Electronic Supplementary Information

for the paper:

Synthesis, regioselective aerobic Pd (II)-catalyzed C-H bond alkenylation and the photophysical properties of pyrenylphenylpyrazoles

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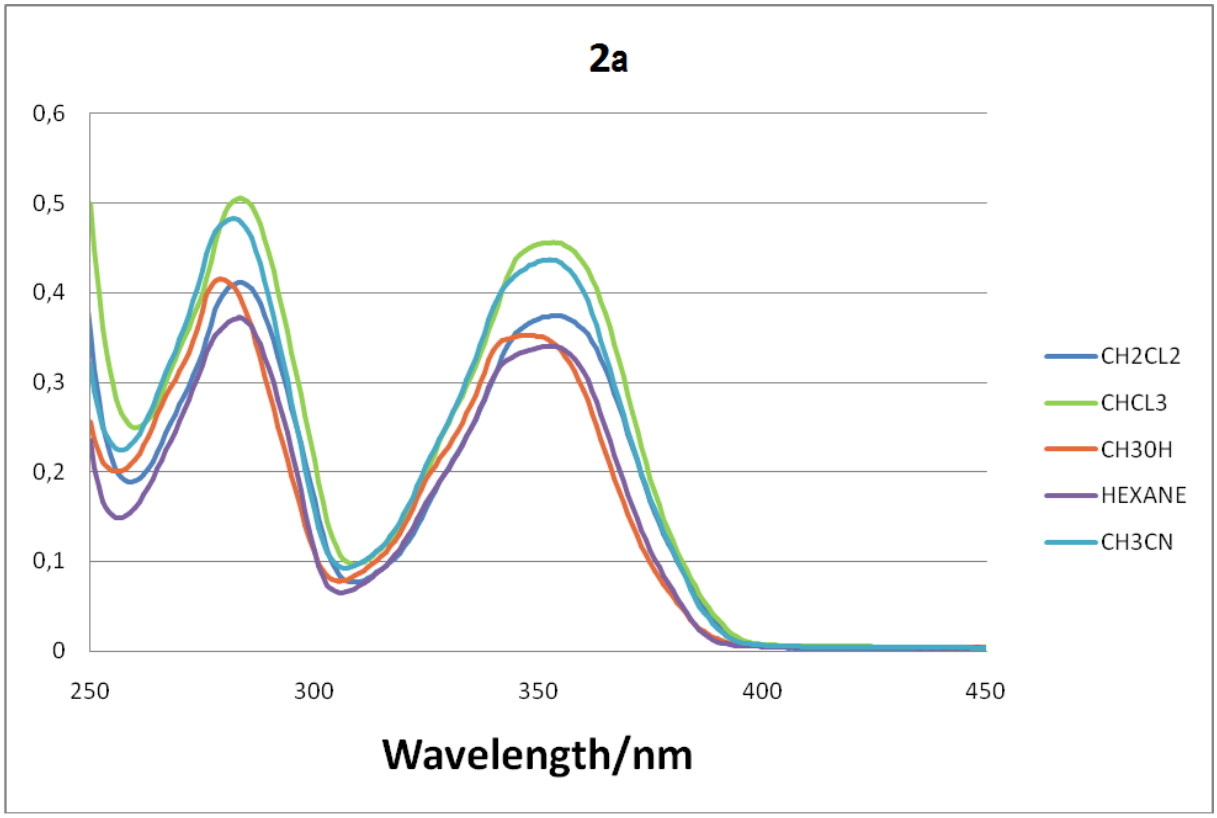
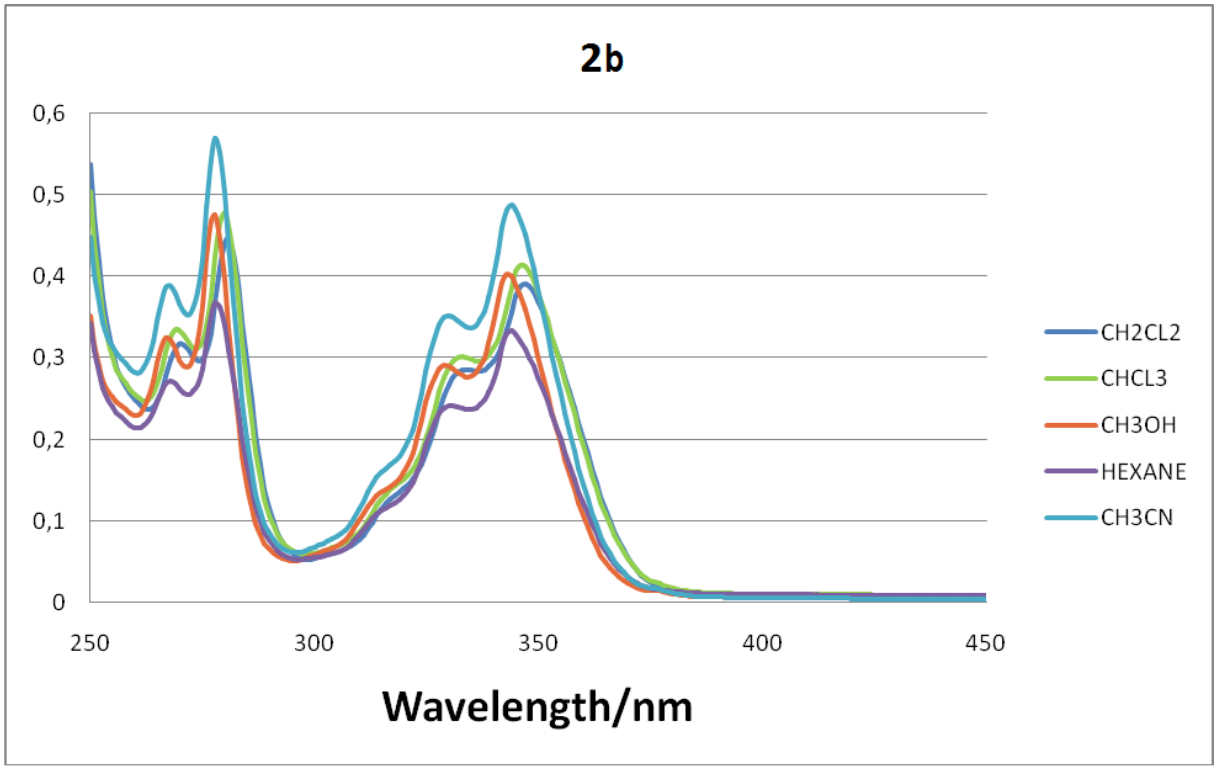
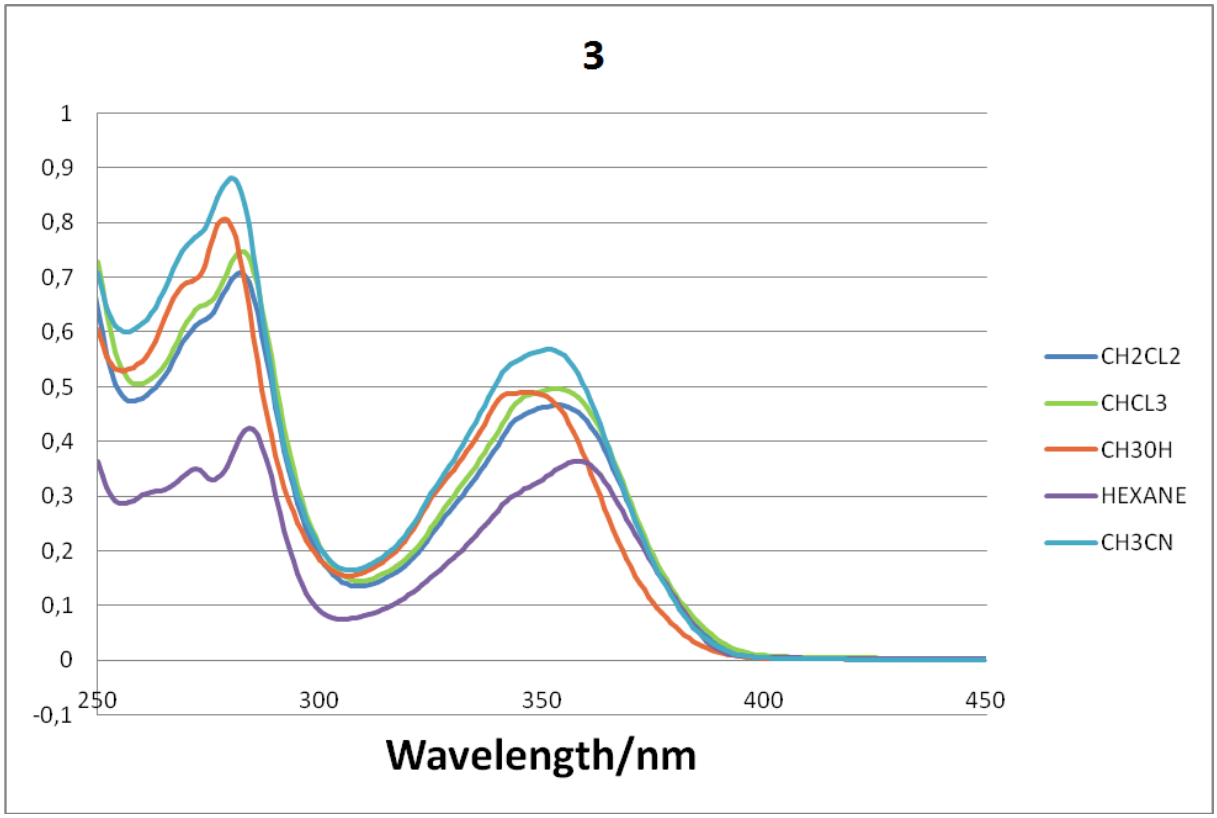
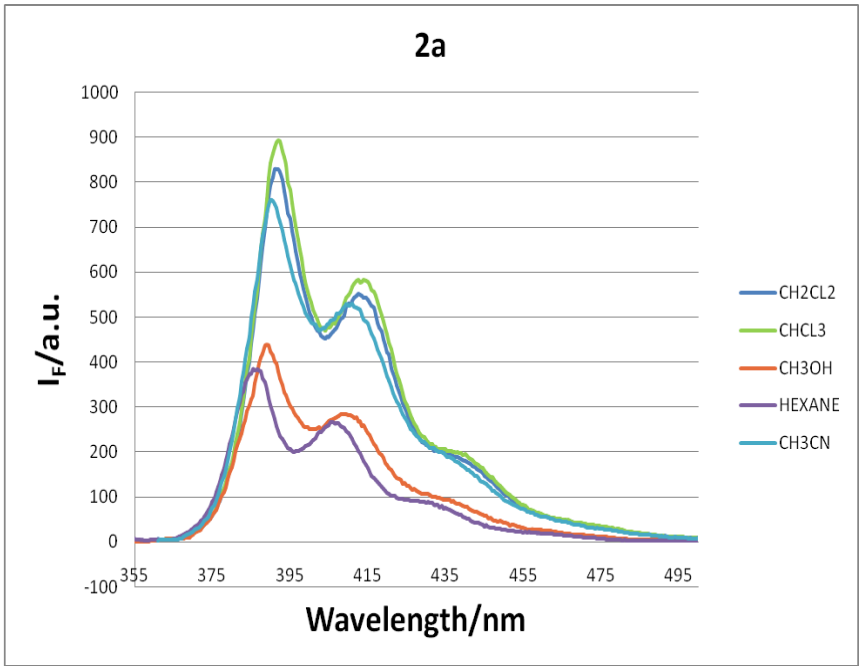
1. **Electronic absorption spectra of 2a-b and 3 in various solvents (c = 10^{-5} M)**

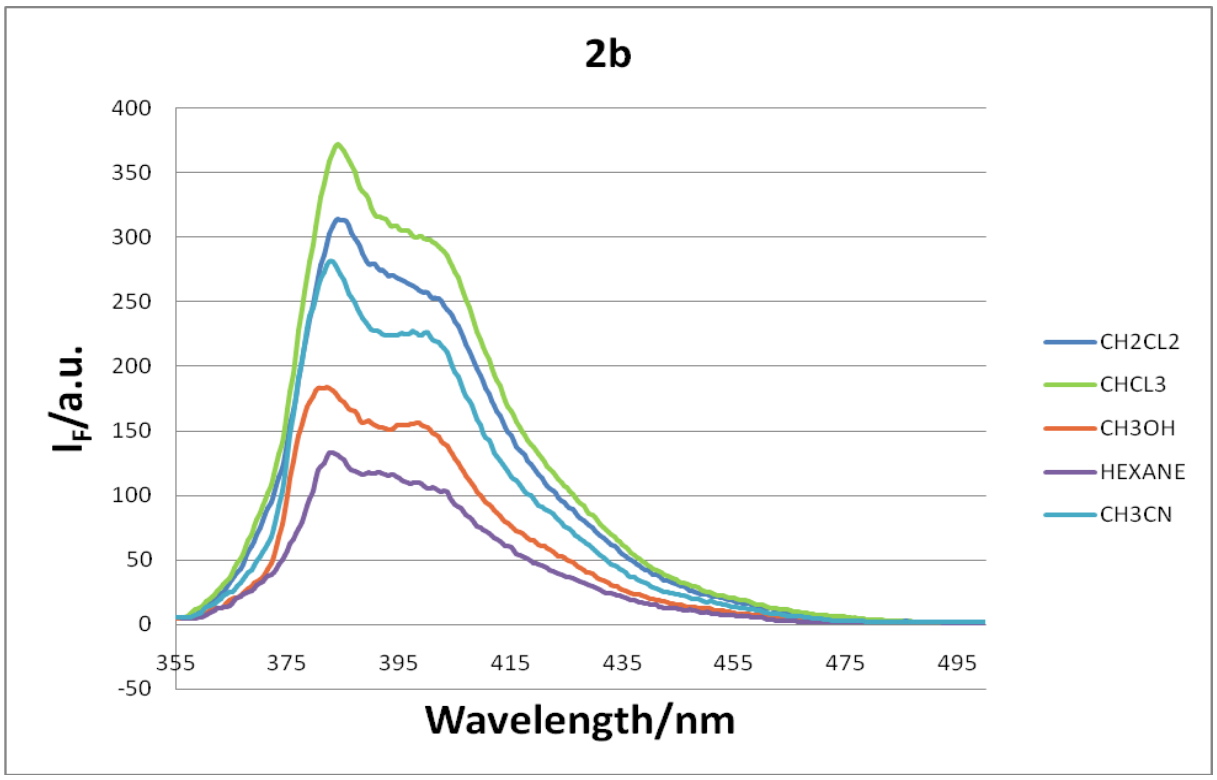



2b
0,6
0,5
0,4
0,3
0,2
0,1
0
250
300
350
400
450
Wavelength/nm
CH2CL2
CHCL3
CH3OH
HEXANE
CH3CN



2. Electronic emission spectra of 2a-b in various solvents (c = 10^{-6} M). ($\lambda_{excit} = \lambda_{abs}$)





3. X-ray diffraction analysis of 2a and 2b

The single crystals - clear light yellow prisms - of **2a** and **2b** suitable for X-ray analysis were obtained by slow diffusion of n-hexane into their respective chloroform solutions.

The data for crystals of **2a** and 2**b** were collected on Agilent Supernova 4 circle diffractometer system equipped with copper and molybdenum microsource and Atlas CCD detector. The data were collected using molybdenum radiation for **2a** and copper radiation for **2b** with CrysAlis171[1] software and integrated with the CrysAlisPRO[2] software. Data were corrected for absorption effects using the multi-scan method (SCALE3 ABSPACK[1]).

The structures were solved by direct methods using SXELXS[3] and refined by full-matrix least squares procedure with SHELXL[3] within OLEX2[4] graphical interface. Figures were produced with Ortep3v2[5] and Mercury_3.3[6].

In both instances all H atoms were visible in the residual density map, but were added geometrically and refined in riding approximation.

The quantitative descriptors of the data processing and structure refinement for all compounds are presented in Table 1.

Table 1.

Identification code	**2a**	**2b**
Empirical formula	$C_{15}H_{16}N_2$	$C_{15}H_{16}N_2$
Formula weight	344.40	344.40
Temperature/K	100.00(10)	100.00(10)
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/n$
a/Å	9.94167(14)	9.13704(10)
b/Å	11.68932(13)	8.80760(13)
c/Å	15.15921(19)	21.4207(2)
α/°	90	90
β/°	107.8620(15)	93.0448(10)
γ/°	90	90
Volume/Å^3	1676.76(4)	1721.41(4)
Z	4	4
ρ_{calc} mg/mm^3	1.364	1.329
μ/mm^{-1}	0.08	0.61
Transmission T_{min}/T_{max}	0.995/0.998	0.806/1.000
F(000)	720	720
Crystal size/mm^3	0.34×0.20×0.14	0.39×0.26×0.15
Radiation Å	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)
2Θ range for data collection	2.152° to 27.496°	4.134° to 74.073°
Index ranges	-12 ≤ h ≤ 12, -15 ≤ k ≤ 15, -19 ≤ l ≤ 19	-11 ≤ h ≤ 11, -10 ≤ k ≤ 10, -26 ≤ l ≤ 26
Reflections collected 84822	16576	
Independent reflections	3838	3437
Rint	0.0328	0.0229
Rsigma	0.0082	0.0137
Data/restraints /parameters	3838/0/244	3437/0/245
Goodness-of-fit on F^2	1.105	1.094
Final R indexes [I>=2σ (I)]	R1 = 0.0422, wR2 = 0.1187	

Final R indexes [all data]	R1 = 0.0398, wR2 = 0.1147 R1 = 0.0443, wR2 = 0.1202	 R1 = 0.0427, wR2 = 0.1170
Largest diff. peak/hole / eÅ^{-3}	0.335/-0.202	0.375/-0.327

4. Photophysical study

Electronic absorption spectra were run on a Perkin Elmer Lambda 45 UV/VIS spectrometer. Corrected emission spectra were obtained on a Fluorolog FL3-221 spectrofluorometer from Horiba Jobin-Yvon, including an integrating sphere accessory which allows recording excitation and emission spectra and determining absolute quantum yield values in the powder state.

Fluorescence decay curves were obtained by the time-correlated single-photon counting (TCSPC) method with femtosecond laser excitation using a Spectra-Physics set-up composed of a Titanium Sapphire laser (Tsunami, Spectra-Physics) pumped by a doubled YAG laser (Millennia, Spectra-Physics), itself pumped by two laser diode arrays. Light pulses at 720 nm were selected by optoacoustic crystals at a repetition rate of 4 MHz, and then doubled to 360 nm by non-linear crystals. Fluorescence photons were detected through a monochromator by means of a Hamamatsu MCP R3809U photomultiplier connected to a constant-fraction discriminator. The time-to-amplitude converter was purchased from Tennelec. The instrumental response function was recorded before each decay measurement. The fluorescence data were analysed using the Globals software package developed at the Laboratory for Fluorescence Dynamics at the University of Illinois at Urbana-Champaign, which includes deconvolution analysis and the global non-linear least-squares minimization method.

REFERENCES

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