ESI For

Contrasted Photochromic and Luminescent Properties in Dinuclear Pt(II) Complexes Linked Through a Central DTE Unit

S1. Methods

S1.a Experiments

General:

All manipulations were performed using Schlenk techniques under argon atmosphere. All solvents were dried and purified by standard procedures. Precursor complex **1** [1] and compounds **2** [2] and **3** [3] were prepared following reported procedures. NMR spectra were recorded on Bruker, AV 400 spectrometer. ^{1}H and ^{13}C chemical shifts are determined by reference to residual ^{1}H and ^{13}C solvent signals. High-resolution mass spectra (HRMS) and Elemental Analysis were performed at the CRMPO (Centre de Mesures Physiques de l'Ouest) in Rennes. UV/Vis absorption spectra were recorded in pure dichloromethane using Specord 205 UV-Vis-NIR spectrophotometer in quartz cuvettes of 1 cm pathlength, against a reference of pure dichloromethane contained within a matched cuvette.

Photoisomerization experiments in solution have been made using a LS series Light Source of ABET technologies, Inc (150 W xenon lamp), with single wavelength light filters "350FS 10-25" or "450FS 40-25" for ring-closure and "650FS 10-25" for cycloreversion. Irradiations for ^{1}H NMR experiments have been made using a Rayonet® with 350 nm light emitting lamps.

Photoluminescence:

Equipment I. Steady state luminescence spectrum was measured at room temperature using an Edinburgh FS920 Steady State Fluorometer (Figure S15a). The emitted light was detected at 90° using a Peltier-cooled R928 PMT after passage through a monochromator. The solutions were degassed via three freeze-pump-thaw cycles in modified Quartz fluorescence cuvettes of 1 cm pathlength.

Equipment II. Steady state excitation and emission spectra at room temperature were recorded on an Edinburgh Instruments Model FLS980 spectrofluorometer equipped with R928P and NIR-PMT detectors (Figures 2b and S15b). The emission spectroscopic investigations of all solution required a degassing procedure on a high-vacuum line in a degassing cell, which contains 10-ml Pyrex bulb and a 1-cm path length quartz cuvette and is sealed from the atmosphere by a Telflon stopper. At least four successive freeze-pump-thaw cycles were performed to degas the solutions prior to the measurement.

Luminescence quantum yield of the sample was determined by optically dilute method [4] using $[Ru(bpy)_3]Cl_2$ ($\Phi_{lum} = 0.062$ in deoxygenated acetonitrile solution) as the standard with the same excitation wavelength at 436 nm and was corrected for changes in the refractive index. The full luminescence spectrum of the standard and partial luminescence spectrum of the sample were obtained by using R928P detector using the same measurement parameters of spectrofluorometer. The full spectrum of the sample, which was corrected for the luminescence intensity with the partial luminescence spectrum, was recorded by using NIR-PMT detector.

NLO measurements:

The second-order nonlinear optical (NLO) properties were determined by the electric-field induced second harmonic generation (EFISH) technique [5]. This method can provide direct information on the intrinsic molecular NLO properties, through equation 1:

$$\gamma_{EFISH} = (\mu\beta_{EFISH}/5kT) + \gamma(-2\omega; \omega, \omega, 0) \quad (1)$$

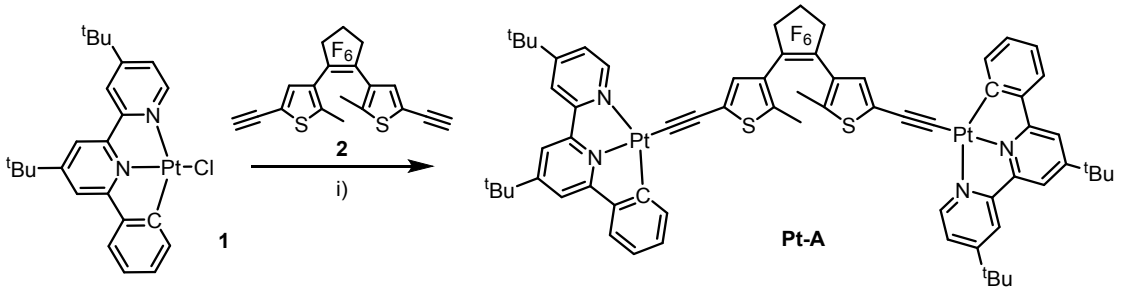
where $\mu\beta_{EFISH}$ /5kT is the dipolar orientational contribution to the molecular nonlinearity, and $\gamma(-2\omega; \omega, \omega, 0)$, the third order polarizability, is a purely electronic cubic contribution to γ_{EFISH} which can usually be neglected when studying the second-order NLO properties of dipolar compounds.
All EFISH measurements were carried out at the Dipartimento di Chimica of the Università degli Studi di Milano, working in solution at a concentration of 1 x 10^{-3} M, with a non-resonant incident wavelength of 1.907 □m, obtained by Raman-shifting the fundamental 1.064 □m wavelength produced by a Q-switched, mode-locked Nd^{3+}:YAG laser manufactured by Atalaser. The apparatus used for EFISH measurements is a prototype made by SOPRA (France). The $\mu\beta_{EFISH}$ values reported are the mean values of 16 successive measurements performed on the same sample. The estimated uncertainty in EFISH measurements is ±10%. The sign of $\mu\beta_{EFISH}$ is determined by comparison with the reference solvent (CH_2Cl_2 or DMF).
The EFISH measurements of complex **Pt-A** were carried out both in CH_2Cl_2 and in DMF, affording similar $\mu\beta_{EFISH}$ values. Due to its poor solubility in CH_2Cl_2, **Pt-B** was characterized in DMF only. As previously observed for related mononuclear Pt(II) complexes [6], **Pt-A** and **Pt-B** are characterized by a negative value of $\mu\beta_{EFISH}$, irrespective of the form of the DTE unit (open or closed), in agreement with a negative value of $\Delta\mu_{eg}$ (difference between the dipole moments of the excited and ground states). The large enhancement (multiplied by a factor of 4.5) of the quadratic NLO response of **Pt-A** upon ring-closing, by irradiation at 350 nm, clearly reflects the delocalization of the π-electron system in the closed form.

S1.b DFT and TD-DFT calculations

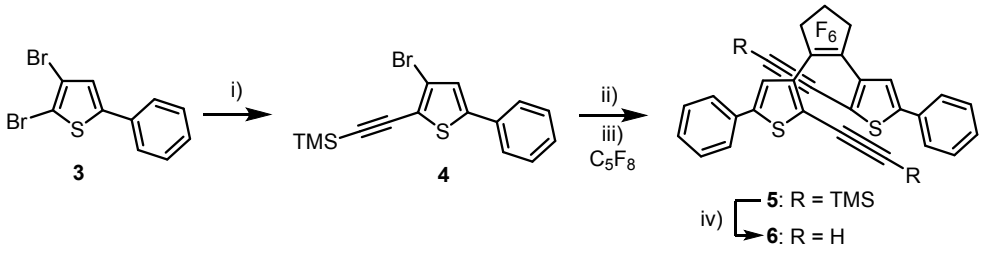
All simulations have been achieved with the Gaussian09 program [7], using Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT), for the ground and excited state properties, respectively. The computational protocol proceeds through several steps:

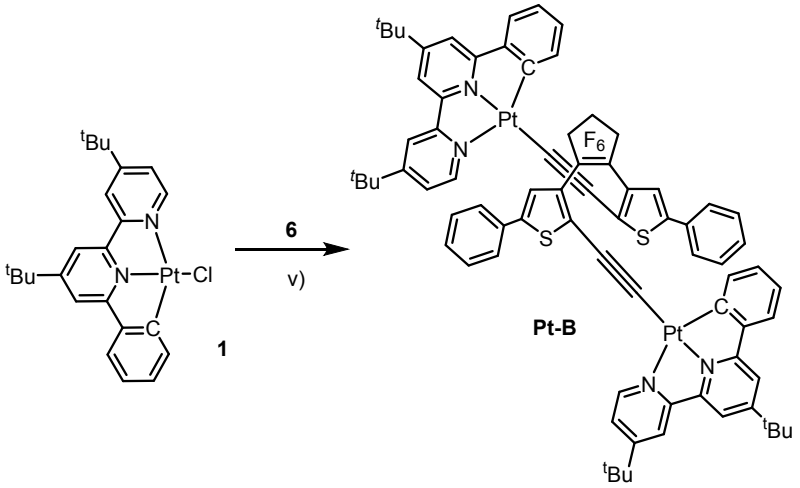
1. The optimal ground-state geometrical parameters have been determined with the PBE0 functional [8] completed with the so-called D3-BJ model [9] to describe weak interactions. These calculations use the LanL2DZ pseudo-potentials and basis set for all atoms completed with additional orbitals [10]. Spherical *d* (5D) and *f* (7F) functions were applied.
2. The vibrational spectrum of each derivative has been determined analytically at the same level of theory and it has been checked that all structures correspond to true minima of the potential energy surface.
3. Single point condensed-phase calculations were performed for all structures using the SMD model [11] and considering dichloromethane as solvent. These single point calculations aimed to reach more accurate total energies and use the more extended 6-311+G(2d,p) basis set for all atoms, except for the Pt centers that are treated with the LanL08+*f* pseudopotential and basis set.
4. From the previous steps, best estimations of the relative free energies of all structures have been obtained.
5. TD-DFT calculations, using the same level of theory as in steps 1 and 2 (PBE0/LanL2DZ+additional functions), were performed to model the excited-states. 120 excited-states were typically determined. These calculations use the PCM model [12], in its linear-response non-equilibrium variant, to account for solvation effects (dichloromethane).

S2. Procedures for the synthesis of complexes Pt-A and Pt-B



Scheme S1 Synthesis of **Pt-A**. i) CH_2Cl_2, Et_3N, CuI, 30°C, 12h.





Scheme S2 Synthesis of **Pt-B**. i) $Pd(PPh_3)_2Cl_2$, CuI, TMSA, THF, Et_3N, 60°C, 12h. ii) ^{n}BuLi, THF, -78°C to r.t., 12h. iv) CH_2Cl_2, MeOH, K_2CO_3, r.t., 3h. v) CH_2Cl_2, Et_3N, CuI, 30°C, 12h.

Synthesis of complex Pt-A. To a dry and degassed CH_2Cl_2/Et_3N (3/2: 15mL) solution of 4,4'-di(*tert*-butyl)-6-phenyl-2,2'-bipyridine platinum chloride **1** (0.400 g, 0.69 mmol), **2** (0.145 g, 0.35 mmol) and CuI (0.026 g, 0.14 mmol) were added. After 15 h of stirring at 30ºC in the dark, the mixture was extracted with dichloromethane and washed with water. The organic layer was dried over $MgSO_4$, filtered and concentrated. The residue was purified by column chromatography (SiO_2, CH_2Cl_2 + 1% Et_3N) to afford **Pt-A** (70 % orange powder). ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.10 (d, J_{H-H} = 8 Hz, 2H, NNC), 7.93 (d, J_{H-H} = 8 Hz, 2H, NNC), 7.82 (m, 2H, NNC), 7.58 (m, 6H, NNC), 7.41 (d, J_{H-H} = 8 Hz, 2H, NNC), 7.20 (t, J_{H-H} = 8 Hz, 2H, NNC), 7.11 (s, 2H, thio), 7.07 (d, J_{H-H} = 8 Hz, 2H, NNC), 1.91 (s, 6H, CH_3), 1.45 (m, 36H, ^{t}Bu). ^{13}C [^{1}H] NMR (100 MHz, CD_2Cl_2): δ 166.1, 164.4, 163.5, 157.3, 154.4, 148.5, 147.2, 142.8, 134.8, 130.6, 124.6, 124.0, 123.8, 119.3, 155.8, 155.0, 35.9, 35.7, 31.9, 30.6, 30.1, 30.0, 29.7, 29.3, 22.7, 20.4, 13.8. HRMS: *m/z* $[M+H]^+$ Calcd. for $C_{67}H_{63}N_4F_6S_2{}^{195}Pt_2$ 1491.3688, found: 1491.3676. Elemental Analysis: Calcd. for $C_{67}H_{62}F_6N_4Pt_2S_2$, 3/2 CH_2Cl_2: C, 50.82; H, 4.05; N, 3.46; S, 3.96. Found: C, 50.89; H, 4.13; N, 3.49; S, 3.90.

Photocyclization of **Pt-A**. Complex **Pt-A(o)** was irradiated in the NMR tube ($CDCl_3$) at 350 nm for 10 hours.

Pt-A(c) (>90% conversion, dark blue solution). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.95 (m, 2H, NNC), 8.15 (d, J_{H-H} = 8 Hz, 2H, NNC), 7.89 (s, 2H, NNC), 7.60 (m, 4H, NNC), 7.39 (m, 2H, NNC), 7.30 (m, 2H, NNC), 7.22 (m, 2H, NNC), 7.05 (m, 2H, NNC), 6.23 (s, 2H, thio), 2.33 (s, 6H, CH_3), 1.46 (s, 18H, ^{t}Bu), 1.44 (s, 18H, ^{t}Bu).

Synthesis of 2-phenyl-4-bromo-5-(trimethylsilylethynyl)thiophene, 4. To a dry THF (40 mL) and Et_3N (30 mL) solution of **3** (1.670 g, 5.25 mmol), $Pd(PPh_3)_2Cl_2$ (0.184 g, 0.26 mmol) and CuI (20 mg, 0.11 mmol), trimethylsilylacetylene (0.822 mL, 5.77 mmol) was added dropwise. The reaction mixture was heating at 60°C overnight under argon atmosphere. After cooling to room temperature, the reaction was extracted with dichloromethane and washed with brine. The organic phases were dried over $MgSO_4$, filtered and concentrated under vacuum. The residue was purified by column chromatography (SiO_2, petroleum ether/CH_2Cl_2, 9:1) to afford **4** (83 %, yellow oil). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53 (d, J_{H-H} = 4 Hz, 2H, Ar), 7.31 to 7.41 (m, 3H, Ar), 7.15 (s, 1H, thio), 0.28 (s, 9H, TMS). ^{13}C [^{1}H] NMR (100 MHz, $CDCl_3$): 145.1, 132.7, 129.1, 128.7, 125.7, 125.1, 119.6, 117.2, 104.2, 95.8, -0.18.

Synthesis of 1,2-bis(2-(trimethylsilylethynyl)-5-phenyl-3-thienyl)perfluorocyclopentene, 5. To a dry THF solution (30 mL) of **4** (1.470 g, 4.38 mmol) at -78°C, ^{n}butyllithium in hexane (1.5 M, 2.9 mL, 4.38 mmol) was added dropwise. The reaction mixture was stirred at -78°C for 1 hour under Ar and a dry THF solution (10 mL) of perfluorocyclopentene (0.25 mL, 2.09 mmol) was transferred by cannula at -78°C. After stirring at -78°C four 1 hour, the reaction mixture was allowed warming up to room temperature overnight. The solvent was evaporated, and the residue was extracted with CH_2Cl_2 and washed with brine. The organic layer was dried over $MgSO_4$, filtered and concentrated. The residue was purified by column chromatography (SiO_2, petroleum ether) to afford **5** (57 %, orange oil). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54 (d, J_{H-H} = 8 Hz, 4H, Ar), 7.32 to 7.42 (m, 6H, Ar), 7.27 (s, 2H, thio), 0.08 (s, 18H, TMS). ^{19}F [^{1}H] NMR (377 MHz, $CDCl_3$): δ -109.42, -131.68. ^{13}C [^{1}H] NMR (100 MHz, $CDCl_3$): δ 145.6, 132.9, 132.5, 129.3, 128.8, 126.0, 124.4, 122.7, 106.8, 95.2, -0.4. Elemental Analysis: Calcd. for $C_{35}H_{30}F_6S_2Si_2$: C, 61.38; H, 4.42; S, 9.36. Found: C, 61.63; H, 4.31; S, 8.99.

Synthesis of 1,2-bis(2-ethynyl-3-thienyl-5-phenyl)perfluorocyclopentene, 6. Compound **5** (0.600 g, 0.88 mmol) was dissolved in a mixture of dichloromethane (10 mL) and methanol (5 mL). Potassium carbonate (1.5 g, 8.80 mmol) was added and the reaction mixture was stirred at room temperature for 3 hours. After washing with brine, the organic layer was dried over $MgSO_4$, filtered and concentrated under vacuum to yield **6** (93 %, orange oil). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57 (d, J_{H-H} = 4 Hz, 4H, Ar), 7.34 to 7.44 (m, 8H, Ar + thio), 3.33 (s, 2H, C≡CH). ^{19}F [^{1}H] NMR (377 MHz, $CDCl_3$): δ -109.49, -131.41. ^{13}C [^{1}H] NMR (100 MHz, $CDCl_3$): δ 146.5, 133.7, 132.8, 129.4, 128.9, 126.1, 123.0, 122.4, 87.9, 74.9. Elemental Analysis: Calcd. for $C_{29}H_{14}F_6S_2$: C, 64.44; H, 2.61; S, 11.86.

Synthesis of complex Pt-B. To a dry and degassed CH_2Cl_2/Et_3N (3/2: 25mL) solution of 4,4'-di(*tert*-butyl)-6-phenyl-2,2'-bipyridine platinum chloride **1** (0.982 g, 1.71 mmol), **6** (0.420 g, 0.77 mmol) and CuI (0.015 g, 0.08 mmol) were added. After 15 hours of stirring at 30ºC under argon atmosphere, the red precipitate was filtered and washed with cold dichloromethane to afford **Pt-B** (80 %, red powder). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.72 (d, J_{H-H} = 4 Hz, 2H, NNC), 7.64 (d, J_{H-H} = 4 Hz, 2H, NNC), 7.62 (s, 2H, NNC), 7.61 (s, 2H, NNC), 7.55 (d, J_{H-H} = 4 Hz, 2H, NNC), 7.47 (d, J_{H-H} = 4 Hz, 2H, NNC), 7.44 (s, 2H, NNC), 7.27 (s, 2H, thio), 7.14 (m, 4H, NNC), 7.01 (d, J_{H-H} = 4 Hz, 4H, Ar), 6.80 (m, 2H, Ar), 6.71 (m, 4H, Ar), 1.50 (s, 18H, ^{t}Bu), 1.45 (s, 18H, ^{t}Bu). HRMS: *m/z* [M+Na] $^{+}$ Calcd. for $C_{77}H_{66}F_6N_4Na^{195}Pt_2S_2$ 1637.3821, found: 1637.3819. Elemental Analysis: Calcd. for $C_{77}H_{66}N_4F_6Pt_2S_2$, 1/2 CH_2Cl_2: C, 56.14; H, 4.07; N, 3.38; S, 3.87. Found: C, 55.99; H, 4.07; N, 3.46; S, 3.66.

S3. NMR Spectra

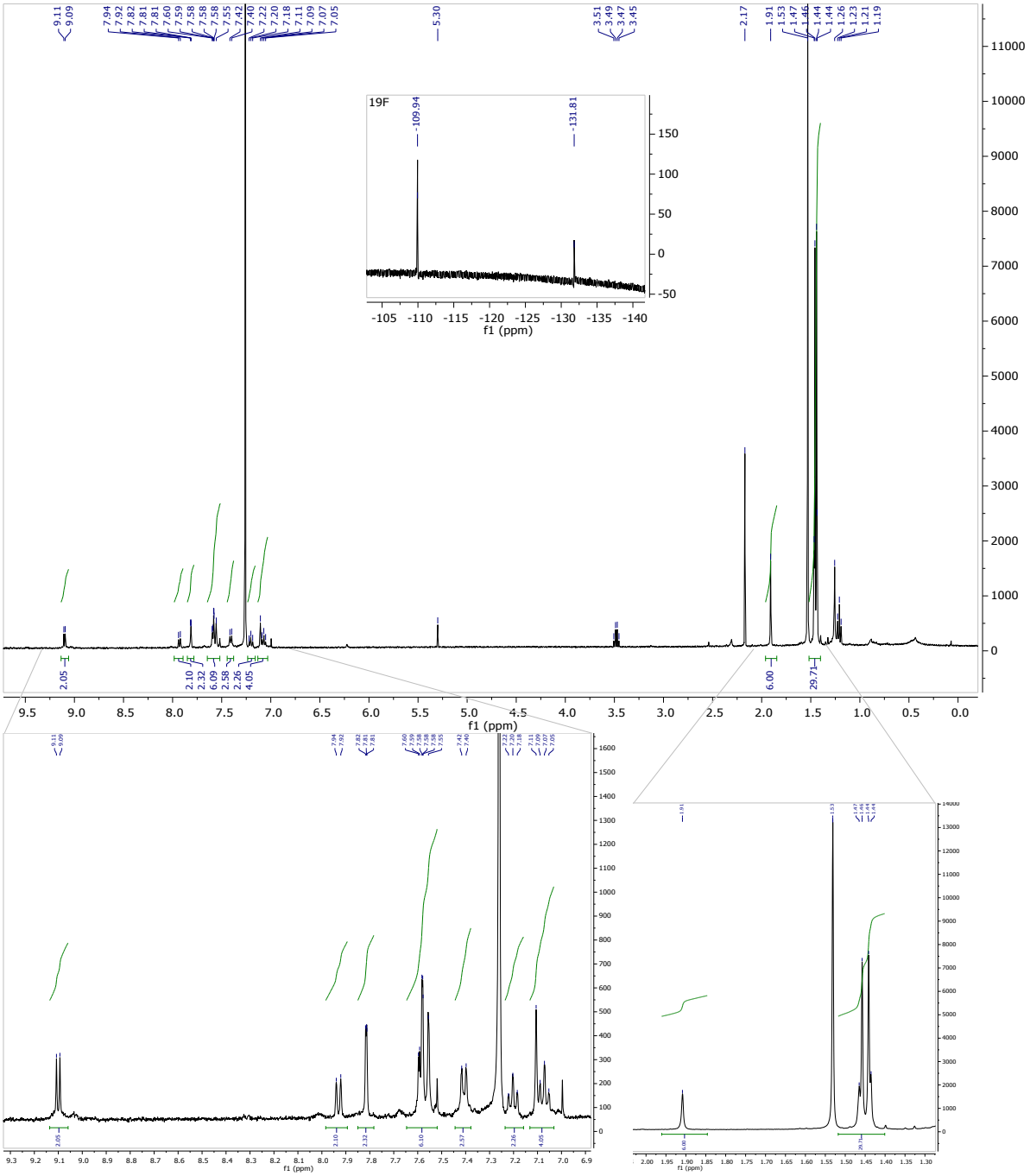


Figure S1 ^{1}H and ^{19}F [^{1}H] NMR of **Pt-A** in $CDCl_3$.

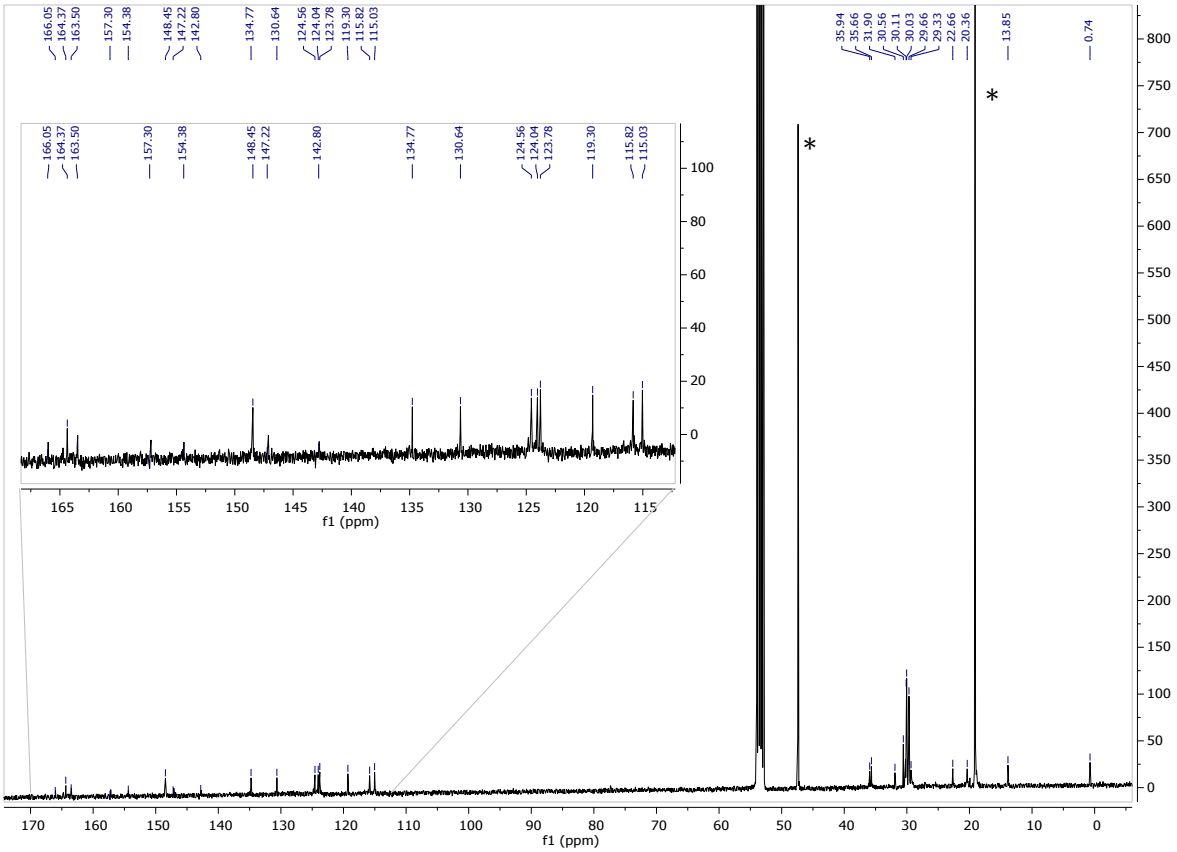


Figure S2 ^{13}C [^{1}H] NMR of **Pt-A** in CD_2Cl_2. * solvents

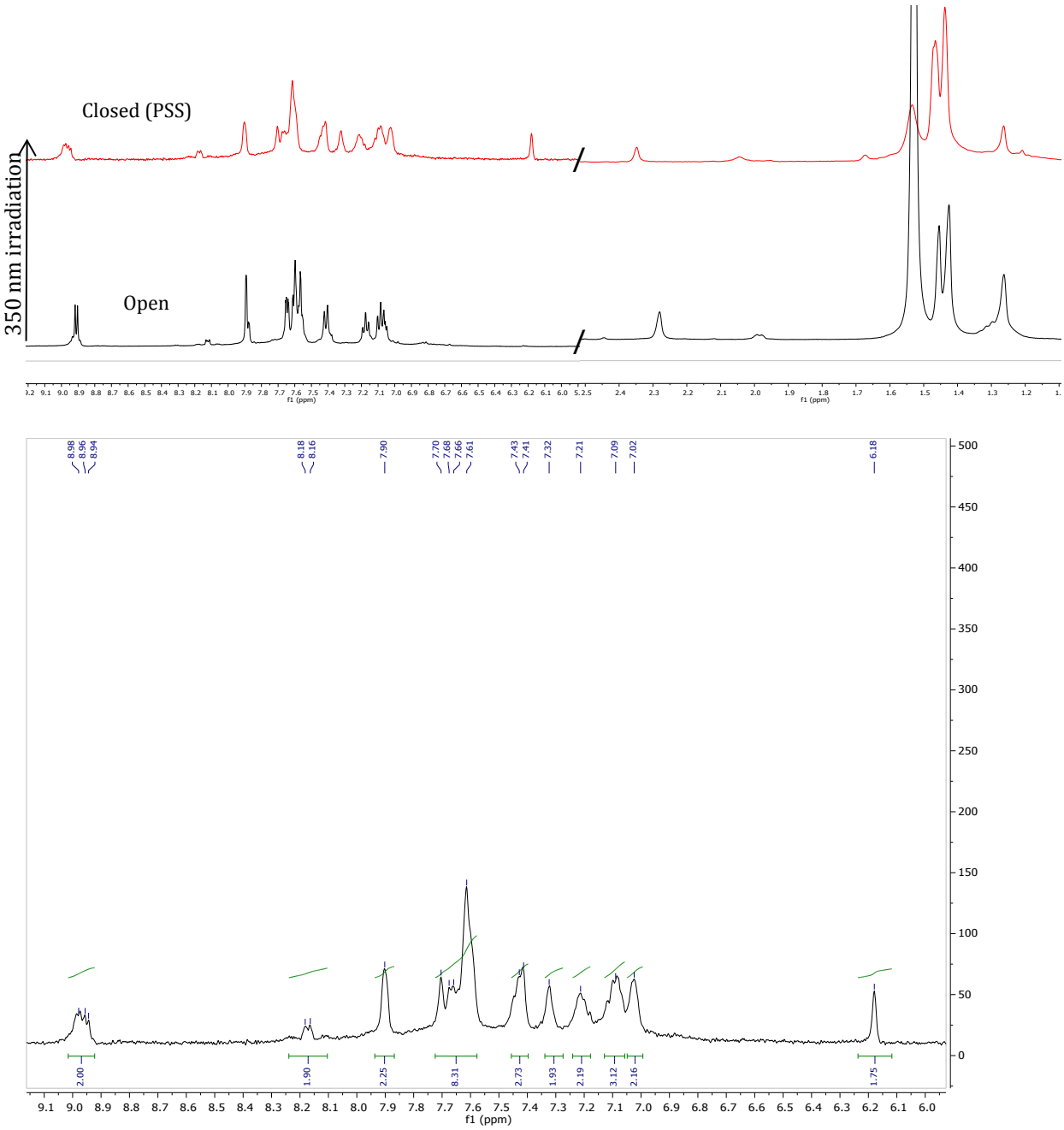


Figure S3 Top: Partial ^{1}H NMR spectra of **Pt-A** before (open) and after (PSS) irradiation at 350 nm, in CD_2Cl_2. The ^{1}H NMR spectrum of the closed (PSS) form shows broad signals due to a lower solubility. Bottom: ^{1}H NMR spectrum of **Pt-A(c)** (PSS) in CD_2Cl_2, from 6.0 to 9.2 ppm.

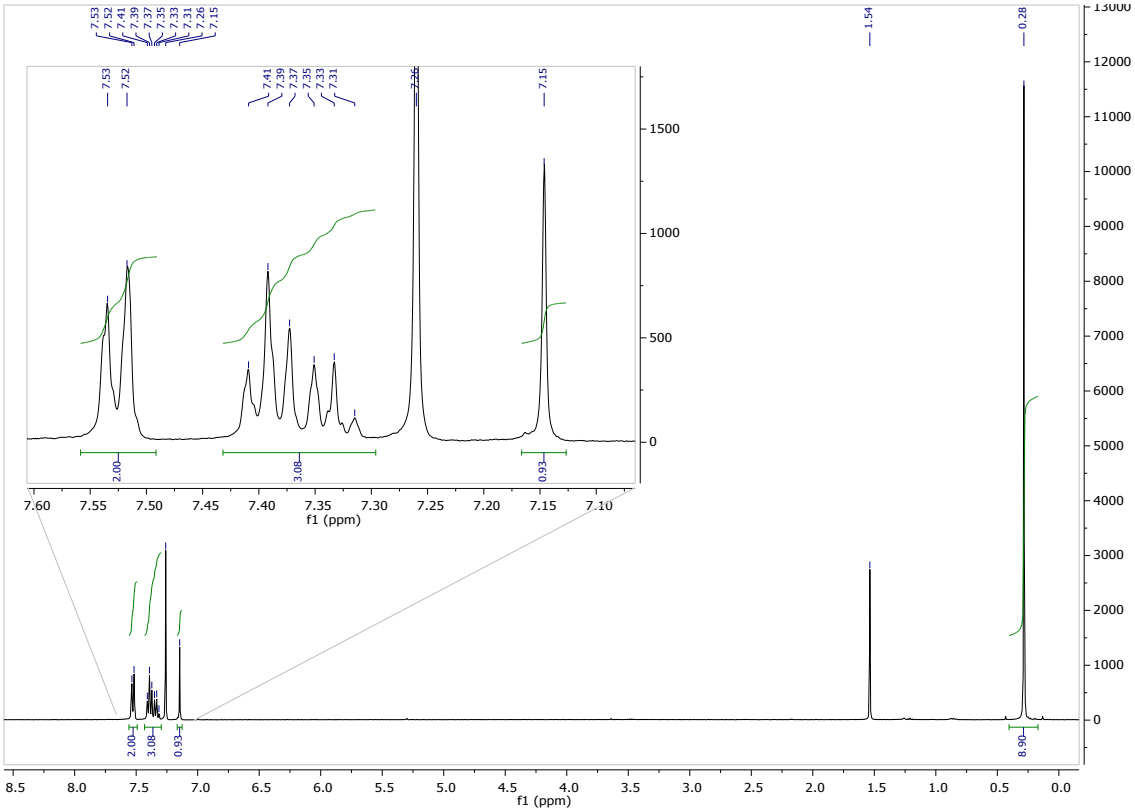


Figure S4 ^{1}H NMR of **4** in $CDCl_3$.

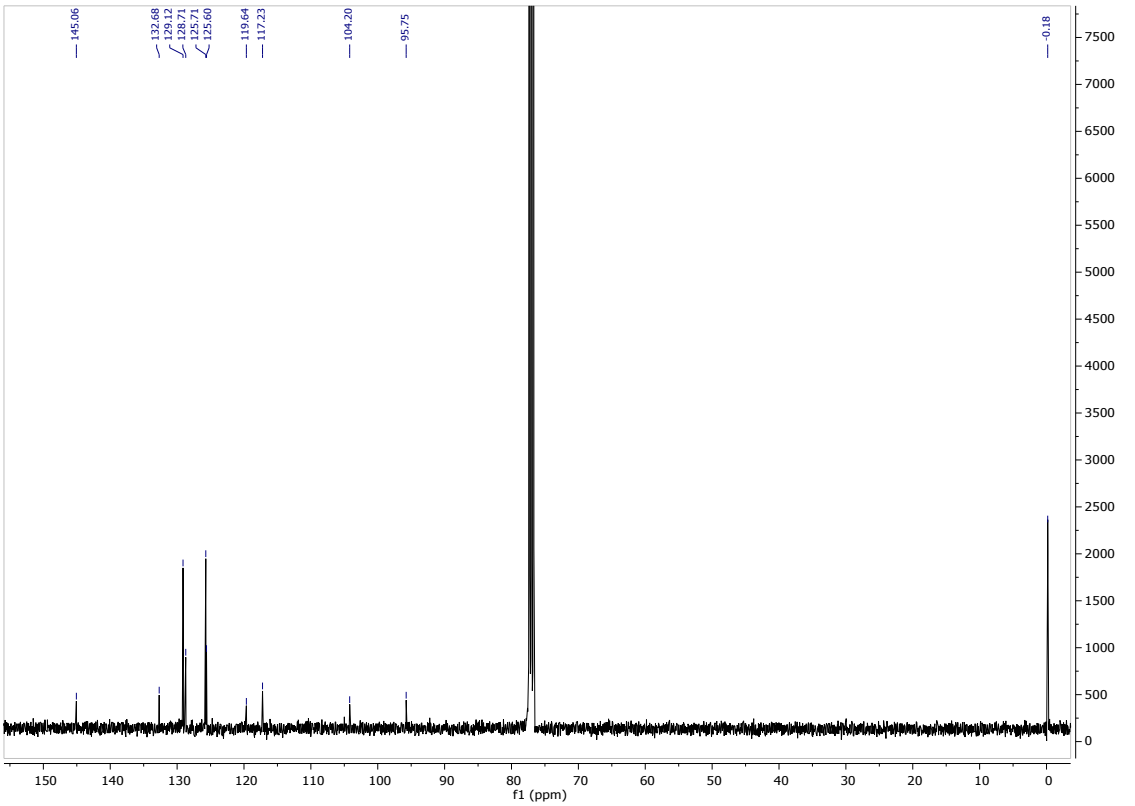


Figure S5 ^{13}C [^{1}H] NMR of **4** in $CDCl_3$.

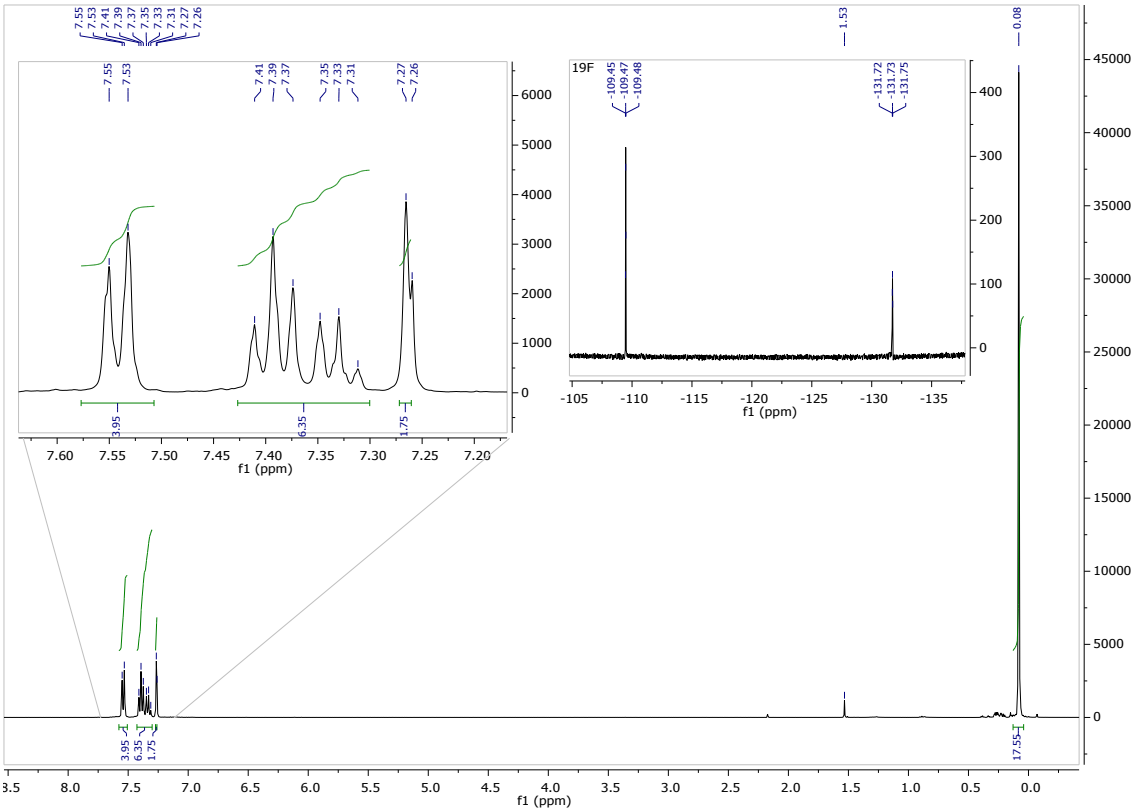


Figure S6 ^{1}H and ^{19}F [^{1}H] NMR of **5** in $CDCl_3$.

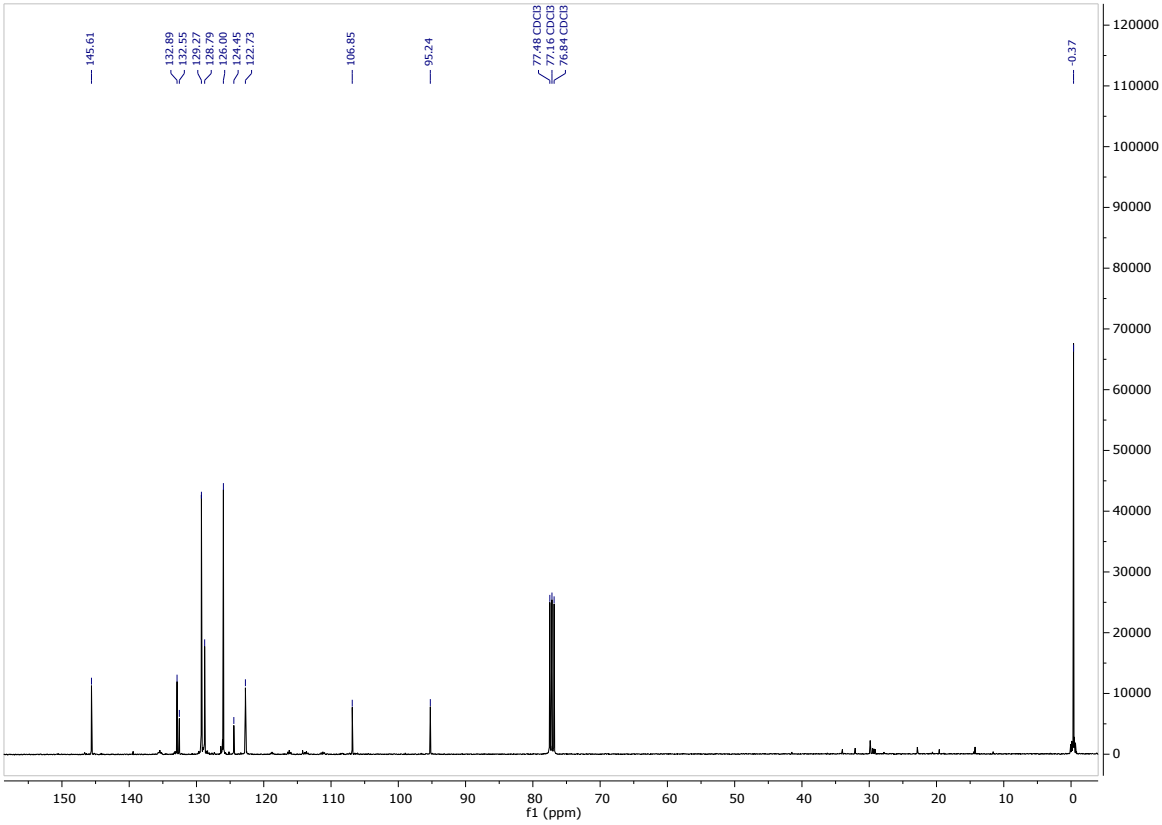


Figure S7 ^{13}C [^{1}H] NMR of **5** in $CDCl_3$.

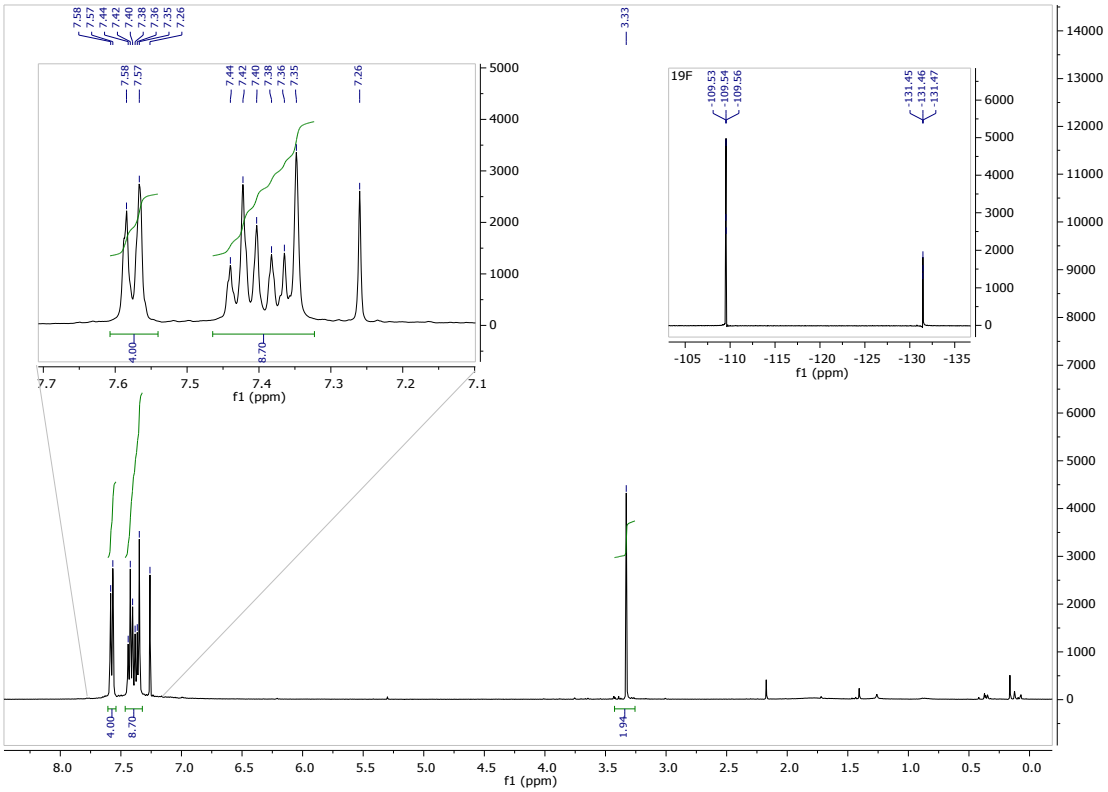


Figure S8 ^{1}H and ^{19}F [^{1}H] NMR of **6** in $CDCl_3$.

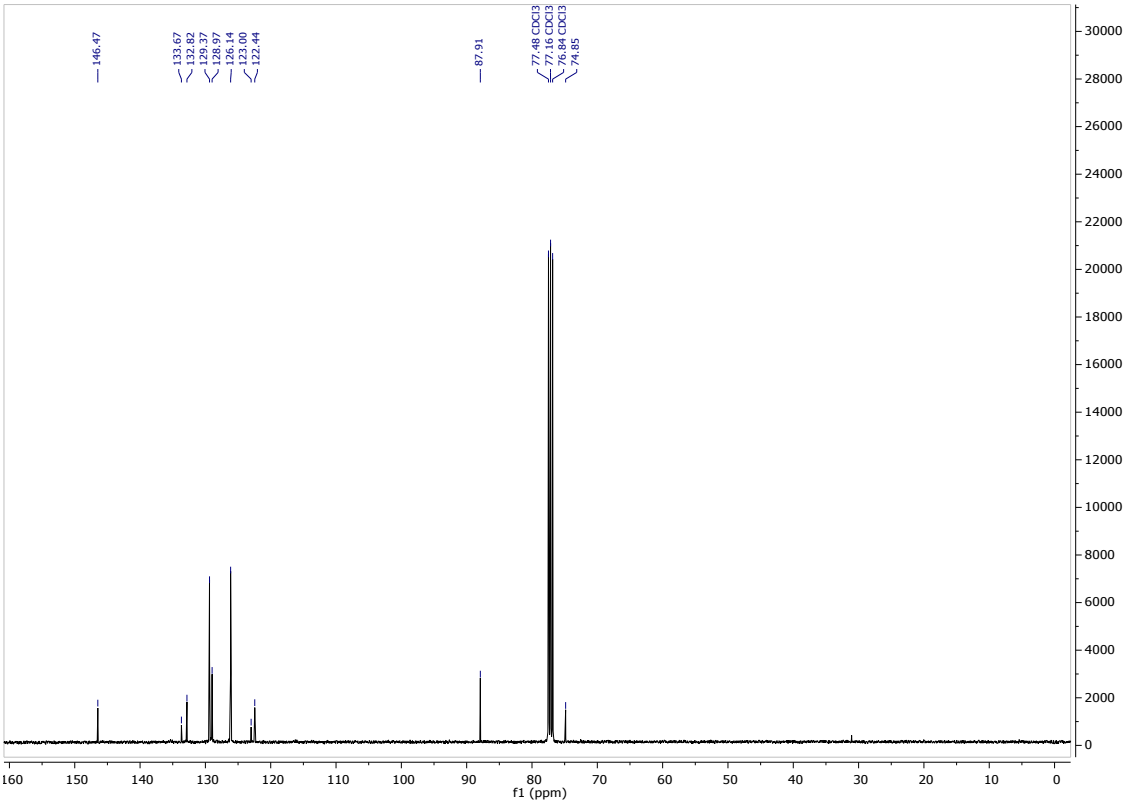


Figure S9 ^{13}C [^{1}H] NMR of **6** in $CDCl_3$.

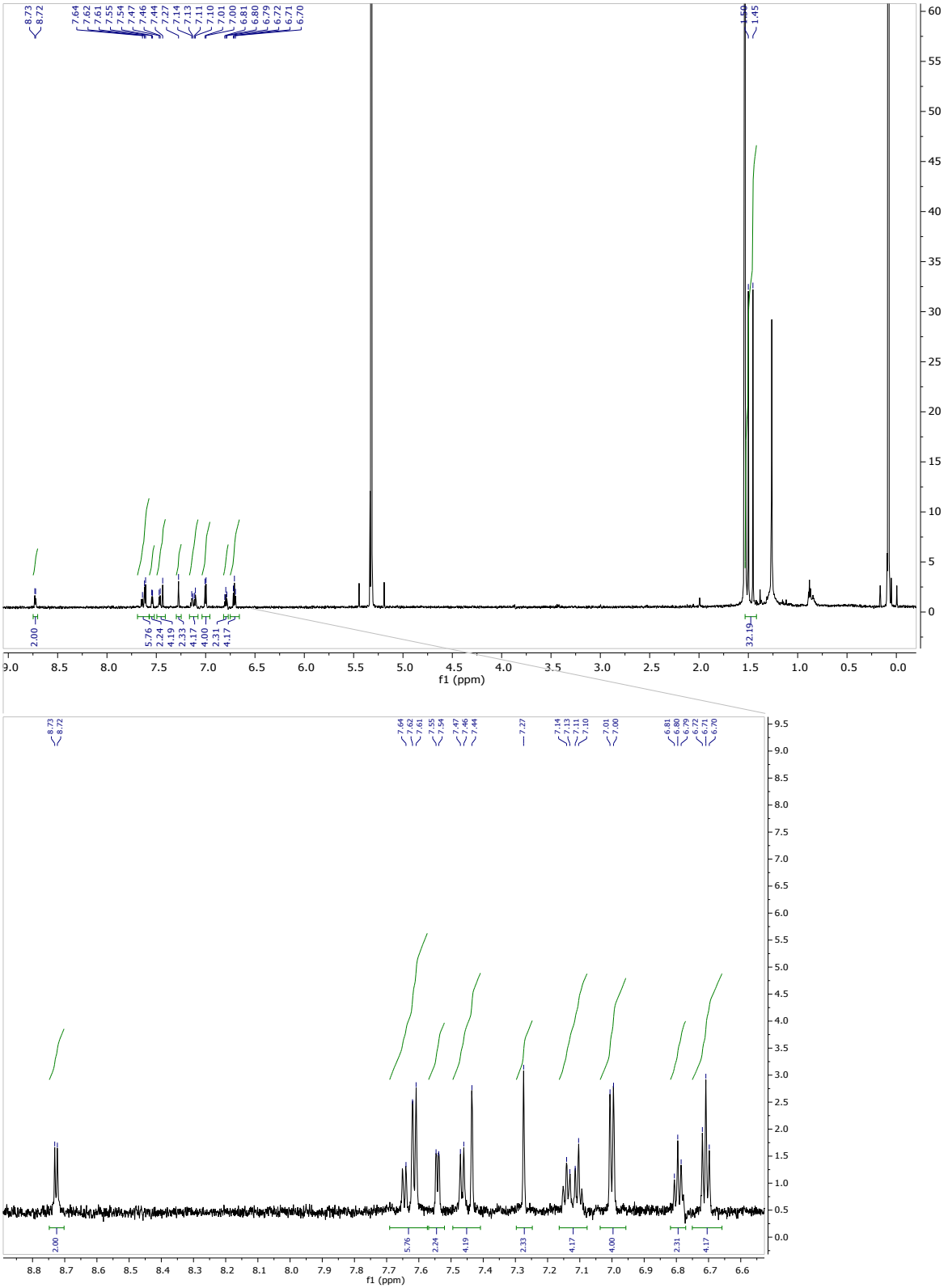


Figure S10 ^{1}H NMR of **Pt-B** in CD_2Cl_2.

S4. VT-NMR Experiments

We have also carried out variable temperature experiments in an effort to obtain more insights into the conformer population of each species. First, we underline that, in this specific organometallic case, the evaluation of the population ratio of P and AP conformers at 293 K by monitoring the chemical shifts of the thiophene signals as a function of the probe's temperature, usual for purely organic DTEs, is not appropriate, because. For **Pt-A**, the chemical shift of the methyl signal as a function of the temperature gives a linear correlation, preventing the determination of the AP/P ratio (see Figures S11 and S12). Moreover, the signal of the thienyl proton is too broad at low temperature to be used here for this purpose.

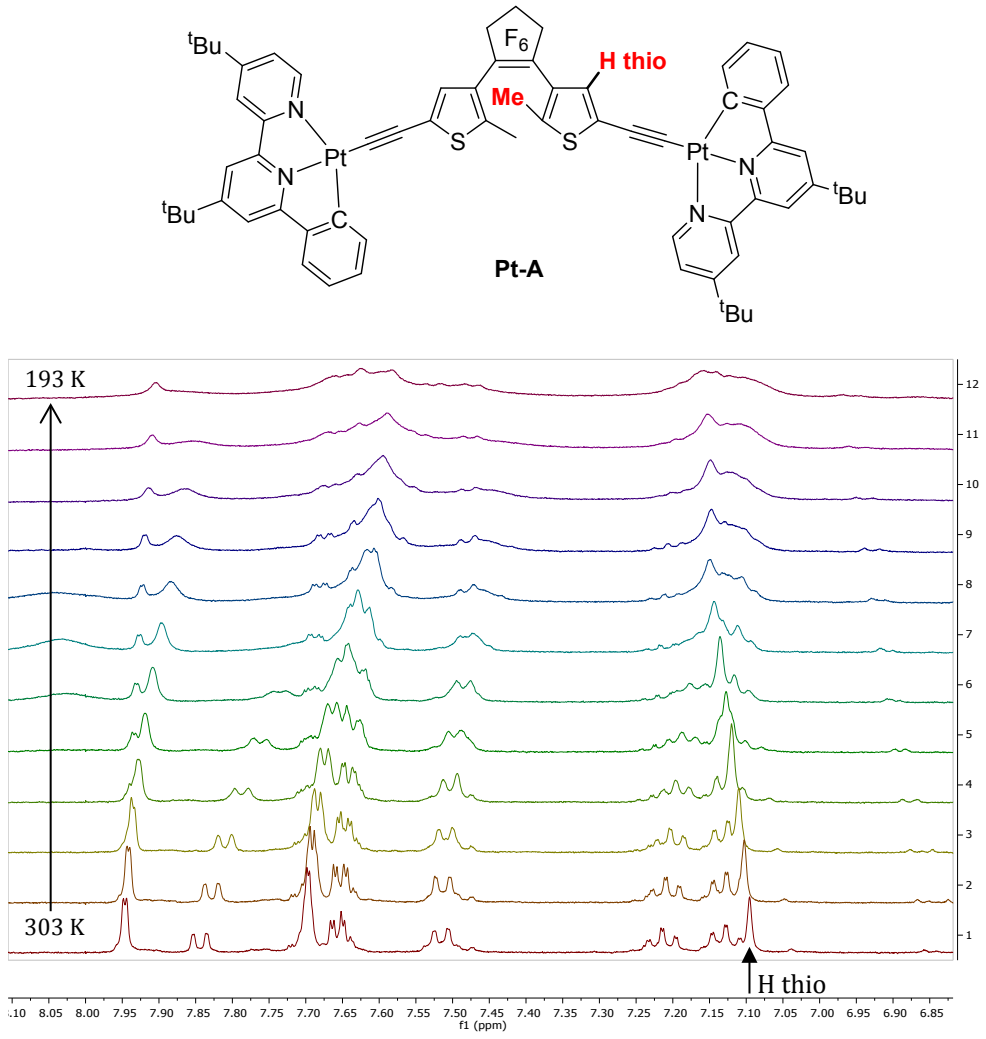


Figure S11. Variable temperature ^{1}H NMR spectra (from 6. 8 to 9.1 ppm) of **Pt-A** in CD_2Cl_2.

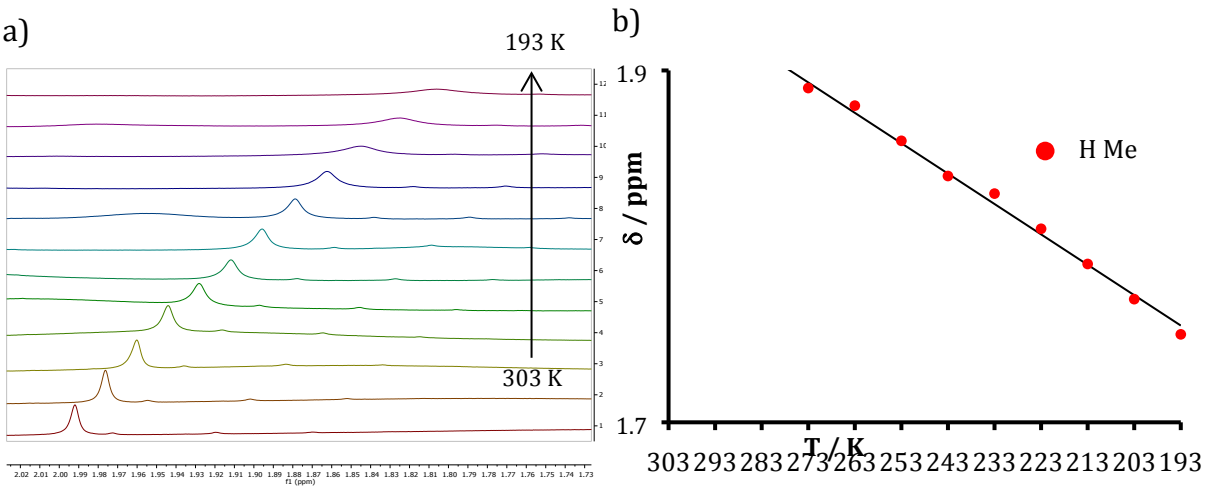
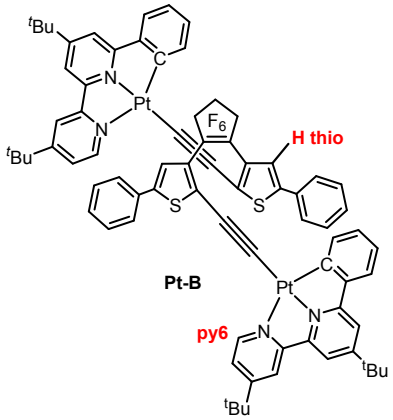


Figure S12. a) Variable temperature ^{1}H NMR spectra (from 1.7 to 2 ppm) of **Pt-A** in CD_2Cl_2. b) Variation of the normalized chemical shift δ (CD_2Cl_2) of singlet attributed to the methyl protons of **Pt-A**, from 303 to 193 K with 10 K step.

For **Pt-B,** we observe a linear correlation between the chemical shift δ *vs*. temperature (Figures S13 and S14), for the singlet attributed to the thienyl proton. From these data, one cannot calculate the ratio of AP/P forms, considering a fast equilibrium. In fact we cannot rule out that **Pt-B** can exist only as the AP form, the form observed by X-Ray structure studies.



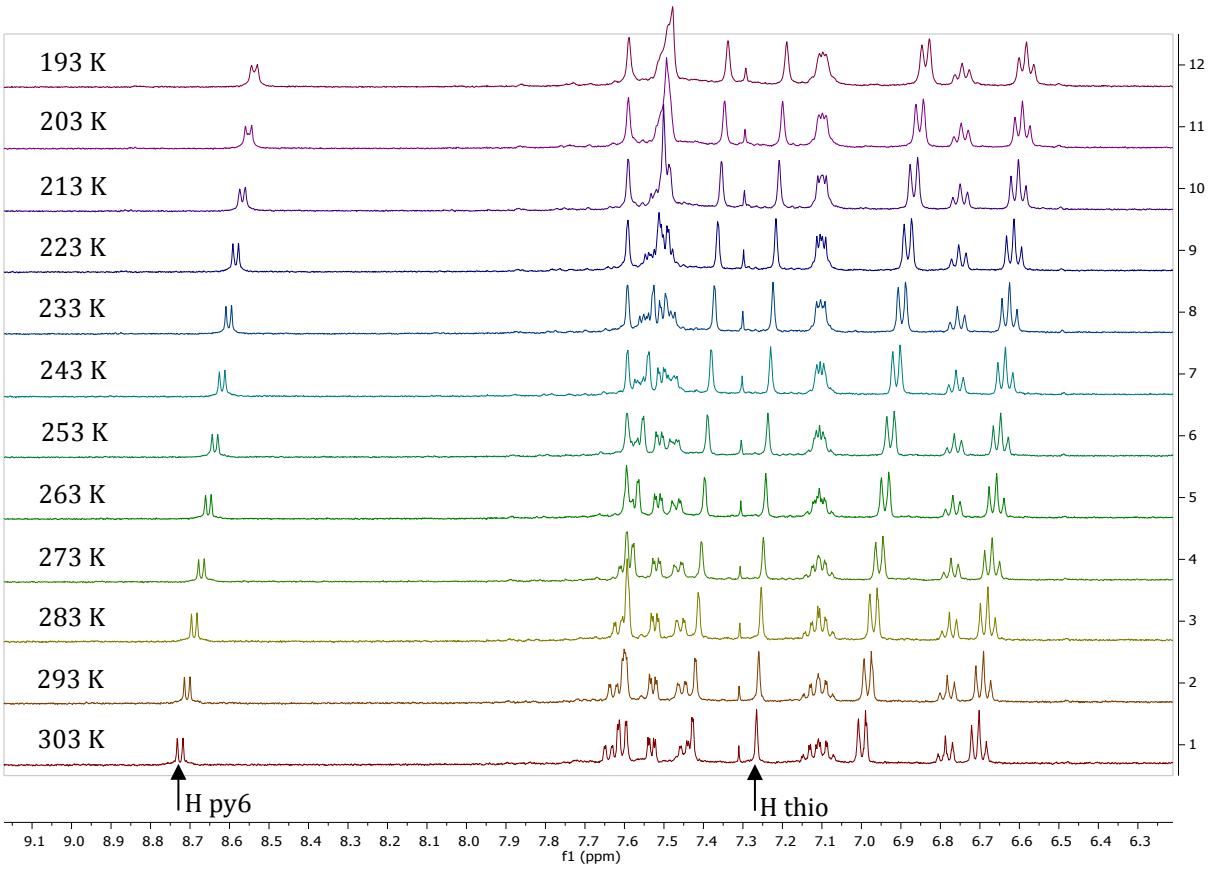


Figure S13. Variable temperature ^{1}H NMR spectra (6.2 - 9.2 ppm) of **Pt-B** in CD_2Cl_2.

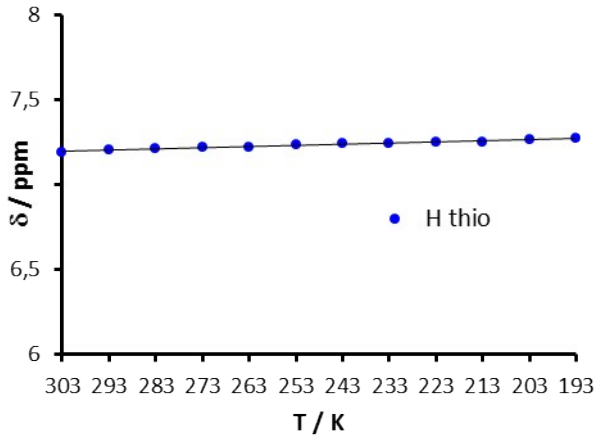


Figure S14. Variation of the normalised chemical shift δ (CD_2Cl_2) of thienyl proton signal of **Pt-B**, from 303 to 193 K with 10 K step.

S5. Crystal structure determination of Pt-B

Orange crystals were grown by slow diffusion of diethyl ether into a concentrated dichloromethane solution of **Pt-B**. An orange crystal of dimensions 0.14 mm x 0.26 mm x 0.33 mm mounted in a glass capillary was used for data collection. Intensity data were collected at 140 K in CCD SuperNova EosS2, Cu α radiation (λ = 1.54184 Å). Crystal data for (C_{77} H_{66} F_6 N_4 Pt_2 S_2); M = 1615.63: Monoclinic P $2_1/c$ (I.T.#14), a = 12.1203(3), b = 21.6638(5), c = 27.3069(9) Å, V = 7168.0(3) Å^3. Z = 4, d = 1.497 g.cm^{-3}, μ = 8.225 mm^{-1}. The structure was solved by direct methods using the *SIR97* program [13], and then refined with full-matrix least-square methods based on F^2 (*SHELXL-97*) [14]. The contribution of the disordered solvents to the calculated structure factors was estimated following the *BYPASS* algorithm [15], implemented as the *SQUEEZE* option in *PLATON* [16]. A new data set, free of solvent contribution, was then used in the final refinement. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 13719 unique intensities and 844 parameters converged at $\omega R(F^2)$ = 0.2789 ($R(F)$ = 0.1088) for 11610 observed reflections with $I > 2\sigma(I)$. Goodness-of-fit of 1.05. CCDC 1446905.

Structural data for **Pt-B**

Empirical formula		C_{77} H_{66} F_6 N_4 Pt_2 S_2
	Formula weight	1615.63
	Temperature	140(2) *K*
	Wavelength	1.54184 Å
	Crystal system, space group	Monoclinic, P $2_1/c$
	Unit cell dimensions	a = 12.1203(3) Å, α = 90 °
		b = 21.6638(5) Å, β = 91.372(3)°
		c = 27.3069(9) Å, γ = 90 °
	Volume	7168.0(3) Å^3
	Z, Calculated density	4, 1.497 (g.cm^{-3})
	Absorption coefficient	8.225 mm^{-1}
	F(000)	3192
	Crystal size	0.138 x 0.027 x 0.017 mm
	Crystal color	red
	Theta range for data collection	3.238 to 70.764 °
	h_min, h_max	-14, 13
	k_min, k_max	-26, 24
	l_min, l_max	-33, 33
	Reflections collected / unique	89426 / 13719 [R(int)[a] =0.1123]
	Reflections [I>2σ]	11610
	Completeness to theta_max	0.995
	Absorption correction type	multi-scan
	Max. and min. transmission	0.857 , 0.470
	Refinement method	Full-matrix least-squares on F^2
	Data / restraints / parameters	13719 / 0 / 844
	Goodness-of-fit	1.057
	Final *R* indices [I>2σ]	$R1^c$ = 0.1088, $wR2^d$ = 0.2789
	R indices (all data)	$R1^c$ = 0.1225, $wR2^d$ = 0.2870
	Largest diff. peak and hole	4.610 and -4.253 e$^-$.Å^{-3}

S6. Photophysical studies of Pt-B

The luminescence behavior of **Pt-B** was determined using two different spectrofluorometers (See S1.a Experiments).

a) *b)*

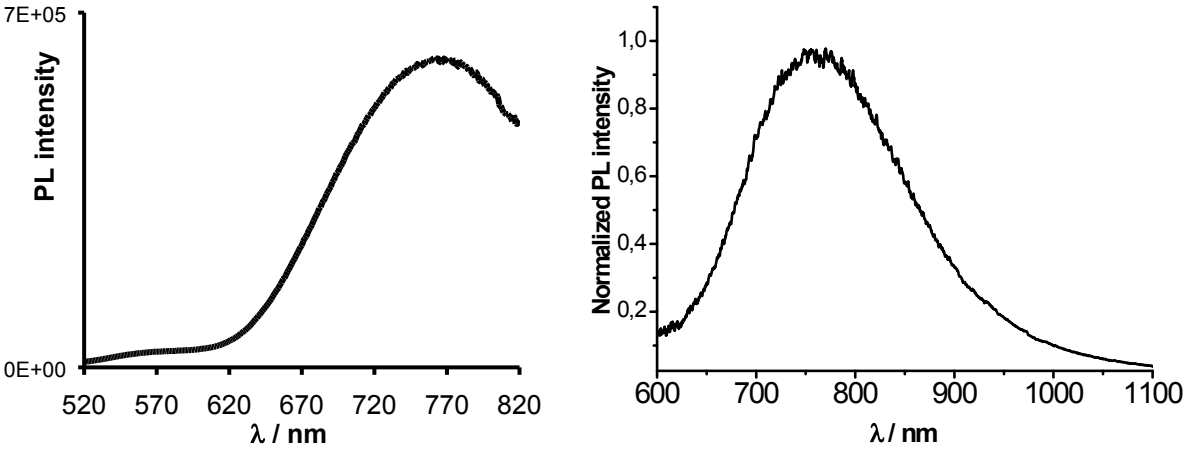


Figure S15 Emission spectra of **Pt-B** recorded in degassed CH_2Cl_2 at 298 K with *a) equipment I*, λ_{ex} = 440 nm; and *b) equipment II*, λ_{ex} = 436 nm (ΦY = 0.0009).

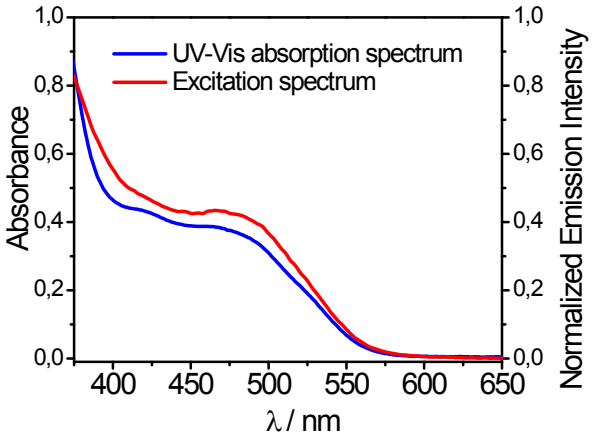


Figure S16 Electronic absorption and excitation (λ_{em}= 765 nm) spectra of **Pt-B** in CH_2Cl_2 at room temperature. (conc. = 3.70×10^{-5} M).

S7. Additional theoretical results

S7.a Conformational search

We have first explored the conformational space for the different structures than can be build. To assess their relative energies, we have considered their gas-phase free energies corrected by single-point solvent calculations. As described in the *Theoretical Methods* section these calculations account for dispersion effects that are essential for the studied systems. We present below only the most stable structures obtained considering both the parallel (P) and anti-parallel (AP) open DTE structures as well as the closed (C) DTE structure

In Figure S17, we report the lowest energy conformers for the P, AP and C forms for the *classical* **Pt-A**. As can be seen, in the AP form, one finds a rather standard structure with the side metallic-containing groups well separated. The situation is similar in the C structure that is only 6.3 kcal.mol^{-1} less stable than the AP one. Such value is in the line of the expected difference between AP and C isomers in DTE photochromes (ca. 5-20 kcal.mol^{-1}) [17]. In contrast, the P conformer that is often almost isoenergetic to its AP counterpart is significantly favoured in **Pt-A**. Indeed, the P conformer of Figure S17 lies 11 kcal.mol^{-1} below its AP counterpart according to theory (and therefore 17.3 kcal.mol^{-1} below the closed form). This is obviously resulting from the stabilising π-stacking interactions between the Pt complexes only present in P. Therefore, in solution, there is, at a given time, only a small fraction of the "photochromically active" AP structures for **Pt-A**.

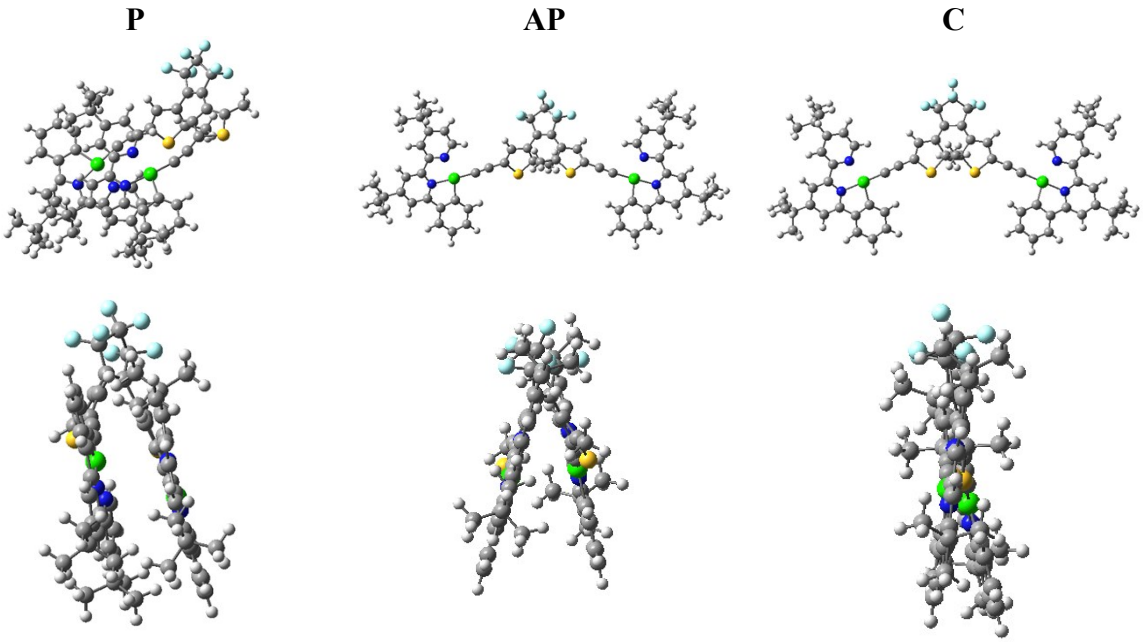


Figure S17 Two views for the most stable conformers of each forms of **Pt-A**

In Figure S18, we report the lowest energy conformers for the P, AP and C forms for the *non-classical* **Pt-B**. The situation is dramatically modified compared to **Pt-A**. Indeed, in **Pt-B** π-stacking interactions involving Pt moieties are present in both the P and AP conformers. In the former, these interactions take place between the two Pt complexes whereas, in the latter, each Pt complex interacts with the thienyl-phenyl groups of the DTE. This obviously corresponds to the XRD structure shown in Figure 1 in the main text. As a consequence, the P and AP forms of **Pt-B** are very close on the energetic scale. Indeed the AP structure is only

0.8 kcal.mol^{-1} more stable than the P conformer (this difference, smaller than 1 kcal.mol^{-1}, is negligible at this level of theory). In solution, one has therefore a blend of P and AP conformers for **Pt-B**. For the closed **Pt-B**, no intramolecular stacking interactions are possible, so that it is much less stable than in "standard" DTE, with a relative free energy of +35.5 kcal.mol^{-1} (compared to AP).

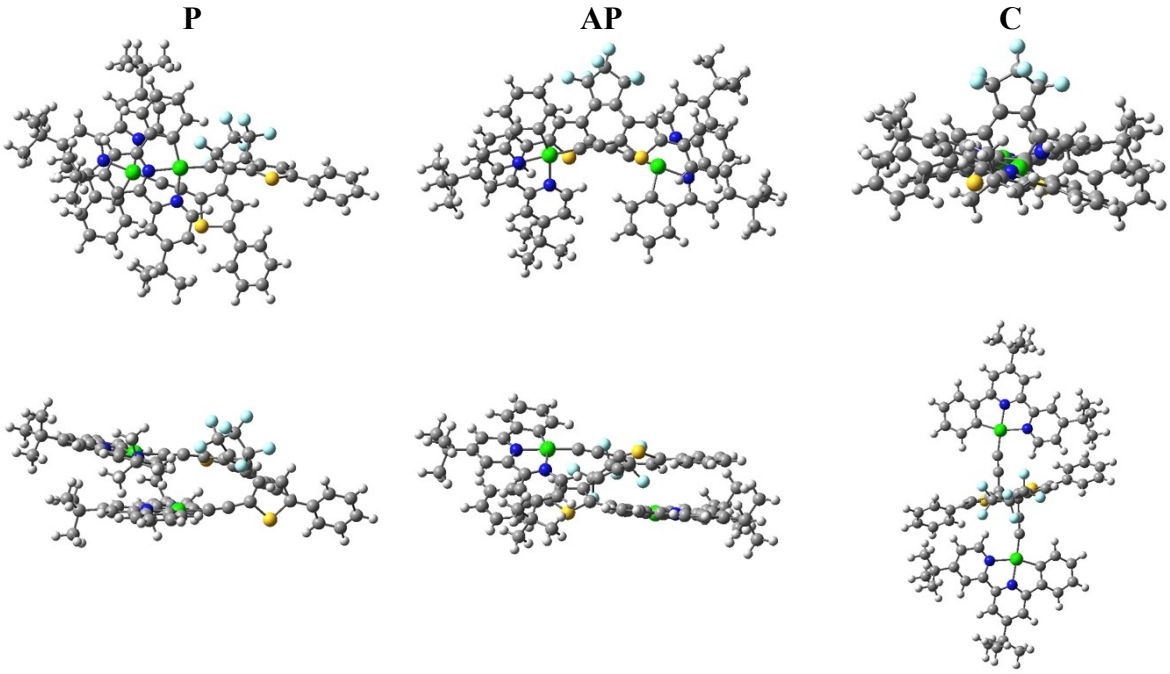


Figure S18 Two views for the most stable conformers of each forms of **Pt-B**

S7.b UV/Vis spectra analysis

In Figure S19, we report the TD-DFT UV/Vis absorption profiles that can be compared directly to the one of the main text (Figure 2). As can be seen, though the hallmark maximum of the closed isomer is shifted to the red compared to the measurements, TD-DFT reproduces correctly the key features and notably the increase of intensity and the redshift of the longest wavelength band when going from **Pt-A** to **Pt-B**.

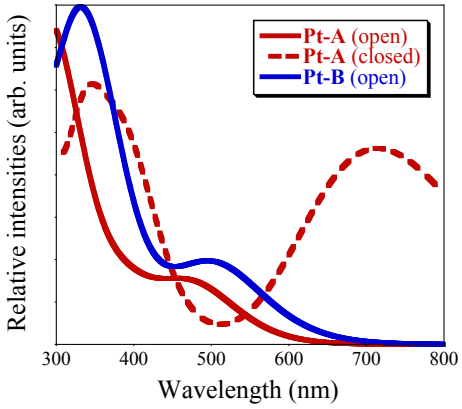


Figure S19 Simulated spectra corresponding to Figure 2 (left) in the main text. This spectra have been obtained on the basis of vertical TD-DFT "stick" transitions broaden with a Gaussian function presenting a HWHM of 0.3 eV. Only the most stable conformers was considered for each forms.

The two main electronic transitions responsible for the intensity of the 400-500 nm band in **Pt-A** (P conformer) are located by TD-DFT at 487 nm (*f*=0.22) and 466 nm (*f*=0.08) and respectively correspond to transitions between the HOMO-1 and the LUMO and the HOMO and the LUMO+1. As can be seen in Figure S20, the occupied orbitals are centered on the thiophene rings, ethynyl linker and Pt atoms, whereas the unoccupied orbitals are centred on the ethynyl and pyrdine ligands. The strong absorption band at 300-400 nm encompasses a very large number of excited-states, the two most intense states being at 354 nm (*f*=0.18) and 305 nm (*f*=0.18). These states present a complex MO blend with a mixed IL/LLCT character.

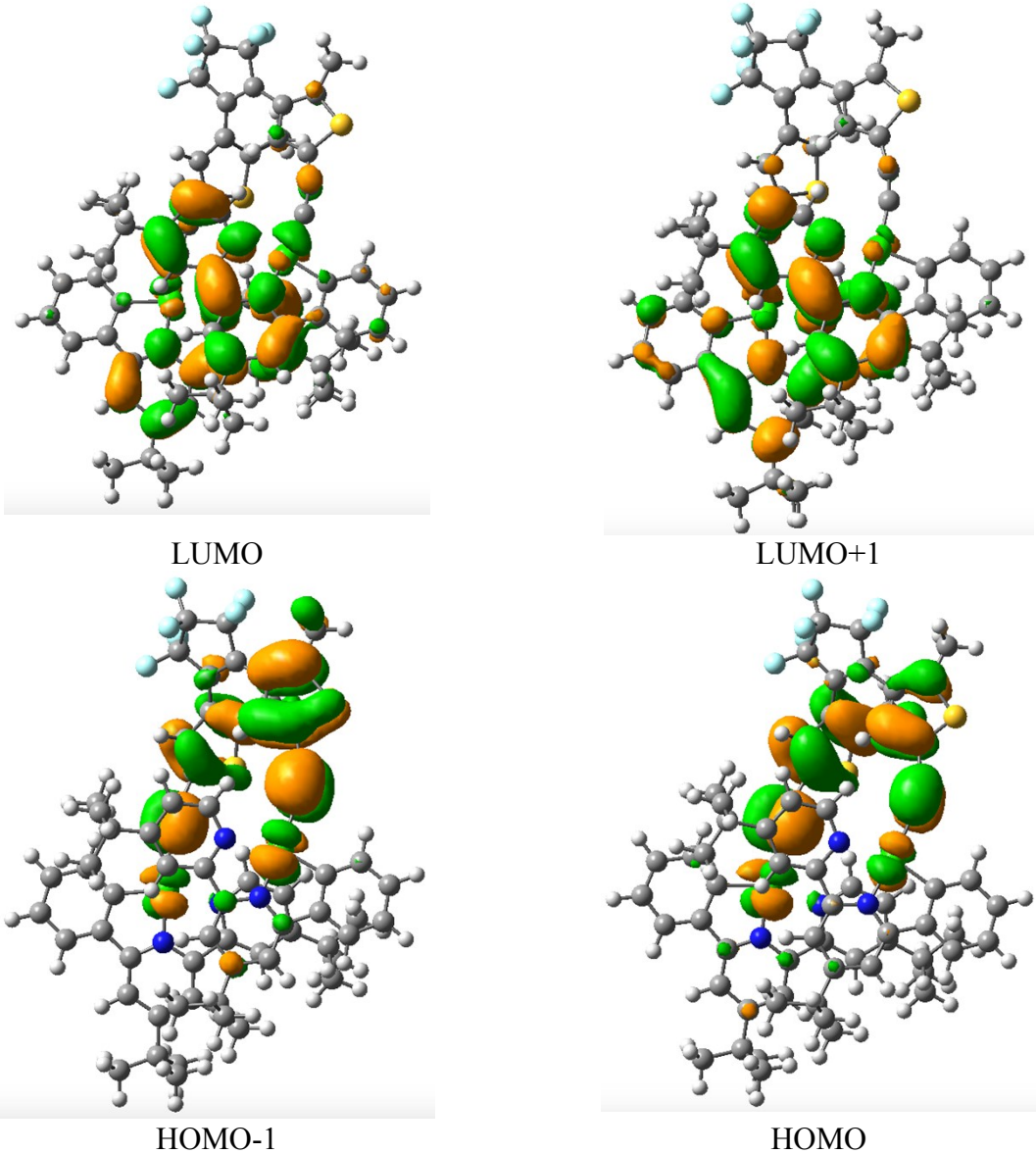


Figure S20 Key fontier MOs in the open form of **Pt-A** (P)

The three main electronic transitions responsible for the 400-500 nm band in **Pt-B** (AP conformer) are located by TD-DFT at 525 nm (*f*=0.10), 515 nm (*f*=0.13) and 500 nm (*f*=0.11) and respectively correspond to transitions between HOMO and LUMO, HOMO-1 and LUMO and HOMO-1 and LUMO+1 orbitals. As can be seen in Figure S21, these transitions have the same nature as in **Pt-A**. The strong absorption band at 300-400 nm encompasses a very large number of excited-states, the two most intense states being at 369 nm (*f*=0.40) and 335 nm (*f*=0.26). Again their character is similar to the one found in **Pt-A**.

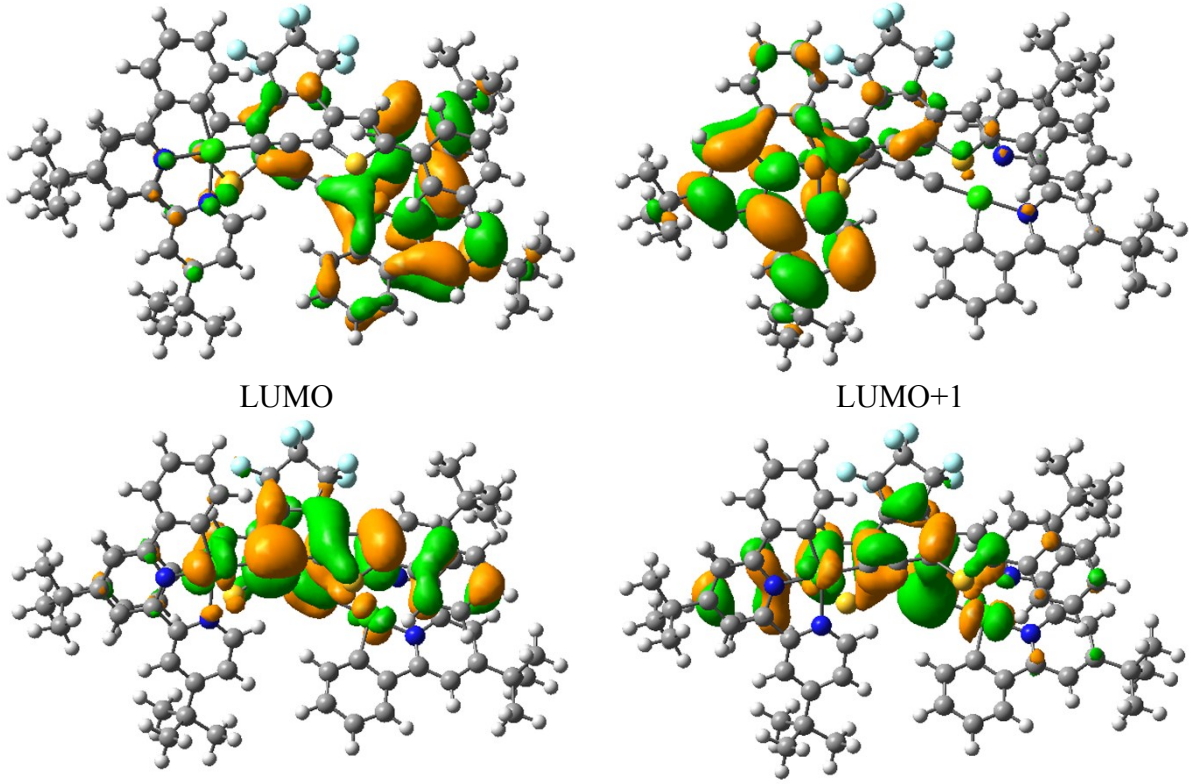


Figure S21 Key fontier MOs in the open form of **Pt-B** (AP)

For the closed **Pt-A** the new intense band in the visible can be mainly ascribed to a HOMO-LUMO transition (See Figure S22). As expected, the former is localised on the DTE core with contributions from the ethynyl, whereas the latter extends on almost the entire π-delocalization path, but with a shape on the photochromic core that remains typical of closed DTE [18].

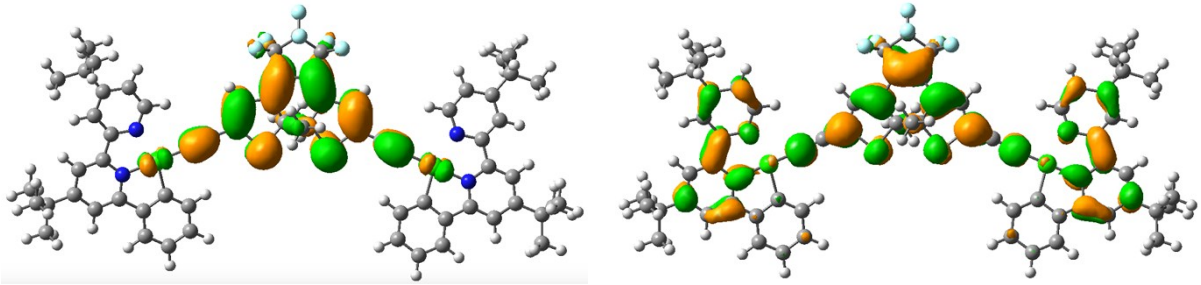


Figure S22 Frontier orbitals (left: HOMO, right: LUMO) in the closed isomer of **Pt-A**.

S7.c Photochromism

For the very large systems investigated here, the theoretical investigation of photochromic reaction cannot in practice rely on refined CAS-PT2 or MR-CI techniques. Consequently we go for a DFT/TD-DFT approach that is more qualitative but was often found very useful to understand photochromic properties of DTE [18]. In Ref. 18, three criteria necessary to reach the closed form are defined: i) an adequate topology for the excited-states; ii) a relatively

short C-C distance in the open (anti-parallel) open form; iii) a thermodynamically stable closed form.

To explain the absence of the closed form the **Pt-B** despite the dominating presence of anti-parallel open structures, we have first investigated the topology of the frontier orbitals and we found that the LUMO of **Pt-B** has indeed a bonding character between the two carbon atoms corresponding to the additional single bond formed in the closed form. This indicates that there is no electronic problem to form the closed form in **Pt-B** [18]. Let us now consider the distance separating the two reactive carbon atoms in the anti-parallel open forms. For **Pt-B** theory predicts a 3.42 Å separation (the XRD value is 3.31 Å), which is actually smaller than in the corresponding **Pt-A** structure (3.49 Å), and in line with expectations for an open DTE. These ca. 3.3-3.5 Å separations are not a problem for photochromism [19]. The third criterion that can explain the lack of photochromism is the unstable character of the putative closed form. In **Pt-A**, the closed form is only 6.3 kcal.mol^{-1} above the anti-parallel form and presents a central C-C distance of 1.537 Å. In contrast in **Pt-B**, the closed form is 35.5 kcal.mol^{-1} above the anti-parallel form and the central C-C distance attains 1.551 Å. It has been shown previously that there is a correlation between the thermal stability of the closed form and this C-C bond, i.e., C-C distance significantly exceeding 1.53 Å lead very unstable products [20]. We have therefore performed relaxed scan of the central C-C distance on both the singlet and triplet potential energy surfaces (Figure S23 below; Figure 3 in the main text). These scans were performed using the methodology given in the *Theoretical Methods* section of the present ESI, optimizing all parameters but the CC distance moved by steps of 0.25 Å going from the open (AP) to the closed DTE form. We are well aware that the singlet energies corresponding to the transition state will be too high energy due to the well-known difficulty to describe single bond formation and breaking with (standard) DFT, but our goal is here to compare two very similar systems. More refined strategies like the broken-symmetry DFT were attempted but were found not to converge for the large compounds investigated here.

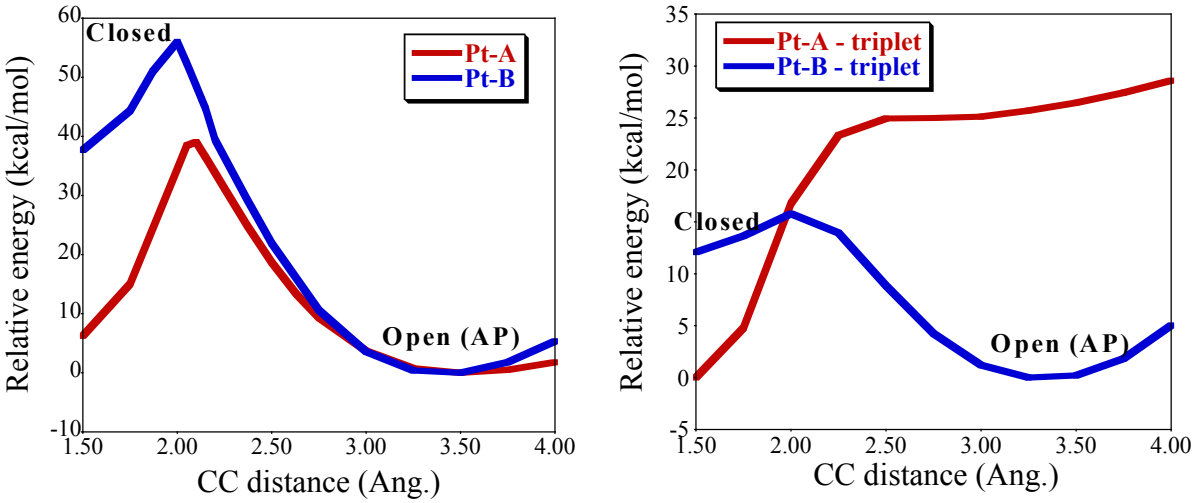


Figure S23 Non-smoothed PES corresponding to Figure 3 in the main text.

S7.d Cartesian coordinates

Below are the Cartesian coordinates (in Å) determined for the compounds displayed in Figures S17 and S18.

Pt-A (P)

16	-3.0149490	-0.7677520	-2.7120520
16	-6.0408420	3.5728720	-0.3620890
9	-7.6420950	-3.1995620	-1.6261070
9	-6.4812110	-3.6494960	0.1557050
9	-9.5097860	-2.8413000	0.1429450
9	-8.0714270	-2.3705020	1.7092100
9	-9.3549980	-0.4761810	-0.8943710
9	-8.8969570	0.0134160	1.1764160
6	-4.7116390	-0.6896240	-2.3951320
6	-5.0338330	-1.4549390	-1.2848010
6	-3.9047410	-2.1280410	-0.7143710
1	-3.9587510	-2.7763800	0.1564660
6	-2.7152660	-1.8346200	-1.3528000
6	-6.3728230	-1.4269370	-0.6917820
6	-7.1813420	-2.6711430	-0.4657200
6	-8.3682860	-2.1944710	0.4081950
6	-8.4524040	-0.6753380	0.1061940
6	-7.0537210	-0.3100960	-0.3130220
6	-6.4938690	1.0391430	-0.2455600
6	-7.1437270	2.2407500	-0.5000460
6	-4.6900020	2.5348260	0.0539410
6	-5.1131090	1.2247050	0.0753660
1	-4.4349160	0.4106280	0.3086680
6	-1.3807850	-2.1869020	-1.0595610
6	-0.1586160	-2.3076090	-0.9140330
6	-3.3731300	2.9714070	0.3102770
6	-2.1656200	3.0647000	0.5648510
78	-0.3139590	2.7903190	1.0264140
6	1.8953880	1.0965180	1.8172640
6	2.4778550	3.3539200	1.3838590
6	3.2314560	0.7618770	2.0481090
6	3.8173050	3.0644470	1.6437180
6	4.2163540	1.7570390	1.9700020
1	3.4916770	-0.2654560	2.2836480
1	4.5504040	3.8659390	1.5859250
6	-1.5842290	0.0426400	1.7574470
6	0.7247610	0.1996880	1.9391260
6	-1.5753910	-1.2443070	2.2782860
1	-2.5029270	0.5473620	1.4655170
6	0.7979990	-1.1025600	2.4303570
6	-0.3648380	-1.8565840	2.6291010
1	-2.5256790	-1.7609070	2.3911010
1	1.7707770	-1.5229020	2.6662970
6	0.4547350	4.5787910	0.7116670
6	-0.1611640	5.7701880	0.2987900
6	1.8617200	4.6265040	0.9850700
6	0.5692440	6.9567430	0.1679470
1	-1.2291690	5.7606460	0.0836170
6	2.5845690	5.8228540	0.8670520
6	1.9415860	6.9905290	0.4559890
1	0.0642130	7.8682080	-0.1550060
1	3.6501980	5.8516460	1.1008830
1	2.5014070	7.9208210	0.3639630

6	5.6876490	1.4702350	2.2555600
6	5.9552920	-0.0230090	2.4723660
6	6.5424690	1.9529480	1.0714560
6	6.0969500	2.2345410	3.5283870
1	5.4209370	-0.4114340	3.3494710
1	5.6731910	-0.6222080	1.5962890
1	7.0271140	-0.1798870	2.6510760
1	6.4331510	3.0292230	0.8912540
1	7.6043720	1.7525480	1.2669450
1	6.2572580	1.4245950	0.1536620
1	7.1562900	2.0514900	3.7554150
1	5.9581880	3.3171010	3.4146370
1	5.5001310	1.9091490	4.3903800
6	-0.3505460	-3.2614980	3.2153370
6	-0.9520700	-3.1957160	4.6320200
6	-1.2098660	-4.1860760	2.3344290
6	1.0695330	-3.8307250	3.3020480
1	-0.3512780	-2.5525000	5.2891210
1	-1.9760450	-2.8005020	4.6175370
1	-0.9834530	-4.2020040	5.0719320
1	-0.9031200	-4.1215070	1.2853020
1	-1.1040000	-5.2256120	2.6718330
1	-2.2757160	-3.9298900	2.3906280
1	1.0282340	-4.8594930	3.6821380
1	1.5556110	-3.8608530	2.3193930
1	1.6992100	-3.2550240	3.9951720
7	-0.4660560	0.7591290	1.5996850
7	1.5699150	2.3555650	1.4798540
6	-8.5689720	2.5012450	-0.8849090
1	-8.8682190	1.8803840	-1.7385210
1	-9.2505380	2.2716700	-0.0555290
1	-8.7161580	3.5517090	-1.1612630
6	-5.6061280	0.1632700	-3.2367550
1	-6.6430920	-0.1851730	-3.1657350
1	-5.5795830	1.2100250	-2.9002900
1	-5.3069660	0.1363950	-4.2919670
78	1.7663470	-2.2401250	-0.8011190
6	2.1654730	-4.1204970	-0.3567840
6	3.5705000	-4.3650280	-0.2124660
6	1.3065310	-5.2166610	-0.1908200
6	4.0588830	-5.6321990	0.1400250
6	1.7980450	-6.4798370	0.1552970
1	0.2381480	-5.0762630	-0.3460300
6	3.1724220	-6.6904700	0.3385190
1	5.1305620	-5.8004370	0.2557510
1	1.1033070	-7.3112720	0.2826330
1	3.5470320	-7.6752760	0.6161910
6	4.3357680	-0.9649870	-1.2129210
6	4.4458900	-3.2297360	-0.5222370
6	5.7197730	-0.9117630	-1.3555340
6	5.8429150	-3.2029560	-0.6253920
6	6.5007510	-2.0471360	-1.0597160
1	6.1906160	-0.0026210	-1.7207550
1	6.4016540	-4.1062740	-0.4008000
6	3.3696130	0.1209990	-1.5008170
6	1.1287850	0.7287370	-1.5653060
6	3.7447790	1.3858360	-1.9352990
6	1.4476470	2.0190920	-1.9910430
1	0.0962810	0.4213380	-1.4033750
6	2.7825120	2.3709750	-2.2158930
1	4.8019350	1.6009700	-2.0721970

1	0.6340610	2.7252490	-2.1312380
7	2.0557730	-0.2057900	-1.3384580
7	3.7502750	-2.1079900	-0.8072060
6	3.2046150	3.7132820	-2.8005420
6	3.6880400	3.4565910	-4.2416870
6	2.0426840	4.7114770	-2.8340550
6	4.3553360	4.3186020	-1.9797710
1	4.5452290	2.7702860	-4.2672650
1	2.8883360	3.0193070	-4.8536050
1	3.9967010	4.4027460	-4.7069200
1	1.6241600	4.8907010	-1.8366280
1	2.3983190	5.6739010	-3.2237130
1	1.2339260	4.3718780	-3.4946080
1	4.6440780	5.2872120	-2.4086130
1	4.0444070	4.4870270	-0.9435190
1	5.2493540	3.6813820	-1.9756710
6	8.0131330	-1.9982130	-1.2646650
6	8.2970770	-1.7443970	-2.7572640
6	8.6130230	-0.8562120	-0.4266250
6	8.6961670	-3.3073360	-0.8551110
1	7.8715080	-2.5421100	-3.3797740
1	7.8738920	-0.7910400	-3.0987070
1	9.3807820	-1.7119970	-2.9336740
1	8.4098210	-1.0027580	0.6421170
1	9.7017420	-0.8212900	-0.5671660
1	8.2098020	0.1221570	-0.7139960
1	9.7795320	-3.2161780	-1.0053550
1	8.5292730	-3.5425580	0.2047770
1	8.3534220	-4.1575580	-1.4595740

Pt-A (AP)

16	2.2618030	-0.4911400	1.8878670
16	-2.2083640	-0.7696350	-1.6120160
9	1.1212830	4.5478680	1.6144130
9	2.3367030	4.3742290	-0.1773330
9	-0.2199010	6.1646720	0.1106860
9	0.4861870	5.2106290	-1.7152660
9	-2.0429880	4.3698060	0.4950280
9	-1.8756150	4.2128560	-1.6666500
6	0.9981720	0.6337520	1.5190470
6	1.4678980	1.6327510	0.6760280
6	2.8547680	1.4861010	0.3544680
1	3.4034210	2.1609400	-0.2956400
6	3.4408350	0.3702840	0.9173020
6	0.6350680	2.7271240	0.1791240
6	1.0939650	4.1551480	0.3174510
6	0.0442740	4.9835600	-0.4642470
6	-1.1889220	4.0494970	-0.5192290
6	-0.6174900	2.6668180	-0.3482890
6	-1.4208030	1.5015410	-0.7036200
6	-0.9388760	0.3821250	-1.3701060
6	-3.4075820	0.2427690	-0.8287990
6	-2.8209340	1.4216610	-0.4171990
1	-3.3799160	2.1991370	0.0969450
6	4.7639220	-0.0986140	0.7931790
6	5.9125970	-0.5486680	0.7025970
6	-4.7440220	-0.1834030	-0.6980980
6	-5.9049670	-0.6020280	-0.6119850
78	-7.7622680	-1.0873060	-0.4352770
6	-10.5586210	-0.6073720	0.1544260

6	-10.0518000	-2.8153270	-0.5401000
6	-11.9123500	-0.9216940	0.2872400
6	-11.3984140	-3.1659420	-0.4187940
6	-12.3523160	-2.2227580	-0.0026360
1	-12.6143390	-0.1600180	0.6116650
1	-11.6978690	-4.1849440	-0.6535070
6	-7.9417630	1.9142440	0.4113140
6	-9.9270500	0.7072090	0.4125650
6	-8.5949440	3.0661890	0.8332420
1	-6.8683300	1.8878070	0.2240730
6	-10.6354560	1.8329300	0.8376200
6	-9.9815070	3.0491470	1.0606590
1	-8.0073680	3.9704770	0.9799380
1	-11.7072150	1.7495060	0.9924320
6	-7.6399460	-2.9803230	-0.9760700
6	-6.5258730	-3.7382290	-1.3635910
6	-8.9114530	-3.6407580	-0.9536390
6	-6.6556620	-5.0865440	-1.7144920
1	-5.5476320	-3.2596830	-1.3882820
6	-9.0351990	-4.9925980	-1.3072970
6	-7.9073240	-5.7189210	-1.6886750
1	-5.7722700	-5.6533110	-2.0122950
1	-10.0088860	-5.4846040	-1.2872650
1	-7.9991770	-6.7692870	-1.9641070
6	-13.8180460	-2.6324930	0.1199850
6	-14.7084610	-1.4738920	0.5818410
6	-14.3206120	-3.1155790	-1.2528400
6	-13.9357680	-3.7750650	1.1454190
1	-14.4181620	-1.1034300	1.5745110
1	-14.6882970	-0.6335120	-0.1254620
1	-15.7484510	-1.8173710	0.6520840
1	-13.7487380	-3.9774850	-1.6177160
1	-15.3742870	-3.4183360	-1.1832220
1	-14.2417870	-2.3186220	-2.0038760
1	-14.9852430	-4.0834970	1.2462640
1	-13.3560500	-4.6564990	0.8451290
1	-13.5752590	-3.4570720	2.1324720
6	-10.7057160	4.3080170	1.5232530
6	-10.0996180	4.7701710	2.8611540
6	-10.5163880	5.4081110	0.4623510
6	-12.2065680	4.0721010	1.7217020
1	-10.2129650	3.9985310	3.6338800
1	-9.0309550	5.0003420	2.7700330
1	-10.6084890	5.6796550	3.2075780
1	-10.9412580	5.1027760	-0.5028710
1	-11.0213130	6.3290750	0.7834160
1	-9.4574300	5.6461570	0.3032560
1	-12.6825430	5.0027810	2.0557020
1	-12.7013790	3.7684750	0.7890600
1	-12.4049580	3.3099310	2.4877200
7	-8.5855200	0.7577910	0.2046710
7	-9.6852140	-1.5448430	-0.2472940
6	0.4358160	0.1060250	-1.8912710
1	0.9493400	1.0446360	-2.1304130
1	1.0525180	-0.4211890	-1.1497080
1	0.3983810	-0.5067570	-2.8003350
6	-0.3642730	0.4575940	2.1110960
1	-0.8755710	1.4242320	2.1860650
1	-0.9924660	-0.1970730	1.4904140
1	-0.3063360	0.0206310	3.1157180
78	7.7547130	-1.0804030	0.4973410

6	7.5892210	-2.9860490	0.9790940
6	8.8424100	-3.6791630	0.9146770
6	6.4614050	-3.7270890	1.3592520
6	8.9354860	-5.0450060	1.2219250
6	6.5608080	-5.0892370	1.6640680
1	5.4965190	-3.2245480	1.4145720
6	7.7945060	-5.7533700	1.5976550
1	9.8951700	-5.5614760	1.1699380
1	5.6672000	-5.6422290	1.9573210
1	7.8620870	-6.8143130	1.8371930
6	10.5551830	-0.6569310	-0.1235280
6	9.9965450	-2.8710390	0.5084330
6	11.8905430	-1.0062110	-0.2956240
6	11.3339440	-3.2597640	0.3463740
6	12.3008810	-2.3337220	-0.0589410
1	12.6102900	-0.2554050	-0.6122310
1	11.6060550	-4.2931860	0.5392960
6	9.9547480	0.6825720	-0.3260000
6	8.0026340	1.9405240	-0.2534880
6	10.6866100	1.8032010	-0.7232720
6	8.6799630	3.0883940	-0.6471350
1	6.9316630	1.9354070	-0.0506770
6	10.0622150	3.0428930	-0.8958810
1	11.7534820	1.6969720	-0.8968690
1	8.1141270	4.0117140	-0.7559350
7	8.6185580	0.7612650	-0.0957240
7	9.6616830	-1.5851730	0.2670460
6	10.8121160	4.2963580	-1.3313590
6	10.2040510	4.8072300	-2.6505320
6	10.6592340	5.3729650	-0.2409780
6	12.3050030	4.0304770	-1.5513070
1	10.2924100	4.0538870	-3.4442630
1	9.1418310	5.0585140	-2.5419260
1	10.7302500	5.7138870	-2.9778790
1	11.0841870	5.0327320	0.7124260
1	11.1842600	6.2890710	-0.5432040
1	9.6079640	5.6334520	-0.0665910
1	12.7997810	4.9584870	-1.8648410
1	12.8013890	3.6897560	-0.6323700
1	12.4779770	3.2855300	-2.3400920
6	13.7676210	-2.7095810	-0.2540650
6	14.1671470	-2.4299850	-1.7146580
6	14.6349510	-1.8577000	0.6909350
6	14.0327870	-4.1886060	0.0453830
1	13.5597440	-3.0250880	-2.4090220
1	14.0415500	-1.3726980	-1.9803220
1	15.2225910	-2.6903540	-1.8723170
1	14.3668610	-2.0376690	1.7401790
1	15.6955610	-2.1113810	0.5592790
1	14.5230470	-0.7836310	0.4955600
1	15.0967690	-4.4084560	-0.1107900
1	13.7935090	-4.4458760	1.0859190
1	13.4600550	-4.8504730	-0.6180040

Pt-A (C)

16	-1.7840480	-0.2921240	-0.1729200
16	1.7904600	-0.2822640	0.1552420
9	-1.6660860	5.3365200	-1.3679000
9	-2.2860430	5.1406270	0.7036220
9	-0.0110300	7.0087730	-0.2799360

9	-0.0203670	5.9473890	1.6225550
9	1.5980070	5.2765070	-1.3831090
9	2.2834970	5.2125300	0.6796620
6	-0.6068180	1.0981360	-0.5016680
6	-1.4261040	2.3711090	-0.2805130
6	-2.8242250	2.1368650	-0.3118450
1	-3.5703400	2.9272760	-0.3243280
6	-3.1757110	0.8032200	-0.2691490
6	-0.7190560	3.5352480	-0.1366630
6	-1.2415870	4.9320940	-0.1381060
6	-0.0129850	5.7926050	0.2833480
6	1.2235360	4.9360140	-0.1151130
6	0.7179670	3.5377300	-0.0177940
6	1.4278560	2.3823160	0.1693990
6	0.6103540	1.1161650	0.4363010
6	3.1805900	0.8181630	0.2175150
6	2.8270210	2.1514830	0.2159810
1	3.5710400	2.9436910	0.2084220
6	0.2261240	1.1168210	1.9296390
1	-0.4146560	1.9774740	2.1588040
1	-0.3091360	0.1996760	2.1975560
1	1.1380130	1.1867100	2.5331320
6	-0.2231540	1.0487720	-1.9944390
1	0.4131430	1.9041350	-2.2539360
1	0.3162860	0.1253480	-2.2303910
1	-1.1357100	1.0936280	-2.5993080
6	4.4736500	0.2766070	0.2368020
6	5.5737800	-0.2936970	0.2478740
78	7.3385830	-1.0572070	0.2433600
6	8.1097900	1.9066140	-0.3843900
6	9.8563830	0.3821280	-0.2345990
6	8.9886390	2.9482240	-0.6565190
1	7.0317960	2.0556080	-0.3254720
6	10.7857520	1.3888070	-0.5022970
6	10.3713250	2.7068810	-0.7215470
1	8.5786550	3.9437770	-0.8159140
1	11.8405210	1.1321450	-0.5382740
6	10.2297240	-1.0327390	0.0018230
6	9.2831760	-3.1534860	0.4730510
6	11.5134670	-1.5676490	-0.0001070
6	10.5620890	-3.7284780	0.4780020
6	11.6961640	-2.9444310	0.2420580
1	12.3688830	-0.9235120	-0.1873160
1	10.6567120	-4.7931990	0.6691670
6	6.8430140	-2.9271840	0.6318140
6	7.9829710	-3.7932010	0.6972940
6	5.5816480	-3.5008530	0.8417960
6	7.8403440	-5.1639330	0.9602200
6	5.4465260	-4.8690650	1.1035140
1	4.6982650	-2.8648330	0.7992790
6	6.5710790	-5.7049600	1.1634450
1	8.7152040	-5.8140920	1.0069190
1	4.4530570	-5.2905370	1.2630350
1	6.4553070	-6.7691160	1.3674690
7	8.5260810	0.6503310	-0.1768310
7	9.1701780	-1.8292460	0.2353980
6	11.3412220	3.8437270	-1.0204250
6	11.0014920	4.4350740	-2.4010780
6	11.1862720	4.9292910	0.0605790
6	12.7990810	3.3725770	-1.0343420
1	11.0974020	3.6774410	-3.1898540

1	9.9787460	4.8300100	-2.4371570
1	11.6872010	5.2607520	-2.6339120
1	11.4194880	4.5306360	1.0566120
1	11.8725560	5.7618560	-0.1444180
1	10.1681310	5.3363010	0.0910740
1	13.4564130	4.2246420	-1.2491150
1	13.1060690	2.9592620	-0.0638020
1	12.9797820	2.6166010	-1.8107860
6	13.1086750	-3.5230400	0.2405120
6	13.7538250	-3.2721920	-1.1350480
6	13.9365220	-2.8259700	1.3359910
6	13.1180590	-5.0310440	0.5122320
1	13.1754820	-3.7536970	-1.9343690
1	13.8240700	-2.2023500	-1.3689380
1	14.7718720	-3.6840210	-1.1527600
1	13.4928230	-2.9885140	2.3269330
1	14.9587330	-3.2278820	1.3480240
1	14.0060000	-1.7430240	1.1729420
1	14.1522890	-5.3981190	0.5009180
1	12.6953320	-5.2730920	1.4965490
1	12.5625280	-5.5894270	-0.2530620
6	-4.4683450	0.2606580	-0.2696500
6	-5.5698850	-0.3070350	-0.2656680
78	-7.3369210	-1.0645410	-0.2425660
6	-9.8449770	0.3843250	0.2575090
6	-8.0910750	1.9014940	0.3959580
6	-10.7681710	1.3944420	0.5334200
6	-8.9635600	2.9463230	0.6761570
1	-7.0129870	2.0463620	0.3290620
6	-10.3466990	2.7105990	0.7509920
1	-11.8236900	1.1420990	0.5770710
1	-8.5482560	3.9399430	0.8337930
6	-10.2259120	-1.0287730	0.0223600
6	-9.2916230	-3.1528820	-0.4581660
6	-11.5118740	-1.5582130	0.0321760
6	-10.5729560	-3.7224910	-0.4551260
6	-11.7020340	-2.9338990	-0.2105640
1	-12.3633540	-0.9107000	0.2255700
1	-10.6734630	-4.7864640	-0.6474160
6	-6.8519750	-2.9361610	-0.6366220
6	-7.9958140	-3.7976250	-0.6933130
6	-5.5946190	-3.5145360	-0.8573250
6	-7.8606980	-5.1687140	-0.9582960
6	-5.4669890	-4.8831000	-1.1210010
1	-4.7084390	-2.8819820	-0.8216600
6	-6.5952530	-5.7145470	-1.1722510
1	-8.7384580	-5.8154010	-0.9981770
1	-4.4765200	-5.3083420	-1.2889300
1	-6.4853250	-6.7790060	-1.3779030
7	-8.5140870	0.6472380	0.1897060
7	-9.1714150	-1.8295400	-0.2192730
6	-11.3097680	3.8511320	1.0577020
6	-10.9581050	4.4398890	2.4364850
6	-11.1577780	4.9370460	-0.0233890
6	-12.7694060	3.3859700	1.0812210
1	-11.0518850	3.6820370	3.2253140
1	-9.9334590	4.8304510	2.4659350
1	-11.6386480	5.2683200	2.6746690
1	-11.3990900	4.5401920	-1.0182100
1	-11.8394820	5.7720580	0.1868680
1	-10.1383070	5.3401900	-0.0602490

1	-13.4218120	4.2405350	1.3009720
1	-13.0845910	2.9745510	0.1125030
1	-12.9479090	2.6302110	1.8583850
6	-13.1170490	-3.5062620	-0.2014280
6	-13.7540270	-3.2527240	1.1774330
6	-13.9473020	-2.8053080	-1.2926230
6	-13.1345700	-5.0141810	-0.4731940
1	-13.1737860	-3.7369150	1.9737540
1	-13.8184810	-2.1826420	1.4118730
1	-14.7737730	-3.6600790	1.2002620
1	-13.5090410	-2.9692540	-2.2857540
1	-14.9712230	-3.2029570	-1.2999270
1	-14.0113870	-1.7221570	-1.1287560
1	-14.1702960	-5.3767490	-0.4556630
1	-12.7188350	-5.2579530	-1.4600530
1	-12.5768310	-5.5749690	0.2887280

Pt-B (P)

16	-3.0149490	-0.7677520	-2.7120520
16	-6.0408420	3.5728720	-0.3620890
9	-7.6420950	-3.1995620	-1.6261070
9	-6.4812110	-3.6494960	0.1557050
9	-9.5097860	-2.8413000	0.1429450
9	-8.0714270	-2.3705020	1.7092100
9	-9.3549980	-0.4761810	-0.8943710
9	-8.8969570	0.0134160	1.1764160
6	-4.7116390	-0.6896240	-2.3951320
6	-5.0338330	-1.4549390	-1.2848010
6	-3.9047410	-2.1280410	-0.7143710
1	-3.9587510	-2.7763800	0.1564660
6	-2.7152660	-1.8346200	-1.3528000
6	-6.3728230	-1.4269370	-0.6917820
6	-7.1813420	-2.6711430	-0.4657200
6	-8.3682860	-2.1944710	0.4081950
6	-8.4524040	-0.6753380	0.1061940
6	-7.0537210	-0.3100960	-0.3130220
6	-6.4938690	1.0391430	-0.2455600
6	-7.1437270	2.2407500	-0.5000460
6	-4.6900020	2.5348260	0.0539410
6	-5.1131090	1.2247050	0.0753660
1	-4.4349160	0.4106280	0.3086680
6	-1.3807850	-2.1869020	-1.0595610
6	-0.1586160	-2.3076090	-0.9140330
6	-3.3731300	2.9714070	0.3102770
6	-2.1656200	3.0647000	0.5648510
78	-0.3139590	2.7903190	1.0264140
6	1.8953880	1.0965180	1.8172640
6	2.4778550	3.3539200	1.3838590
6	3.2314560	0.7618770	2.0481090
6	3.8173050	3.0644470	1.6437180
6	4.2163540	1.7570390	1.9700020
1	3.4916770	-0.2654560	2.2836480
1	4.5504040	3.8659390	1.5859250
6	-1.5842290	0.0426400	1.7574470
6	0.7247610	0.1996880	1.9391260
6	-1.5753910	-1.2443070	2.2782860
1	-2.5029270	0.5473620	1.4655170
6	0.7979990	-1.1025600	2.4303570
6	-0.3648380	-1.8565840	2.6291010
1	-2.5256790	-1.7609070	2.3911010

1	1.7707770	-1.5229020	2.6662970
6	0.4547350	4.5787910	0.7116670
6	-0.1611640	5.7701880	0.2987900
6	1.8617200	4.6265040	0.9850700
6	0.5692440	6.9567430	0.1679470
1	-1.2291690	5.7606460	0.0836170
6	2.5845690	5.8228540	0.8670520
6	1.9415860	6.9905290	0.4559890
1	0.0642130	7.8682080	-0.1550060
1	3.6501980	5.8516460	1.1008830
1	2.5014070	7.9208210	0.3639630
6	5.6876490	1.4702350	2.2555600
6	5.9552920	-0.0230090	2.4723660
6	6.5424690	1.9529480	1.0714560
6	6.0969500	2.2345410	3.5283870
1	5.4209370	-0.4114340	3.3494710
1	5.6731910	-0.6222080	1.5962890
1	7.0271140	-0.1798870	2.6510760
1	6.4331510	3.0292230	0.8912540
1	7.6043720	1.7525480	1.2669450
1	6.2572580	1.4245950	0.1536620
1	7.1562900	2.0514900	3.7554150
1	5.9581880	3.3171010	3.4146370
1	5.5001310	1.9091490	4.3903800
6	-0.3505460	-3.2614980	3.2153370
6	-0.9520700	-3.1957160	4.6320200
6	-1.2098660	-4.1860760	2.3344290
6	1.0695330	-3.8307250	3.3020480
1	-0.3512780	-2.5525000	5.2891210
1	-1.9760450	-2.8005020	4.6175370
1	-0.9834530	-4.2020040	5.0719320
1	-0.9031200	-4.1215070	1.2853020
1	-1.1040000	-5.2256120	2.6718330
1	-2.2757160	-3.9298900	2.3906280
1	1.0282340	-4.8594930	3.6821380
1	1.5556110	-3.8608530	2.3193930
1	1.6992100	-3.2550240	3.9951720
7	-0.4660560	0.7591290	1.5996850
7	1.5699150	2.3555650	1.4798540
6	-8.5689720	2.5012450	-0.8849090
1	-8.8682190	1.8803840	-1.7385210
1	-9.2505380	2.2716700	-0.0555290
1	-8.7161580	3.5517090	-1.1612630
6	-5.6061280	0.1632700	-3.2367550
1	-6.6430920	-0.1851730	-3.1657350
1	-5.5795830	1.2100250	-2.9002900
1	-5.3069660	0.1363950	-4.2919670
78	1.7663470	-2.2401250	-0.8011190
6	2.1654730	-4.1204970	-0.3567840
6	3.5705000	-4.3650280	-0.2124660
6	1.3065310	-5.2166610	-0.1908200
6	4.0588830	-5.6321990	0.1400250
6	1.7980450	-6.4798370	0.1552970
1	0.2381480	-5.0762630	-0.3460300
6	3.1724220	-6.6904700	0.3385190
1	5.1305620	-5.8004370	0.2557510
1	1.1033070	-7.3112720	0.2826330
1	3.5470320	-7.6752760	0.6161910
6	4.3357680	-0.9649870	-1.2129210
6	4.4458900	-3.2297360	-0.5222370
6	5.7197730	-0.9117630	-1.3555340

6	5.8429150	-3.2029560	-0.6253920
6	6.5007510	-2.0471360	-1.0597160
1	6.1906160	-0.0026210	-1.7207550
1	6.4016540	-4.1062740	-0.4008000
6	3.3696130	0.1209990	-1.5008170
6	1.1287850	0.7287370	-1.5653060
6	3.7447790	1.3858360	-1.9352990
6	1.4476470	2.0190920	-1.9910430
1	0.0962810	0.4213380	-1.4033750
6	2.7825120	2.3709750	-2.2158930
1	4.8019350	1.6009700	-2.0721970
1	0.6340610	2.7252490	-2.1312380
7	2.0557730	-0.2057900	-1.3384580
7	3.7502750	-2.1079900	-0.8072060
6	3.2046150	3.7132820	-2.8005420
6	3.6880400	3.4565910	-4.2416870
6	2.0426840	4.7114770	-2.8340550
6	4.3553360	4.3186020	-1.9797710
1	4.5452290	2.7702860	-4.2672650
1	2.8883360	3.0193070	-4.8536050
1	3.9967010	4.4027460	-4.7069200
1	1.6241600	4.8907010	-1.8366280
1	2.3983190	5.6739010	-3.2237130
1	1.2339260	4.3718780	-3.4946080
1	4.6440780	5.2872120	-2.4086130
1	4.0444070	4.4870270	-0.9435190
1	5.2493540	3.6813820	-1.9756710
6	8.0131330	-1.9982130	-1.2646650
6	8.2970770	-1.7443970	-2.7572640
6	8.6130230	-0.8562120	-0.4266250
6	8.6961670	-3.3073360	-0.8551110
1	7.8715080	-2.5421100	-3.3797740
1	7.8738920	-0.7910400	-3.0987070
1	9.3807820	-1.7119970	-2.9336740
1	8.4098210	-1.0027580	0.6421170
1	9.7017420	-0.8212900	-0.5671660
1	8.2098020	0.1221570	-0.7139960
1	9.7795320	-3.2161780	-1.0053550
1	8.5292730	-3.5425580	0.2047770
1	8.3534220	-4.1575580	-1.4595740

Pt-B (AP)

16	-2.4239310	-0.9261740	1.6289570
16	2.3227530	-0.7092530	-1.4162450
9	-1.2520170	-5.9677220	1.6133220
9	-2.2937650	-5.8493090	-0.2896500
9	0.2267460	-7.6199340	0.2812140
9	-0.2947350	-6.7047670	-1.6255800
9	1.9911000	-5.7982400	0.8152160
9	2.0528400	-5.7012190	-1.3563370
6	-1.1367390	-2.0669720	1.4282840
6	-1.5200430	-3.0788070	0.5582340
6	-2.8604290	-2.9299760	0.0777710
1	-3.3423380	-3.6183880	-0.6100880
6	-3.4952540	-1.7980150	0.5470460
6	-0.6406970	-4.1851480	0.1802310
6	-1.1056890	-5.6121160	0.3137330
6	0.0191180	-6.4527490	-0.3412490

6	1.2496540	-5.5139840	-0.2918760
6	0.6573910	-4.1310120	-0.2194310
6	1.4818500	-2.9654220	-0.5250540
6	1.0556750	-1.8819460	-1.2813170
6	3.4442630	-1.6659360	-0.4636600
6	2.8380310	-2.8445460	-0.0816550
1	3.3520530	-3.5927090	0.5161450
6	-4.7872080	-1.3069600	0.2728260
6	-5.9109790	-0.8470430	0.0367000
6	4.7443730	-1.1903580	-0.2019630
6	5.8799330	-0.7496420	0.0135050
78	7.6242290	0.0427440	0.2316560
6	9.7264130	1.9581490	-0.3276860
6	10.2666200	0.3364010	1.3130020
6	10.9821790	2.5551880	-0.2024780
6	11.5330150	0.9062140	1.4635470
6	11.9119010	2.0272000	0.7070660
1	11.2317810	3.4201280	-0.8090030
1	12.2245000	0.4647980	2.1778000
6	6.4726120	1.9407040	-1.9665340
6	8.6356320	2.3765700	-1.2381920
6	6.5172320	3.0020710	-2.8623850
1	5.5959570	1.3011570	-1.8644190
6	8.7376550	3.4544560	-2.1203400
6	7.6731310	3.7949100	-2.9614960
1	5.6416510	3.1960250	-3.4790760
1	9.6616510	4.0249500	-2.1453510
6	8.3460980	-1.1650970	1.6130580
6	7.7548220	-2.2680530	2.2452160
6	9.6831310	-0.8223400	1.9978930
6	8.4477320	-3.0016750	3.2146040
1	6.7393060	-2.5495800	1.9692940
6	10.3723470	-1.5616590	2.9706300
6	9.7558670	-2.6532500	3.5817240
1	7.9648440	-3.8562390	3.6908470
1	11.3902700	-1.2910610	3.2554500
1	10.2875280	-3.2307290	4.3376370
6	13.3045530	2.6255960	0.8891320
6	13.5346610	3.8450530	-0.0101870
6	13.4775400	3.0628290	2.3552960
6	14.3572130	1.5575560	0.5396240
1	13.4571970	3.5893670	-1.0757460
1	12.8266580	4.6560530	0.2085520
1	14.5453020	4.2384690	0.1583960
1	13.3682260	2.2212320	3.0503740
1	14.4777570	3.4918430	2.5043270
1	12.7340340	3.8226900	2.6297190
1	15.3678270	1.9682120	0.6690790
1	14.2710450	0.6721130	1.1814210
1	14.2520180	1.2270860	-0.5021080
6	7.7312440	4.9555540	-3.9473540
6	7.5060880	4.4119270	-5.3702580
6	6.6206600	5.9627860	-3.5960790
6	9.0802220	5.6810580	-3.9085460
1	8.2828850	3.6854720	-5.6426650
1	6.5327310	3.9161450	-5.4705790
1	7.5377920	5.2358030	-6.0957700
1	6.7559190	6.3615100	-2.5821050
1	6.6412210	6.8049150	-4.3009090
1	5.6237790	5.5078990	-3.6482760
1	9.0756480	6.5021540	-4.6366130

1	9.2825670	6.1198410	-2.9219040
1	9.9122910	5.0142830	-4.1728590
7	7.5035440	1.6285170	-1.1701670
7	9.4109970	0.8882550	0.4199410
6	-0.2566420	-1.6541370	-1.9618370
1	-0.7313390	-2.6116800	-2.2053050
1	-0.9557660	-1.0987330	-1.3208140
1	-0.1266110	-1.0893020	-2.8933520
6	0.1550690	-1.8843260	2.1604030
1	0.6390000	-2.8533840	2.3293660
1	0.8594720	-1.2632160	1.5889230
1	-0.0055570	-1.4080990	3.1356060
78	-7.6321280	-0.0184730	-0.2279750
6	-8.2824940	-1.1218070	-1.7271370
6	-9.5858630	-0.7270070	-2.1742900
6	-7.6711780	-2.1961110	-2.3886690
6	-10.2237440	-1.3899600	-3.2336260
6	-8.3131090	-2.8536930	-3.4439540
1	-6.6806330	-2.5157360	-2.0673110
6	-9.5884320	-2.4551370	-3.8711500
1	-11.2161970	-1.0805680	-3.5648370
1	-7.8158220	-3.6878550	-3.9411570
1	-10.0800850	-2.9737670	-4.6938580
6	-9.7349450	1.9038360	0.3157990
6	-10.1908250	0.3987950	-1.4559280
6	-10.9622090	2.5350360	0.1412840
6	-11.4366720	1.0088010	-1.6597370
6	-11.8413810	2.0867060	-0.8651570
1	-11.2369660	3.3697030	0.7814350
1	-12.0816170	0.6288360	-2.4465440
6	-8.6985010	2.2399480	1.3201370
6	-6.5977030	1.7105680	2.1599140
6	-8.8375930	3.2654590	2.2576820
6	-6.6814520	2.7165310	3.1148350
1	-5.7284530	1.0585750	2.0748030
6	-7.8249050	3.5302380	3.1854940
1	-9.7496160	3.8555420	2.2563090
1	-5.8454870	2.8520900	3.7985220
7	-7.5789210	1.4717340	1.2795830
7	-9.3905140	0.8708150	-0.4758170
6	-7.9236810	4.6341320	4.2315430
6	-7.8087850	4.0056720	5.6325690
6	-6.7693050	5.6299440	4.0152020
6	-9.2501380	5.3961980	4.1447070
1	-8.6227720	3.2914390	5.8131550
1	-6.8590500	3.4733770	5.7666910
1	-7.8636300	4.7893700	6.4000810
1	-6.8258940	6.0896560	3.0197960
1	-6.8200380	6.4299940	4.7658850
1	-5.7887430	5.1469550	4.1073390
1	-9.2757700	6.1760620	4.9163960
1	-9.3753470	5.8931800	3.1729510
1	-10.1130110	4.7382220	4.3159290
6	-13.1861000	2.7844030	-1.0518350
6	-13.9939860	2.6792990	0.2547930
6	-12.9391180	4.2663660	-1.3893750
6	-14.0105010	2.1601270	-2.1826870
1	-14.1772120	1.6299850	0.5203840
1	-13.4760480	3.1534850	1.0981250
1	-14.9658070	3.1780270	0.1379420
1	-12.3571280	4.3669030	-2.3147970

1	-13.8969640	4.7857280	-1.5284920
1	-12.3922020	4.7838050	-0.5909740
1	-14.9644720	2.6945620	-2.2778180
1	-13.4972320	2.2291930	-3.1511400
1	-14.2430940	1.1049940	-1.9859800

Pt-B (C)

16	-1.8094540	1.2067840	0.0202670
16	1.7758300	1.1934590	-0.0521010
9	-1.7938590	6.8414370	-1.1228570
9	-2.1671500	6.6309680	1.0063200
9	-0.0124810	8.4963690	-0.2189550
9	0.1988210	7.4107420	1.6585740
9	1.4322430	6.7602300	-1.5293370
9	2.3677890	6.6761330	0.4327100
6	-0.6691960	2.5937110	-0.4260190
6	-1.4515310	3.8672220	-0.0974240
6	-2.8477120	3.6416880	0.0267280
1	-3.5867340	4.4351950	0.1041690
6	-3.2015390	2.3111360	0.0862150
6	-0.7237910	5.0245930	-0.0266050
6	-1.2326620	6.4263070	0.0458980
6	0.0441370	7.2744850	0.3264520
6	1.2172310	6.4149730	-0.2273890
6	0.7172860	5.0175540	-0.0793010
6	1.4372810	3.8580070	0.0169460
6	0.6456380	2.5964890	0.3705220
6	3.1766940	2.2861550	-0.1330380
6	2.8329770	3.6197520	-0.0957690
1	3.5775920	4.4069740	-0.1797210
6	0.4319370	2.5894760	1.8970210
1	-0.1689710	3.4543780	2.2037770
1	-0.0812150	1.6761450	2.2167190
1	1.4068770	2.6460910	2.3942060
6	-0.4551570	2.5595090	-1.9522590
1	0.1506530	3.4158220	-2.2732880
1	0.0527570	1.6379200	-2.2562280
1	-1.4296050	2.6137500	-2.4506830
6	4.4537730	1.7160820	-0.2262960
6	5.5372060	1.1174700	-0.2828750
78	7.1179390	0.0234150	-0.2374760
6	5.1529500	-1.7589020	1.4113710
6	7.3039720	-2.5839570	1.1033030
6	4.7852750	-2.8802090	2.1453700
1	4.4591130	-0.9419300	1.2126250
6	6.9901980	-3.7328030	1.8317540
6	5.7127340	-3.9101880	2.3744890
1	3.7689320	-2.9339280	2.5307130
1	7.7560730	-4.4902750	1.9714230
6	8.6368490	-2.3326950	0.5044540
6	9.8340630	-0.7317830	-0.7686290
6	9.7495040	-3.1644580	0.5680410
6	10.9765160	-1.5437090	-0.7248060
6	10.9514230	-2.7720710	-0.0559480
1	9.6884950	-4.1112890	1.0986150
1	11.8808470	-1.2014210	-1.2188260
6	8.3525250	1.1603680	-1.2743750
6	9.6539100	0.5753000	-1.4088990
6	8.1416590	2.4110950	-1.8704230
6	10.6765380	1.2298290	-2.1115780

6	9.1663110	3.0590130	-2.5699950
1	7.1619530	2.8791100	-1.7819350
6	10.4346870	2.4737380	-2.6941570
1	11.6633720	0.7745540	-2.2072740
1	8.9758460	4.0323280	-3.0243750
1	11.2259000	2.9861500	-3.2407840
7	6.3818470	-1.6079600	0.8993530
7	8.7120080	-1.1599660	-0.1522340
6	5.3142150	-5.1445730	3.1747700
6	4.8765570	-4.7054920	4.5843820
6	4.1402710	-5.8409170	2.4621750
6	6.4672130	-6.1448230	3.3088750
1	5.6947830	-4.1982440	5.1120790
1	4.0209630	-4.0197670	4.5533950
1	4.5803070	-5.5832840	5.1741970
1	4.4259380	-6.1613150	1.4516510
1	3.8324930	-6.7293790	3.0296950
1	3.2673700	-5.1827900	2.3722720
1	6.1313960	-7.0143830	3.8881060
1	6.8055950	-6.5142250	2.3311140
1	7.3274560	-5.7121940	3.8376960
6	12.1690920	-3.6894960	0.0204810
6	12.5482930	-3.8978660	1.4982770
6	11.8175290	-5.0450760	-0.6199580
6	13.3806880	-3.1068740	-0.7142710
1	12.7932140	-2.9422940	1.9799840
1	11.7357230	-4.3635600	2.0703330
1	13.4262570	-4.5537750	1.5725440
1	11.5379380	-4.9212080	-1.6743420
1	12.6832640	-5.7195050	-0.5723910
1	10.9826530	-5.5391940	-0.1070880
1	14.2263640	-3.8017640	-0.6334500
1	13.1789110	-2.9580690	-1.7835100
1	13.7003950	-2.1488710	-0.2828870
6	-4.4813940	1.7496630	0.1909580
6	-5.5623310	1.1472290	0.2557110
78	-7.1325350	0.0380220	0.2227520
6	-7.2910560	-2.5809230	-1.0987330
6	-5.1511750	-1.7323750	-1.4199260
6	-6.9661470	-3.7308150	-1.8205980
6	-4.7725670	-2.8543550	-2.1473270
1	-4.4661960	-0.9060960	-1.2290600
6	-5.6885000	-3.8967100	-2.3665430
1	-7.7235180	-4.4981290	-1.9526420
1	-3.7567930	-2.8987720	-2.5353580
6	-8.6245030	-2.3421670	-0.4959800
6	-9.8369430	-0.7473000	0.7703190
6	-9.7258280	-3.1896910	-0.5464980
6	-10.9683380	-1.5751960	0.7394260
6	-10.9296140	-2.8088570	0.0810460
1	-9.6543280	-4.1403720	-1.0687970
1	-11.8745500	-1.2415640	1.2359390
6	-8.3773940	1.1670700	1.2560520
6	-9.6708480	0.5668400	1.3999330
6	-8.1797490	2.4245620	1.8422580
6	-10.6988410	1.2137710	2.1018030
6	-9.2097200	3.0648360	2.5410840
1	-7.2062490	2.9040000	1.7467740
6	-10.4702460	2.4648430	2.6743550
1	-11.6795760	0.7470020	2.2046120
1	-9.0295930	4.0436940	2.9877030

1	-11.2657040	2.9714130	3.2202640
7	-6.3801600	-1.5924330	-0.9049500
7	-8.7123890	-1.1652010	0.1514660
6	-5.2779010	-5.1316860	-3.1598240
6	-4.8486270	-4.6968750	-4.5733200
6	-4.0942920	-5.8098590	-2.4456370
6	-6.4197790	-6.1457700	-3.2847930
1	-5.6740690	-4.2031130	-5.1025600
1	-4.0012910	-4.0007110	-4.5489150
1	-4.5431030	-5.5750260	-5.1578570
1	-4.3735520	-6.1266130	-1.4321770
1	-3.7781340	-6.6985900	-3.0080750
1	-3.2286860	-5.1413040	-2.3625990
1	-6.0754100	-7.0150760	-3.8593660
1	-6.7518610	-6.5128830	-2.3040310
1	-7.2859710	-5.7261490	-3.8143960
6	-12.1336200	-3.7453780	0.0213320
6	-12.5179900	-3.9757890	-1.4518850
6	-11.7575150	-5.0881750	0.6744720
6	-13.3498880	-3.1733610	0.7566690
1	-12.7806000	-3.0295260	-1.9425840
1	-11.7016260	-4.4351190	-2.0236840
1	-13.3860270	-4.6460110	-1.5139250
1	-11.4735500	-4.9481920	1.7256470
1	-12.6131870	-5.7760830	0.6396350
1	-10.9182450	-5.5751760	0.1619350
1	-14.1854700	-3.8815900	0.6874410
1	-13.1448900	-3.0106880	1.8232750
1	-13.6861170	-2.2246500	0.3173620

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[10] The additional atomic orbitals are: on C: *d* with α= 0.587; on N : *d* with α= 0.736; on F: *d* with α= 1.577; on S: *d* with α= 0.496; on Pt: *f* with α= 0.802.

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