the number of absorbed photons. The error made was estimated at around 5%.

Time-resolved fluorescence measurements were performed through the time-correlated single photon counting technique, and time-resolved fluorescence curves were fitted using a multi-exponential function:

$$I(\lambda, t) = \sum_{i=1}^m \alpha_i(\lambda) \exp\left(\frac{-t}{\tau_i}\right)$$

where m is the number of exponentials, $\alpha_i(\lambda)$ is the amplitude at wavelength λ and τ_i is the lifetime of the component i . The quality of the fit was evaluated through the reduced χ^2 values.

In case of multi-exponential decay, it is possible to define an average lifetime as:

$$\tau_{av} = \frac{\sum_{n=1}^m \alpha_n \tau_n^2}{\sum_{n=1}^m \alpha_n \tau_n}, \quad m = \text{multi-exponential decay number of the fit.}$$

Absorption vs Concentration

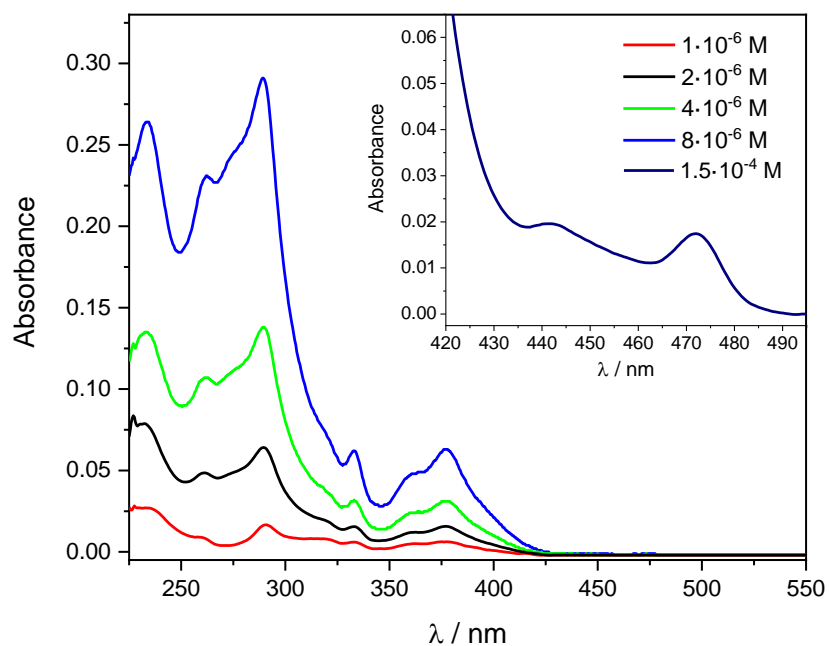


Figure S4. Absorption spectra of complex **1** in CH₂Cl₂ at different concentrations. The weak bands at longer wavelengths are shown on an expanded scale for clarity.

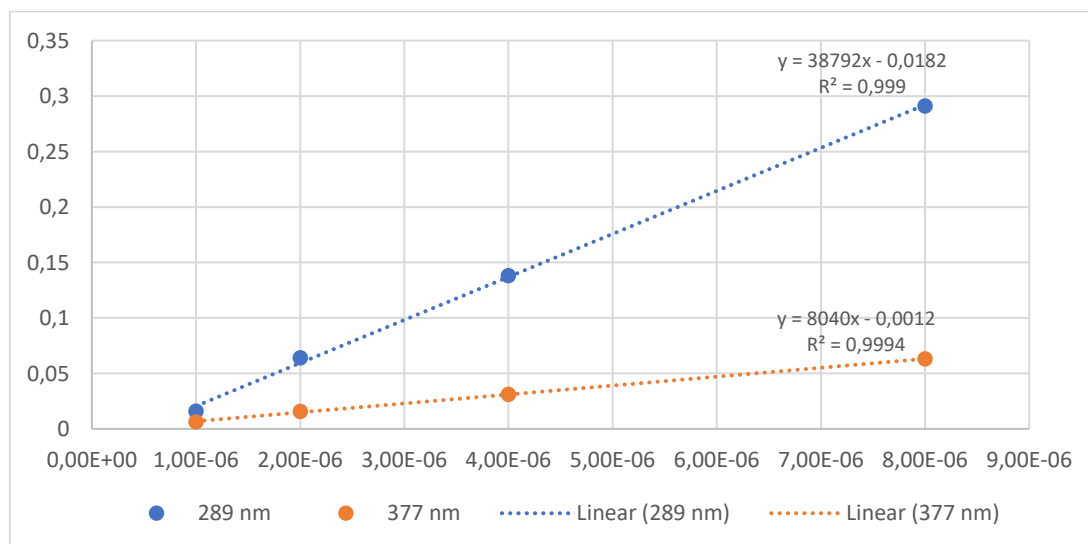


Figure S5. Lambert-Beer relationship for complex **1** in CH₂Cl₂.

Excitation spectra

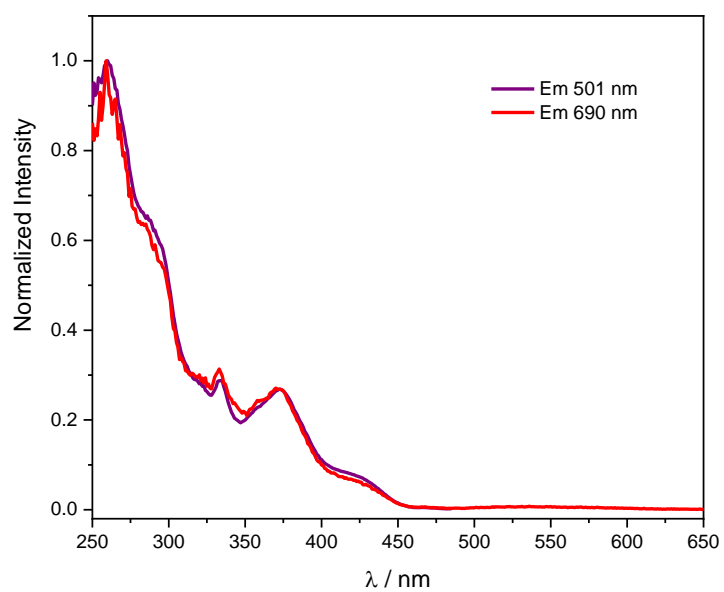


Figure S6. Excitation spectra of complex **1** in CH₂Cl₂ at 1·10⁻⁵ M at different emission wavelengths.

Excited state decay measurement

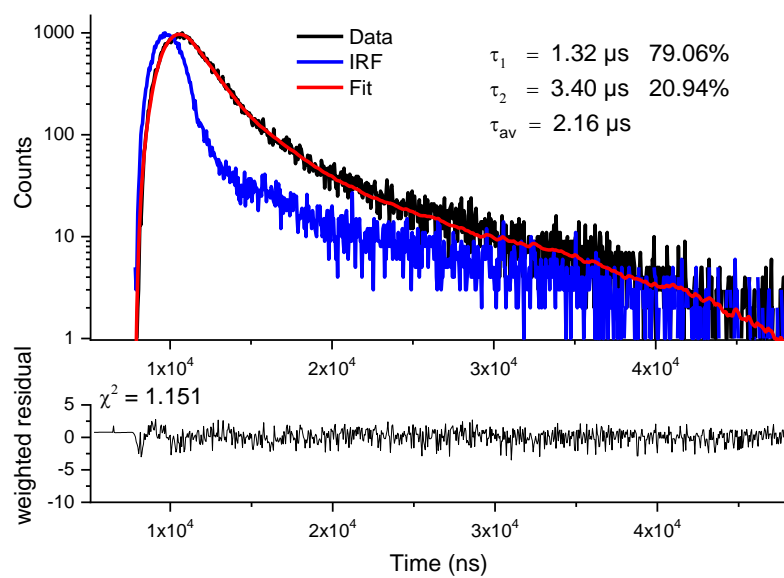


Figure S7. Excited state decay measurement of complex **1** in CH_2Cl_2 at $1 \cdot 10^{-5}$ M, excitation wavelength 427 nm, emission wavelength 496 nm.

IV. X-ray diffraction data

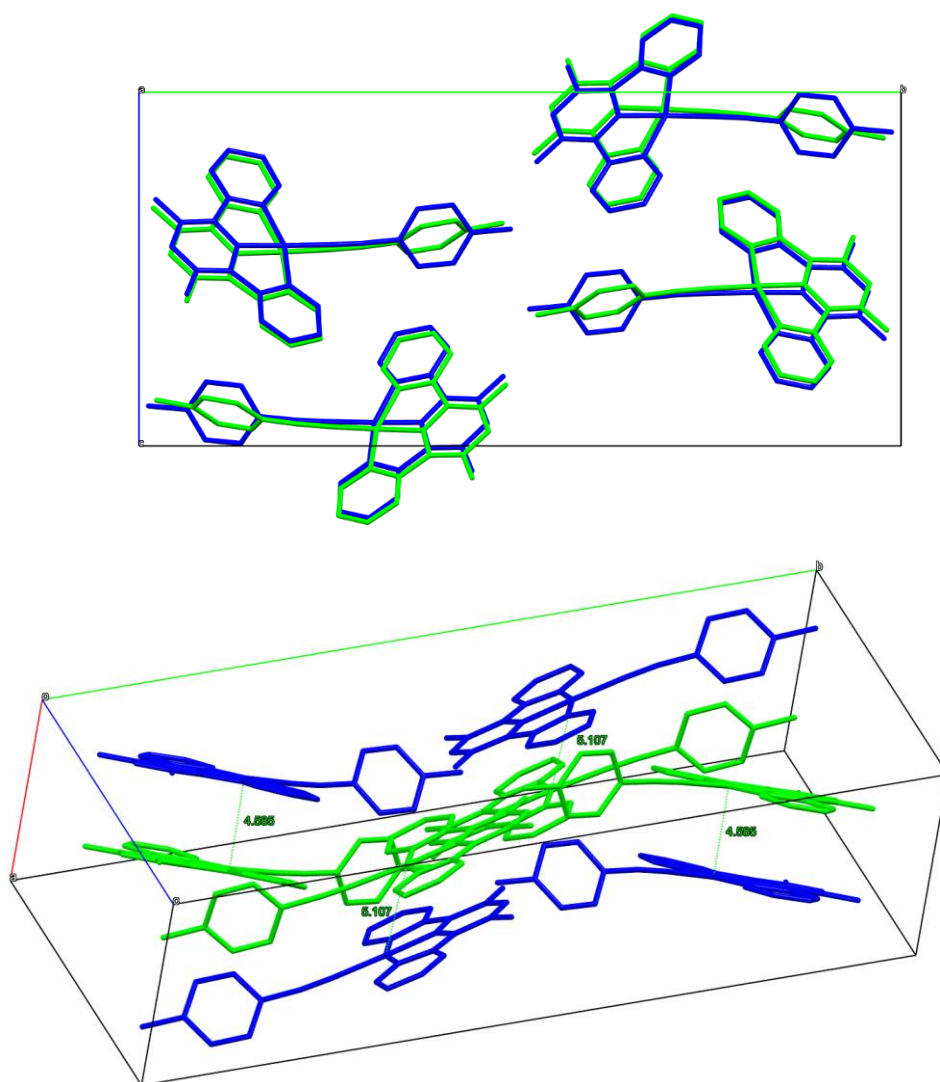


Figure S8. Different views of the crystal packing of complex **1**. Different colors indicate symmetry-independent molecules.

Table S1. Key crystallographic data for complex **1**.

CCDC number	2357874
Empirical formula	C ₂₅ H ₁₆ F ₂ N ₂ Pt
Formula weight	577.49 g/mol
Temperature	150 K
Wavelength	0.71073 Å
Crystal system, space group	monoclinic, P 2 ₁ /n (I.T.#14)
Unit cell dimensions	a = 9.6784(11) Å
	b = 29.183(3) Å
	c = 14.1219(14) Å
	β = 106.454(4) °
Volume	3825.4(7) Å ³
Z	8
Calculated density	2.005 g cm ⁻³
Absorption coefficient	7.370 mm ⁻¹
F(000)	2208
Crystal size	0.360 x 0.220 x 0.070 mm
Theta range for data collection	2.282 to 27.489 °
Limiting indices	-12 ≤ h ≤ 12, -37 ≤ k ≤ 37, -16 ≤ l ≤ 18
Reflections collected / unique	28200 / 8715 [R(int) ^a = 0.0368]
Reflections [I > 2σ]	7300
Completeness to theta max	0.992
Absorption correction	Multi-scan
Max. and min. transmission	0.597, 0.336
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8715 / 0 / 543
Goodness-of-fit on F ²	0.867
Final R indices [I > 2σ(I)]	R1 ^c = 0.0377, wR2 ^d = 0.1258
R indices (all data)	R1 ^c = 0.0474, wR2 ^d = 0.1370
Largest diff. peak and hole	1.967 and -1.866 e ⁻ .Å ⁻³