

Investigation of Second-Order Nonlinear Optical Responses in a Series of V-Shaped Binuclear Platinum (II) Complexes

Raphaël J. Durand,^a Sylvain Achelle,^a Françoise Robin-Le Guen,^a Elsa Caytan,^a
Nicolas Le Poul,^b Alberto Barsella,^c Patricia Guevara Level,^d
Denis Jacquemin,^{*d} and Sébastien Gauthier^{*a}

^a Univ. Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) - UMR 6226, F-35000 Rennes, France. E-mail: sebastien.gauthier@univ-rennes1.fr, Tel: +33 2 96 46 93 44.

^b Laboratoire de Chimie, Électrochimie Moléculaires et Chimie Analytique, UMR CNRS 6521, Université de Bretagne Occidentale, UFR Sciences et Techniques, 6 avenue Victor Le Gorgeu – CS 93837, F-29238 Brest Cedex 3, France.

^c Département d'Optique ultra-rapide et Nanophotonique, IPCMS-CNRS, 23 rue du Loess, BP 43, 67034 Strasbourg Cedex 2, France.

^[d] Université de Nantes, CNRS, CEISAM UMR 6230, F-44000 Nantes, France. E-mail: denis.jacquemin@univ-nantes.fr, Tel: +33 2 51 12 55 64.

Table of content

NMR Spectra of complexes 1-7	2
DOSY of complex 6	16
Cyclic Voltammetry	18
Additional Theoretical Results	20

Complex 1:

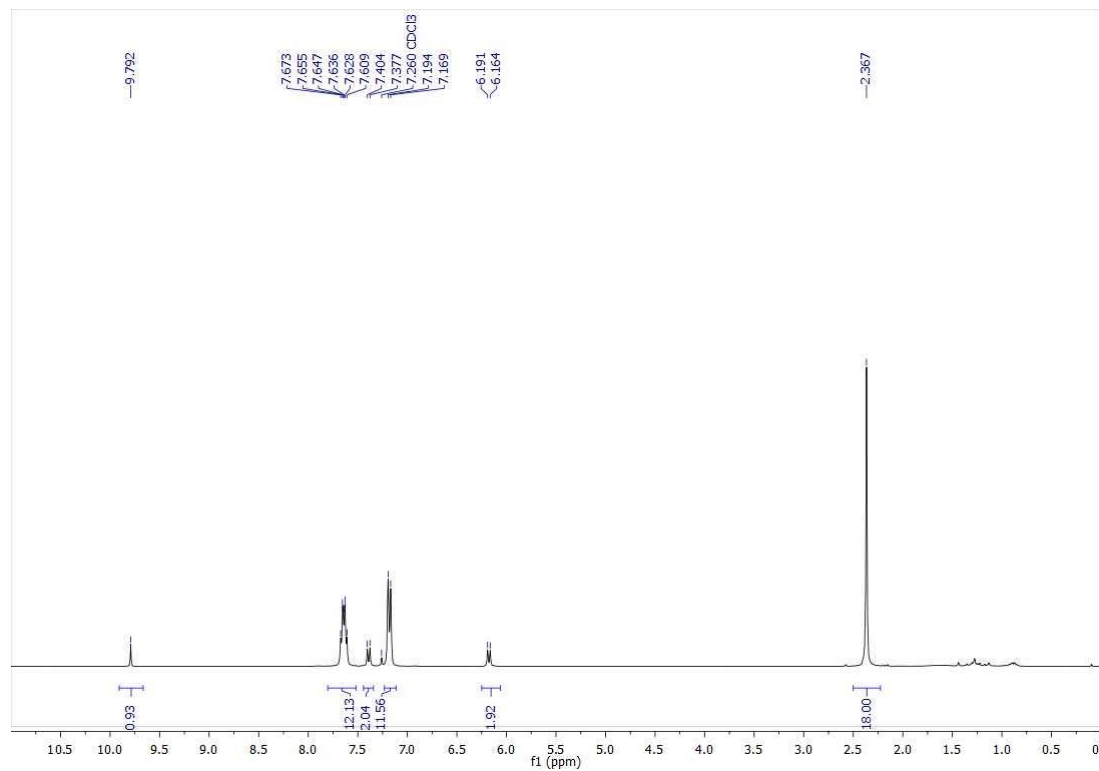
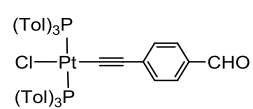


Figure S1. ¹H NMR spectrum (300 MHz, CDCl₃) of **1**.

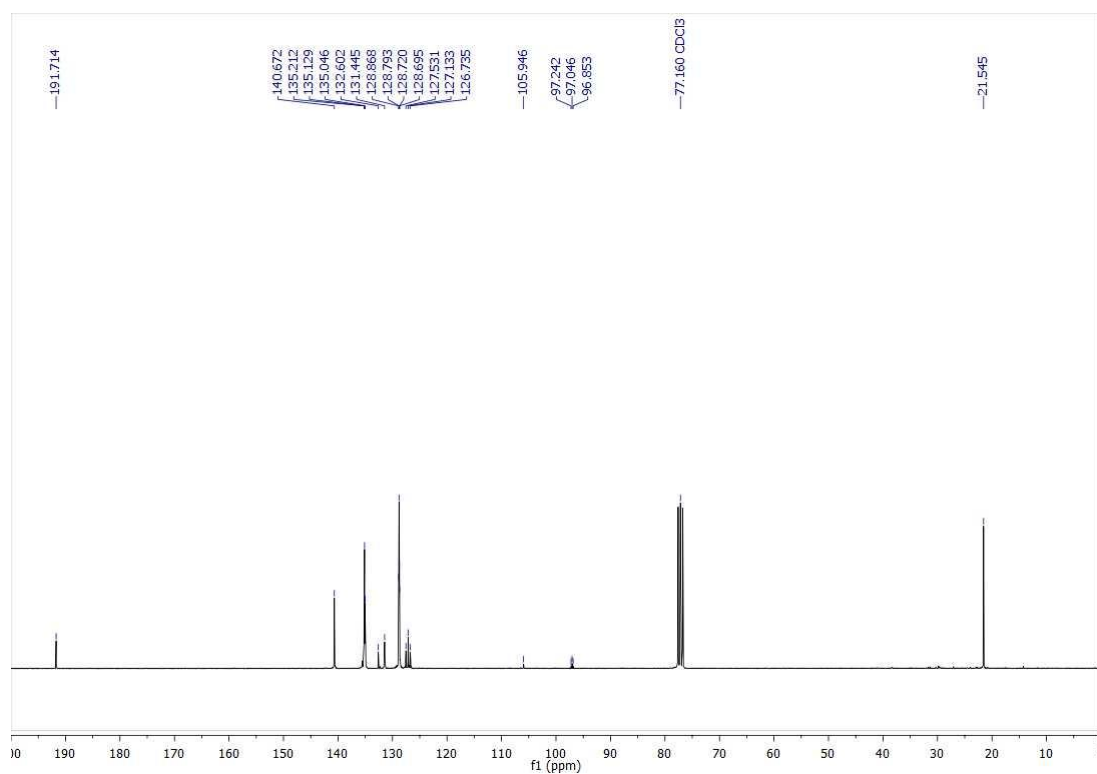


Figure S2. ¹³C NMR spectrum (75 MHz, CDCl₃) of **1**.

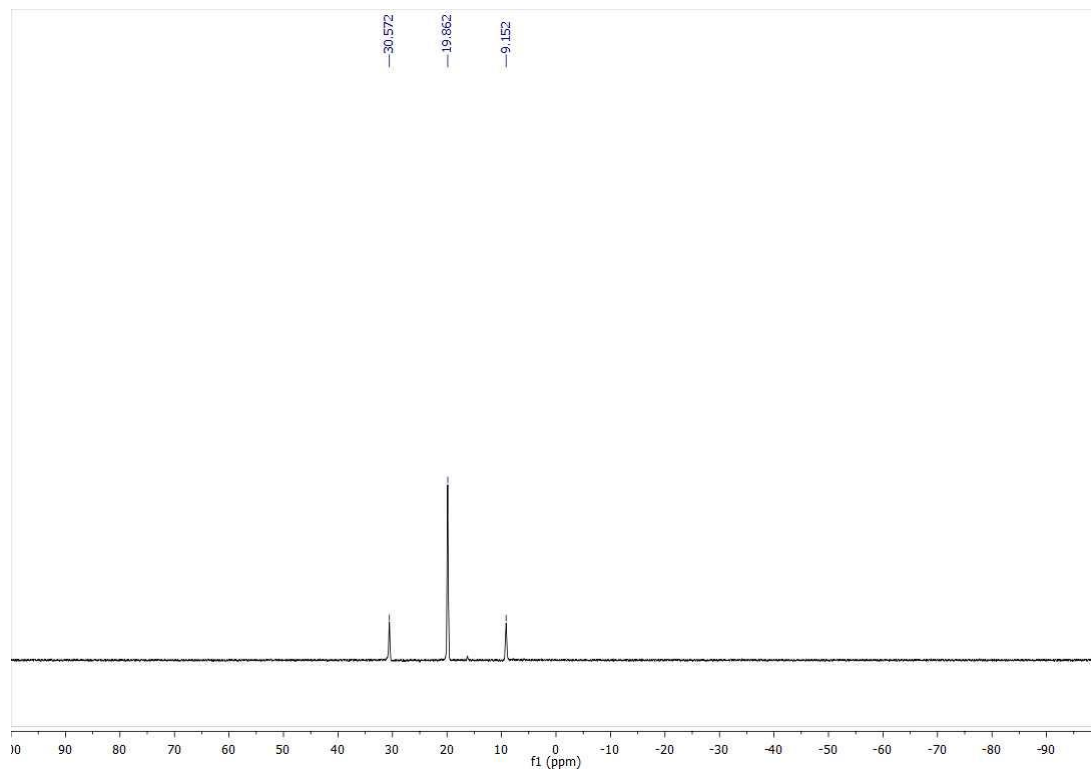


Figure S3. ³¹P NMR spectrum (121 MHz, CDCl₃) of **1**.

Complex 2:

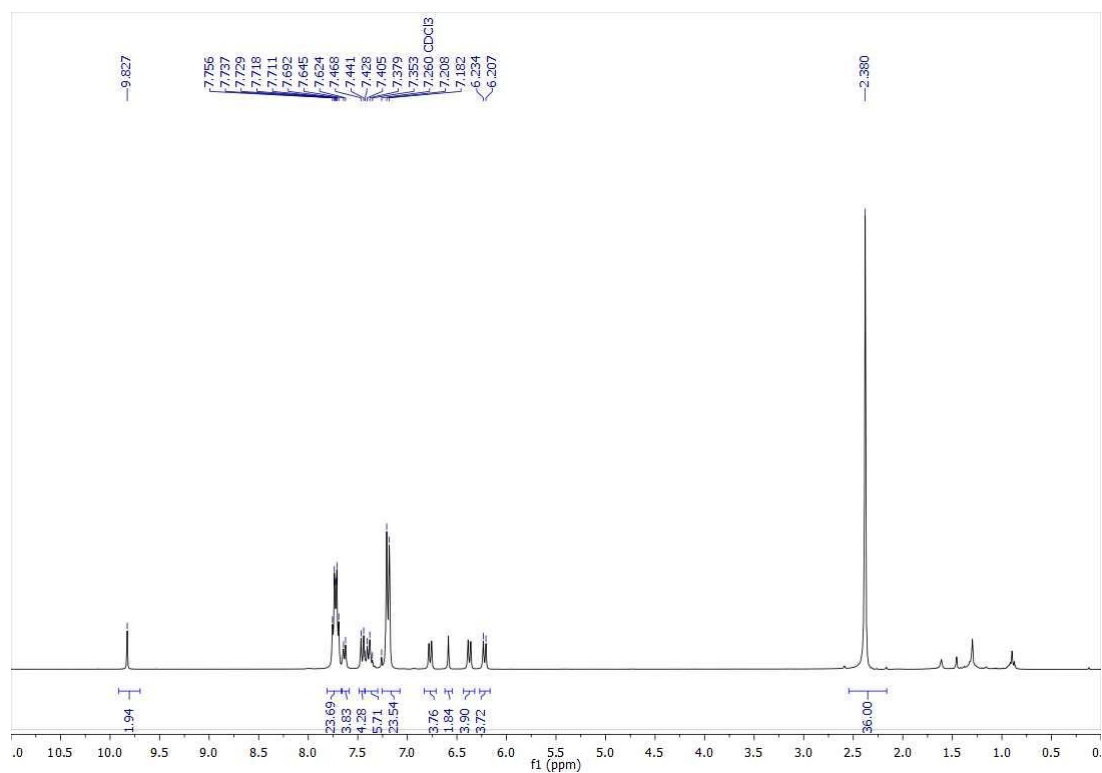
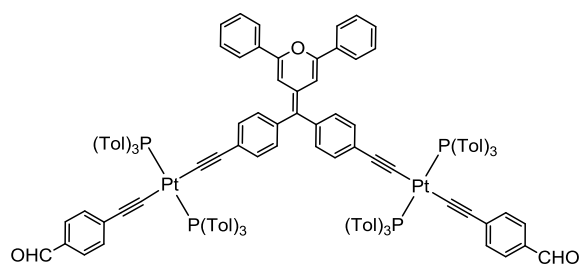


Figure S4. ¹H NMR spectrum (300 MHz, CDCl₃) of 2.

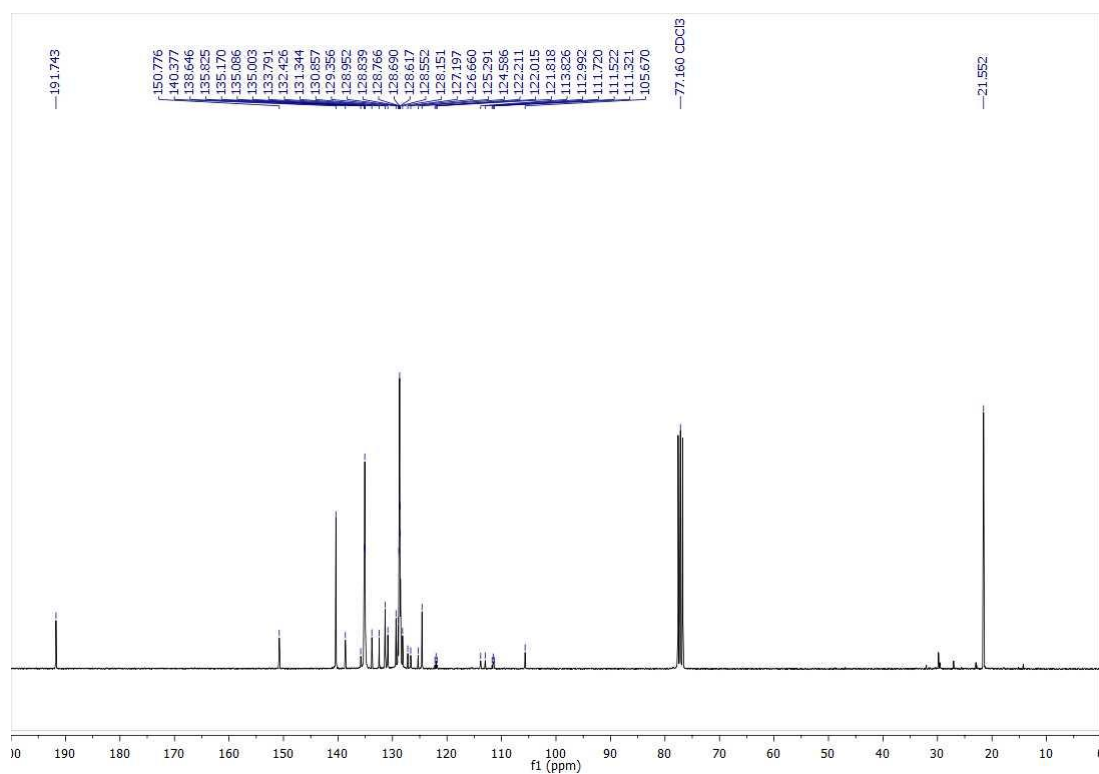


Figure S5. ^{13}C NMR spectrum (75 MHz, CDCl_3) of **2**.

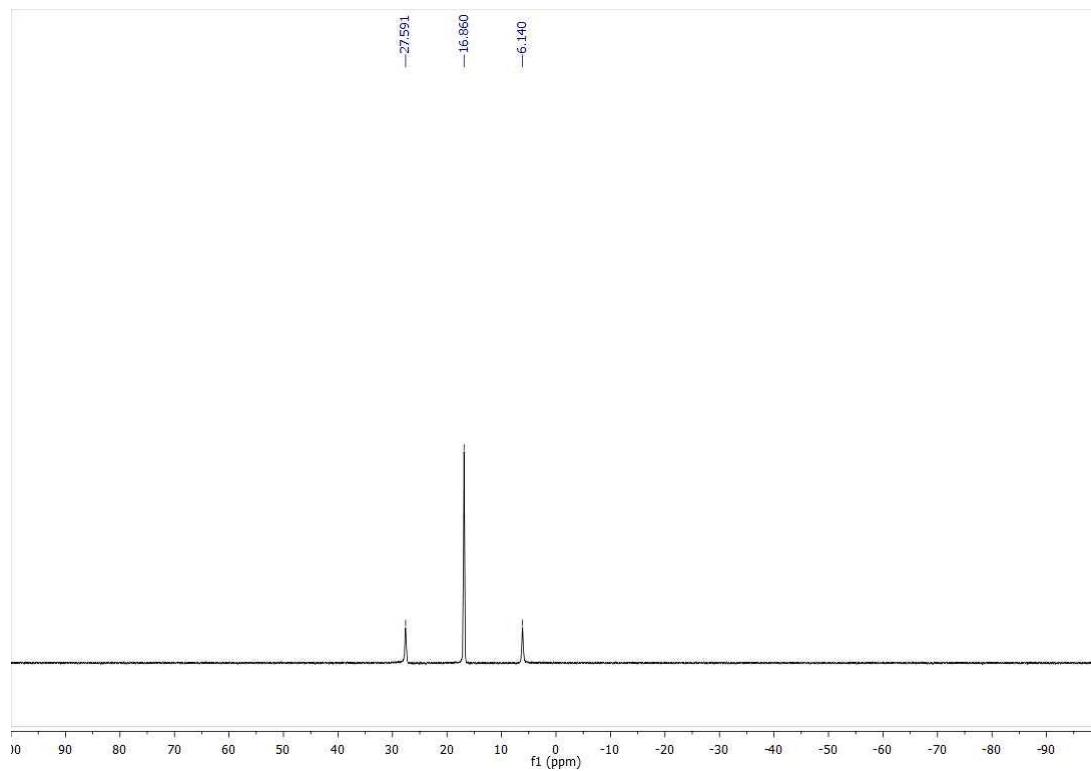


Figure S6. ^{31}P NMR spectrum (121 MHz, CDCl_3) of **2**.

Complex 3:

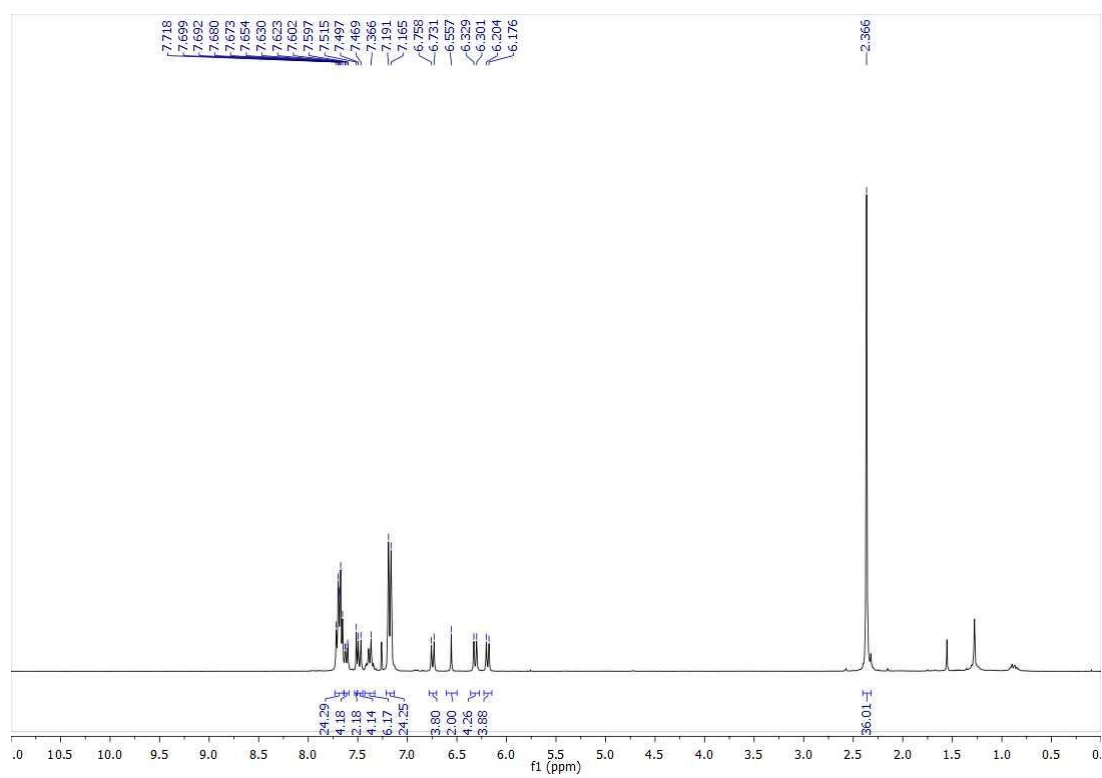
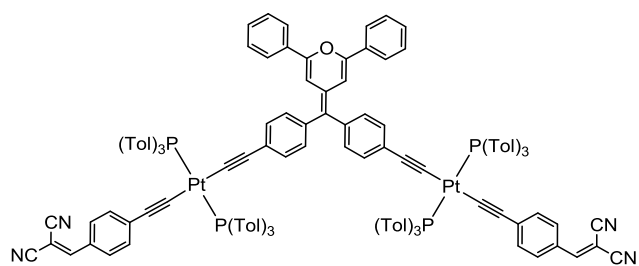


Figure S7. ^1H NMR spectrum (300 MHz, CDCl_3) of **3**.

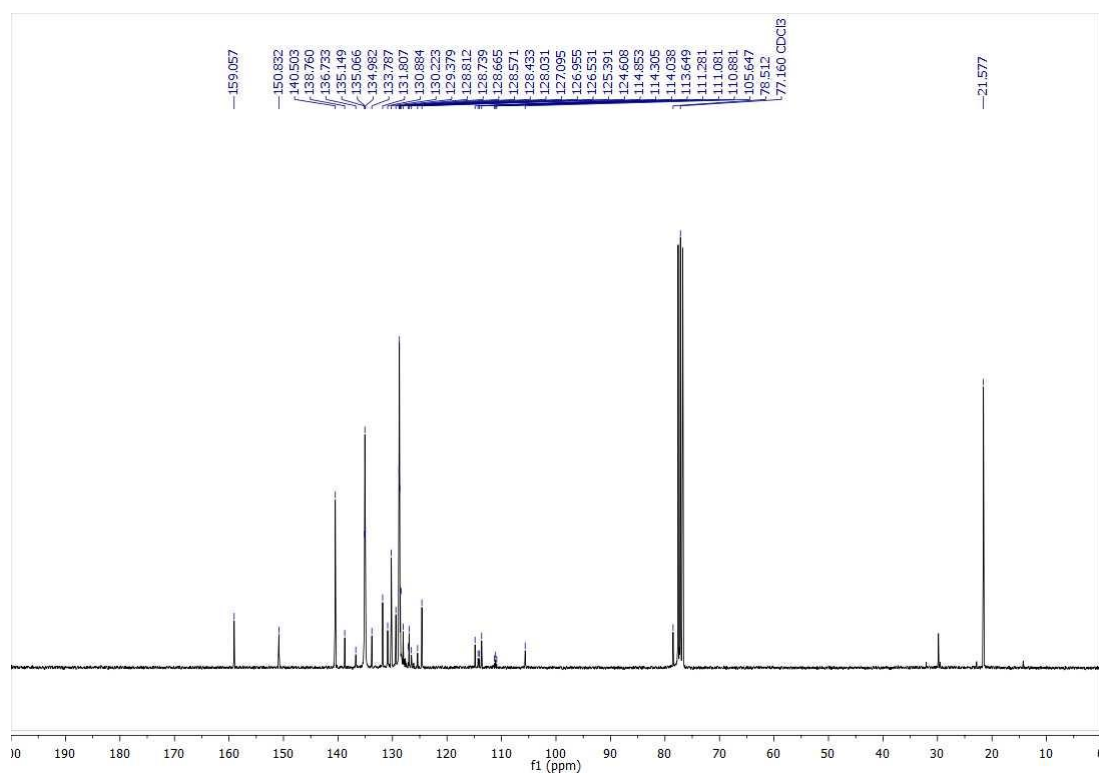


Figure S8. ^{13}C NMR spectrum (75 MHz, CDCl_3) of **3**.

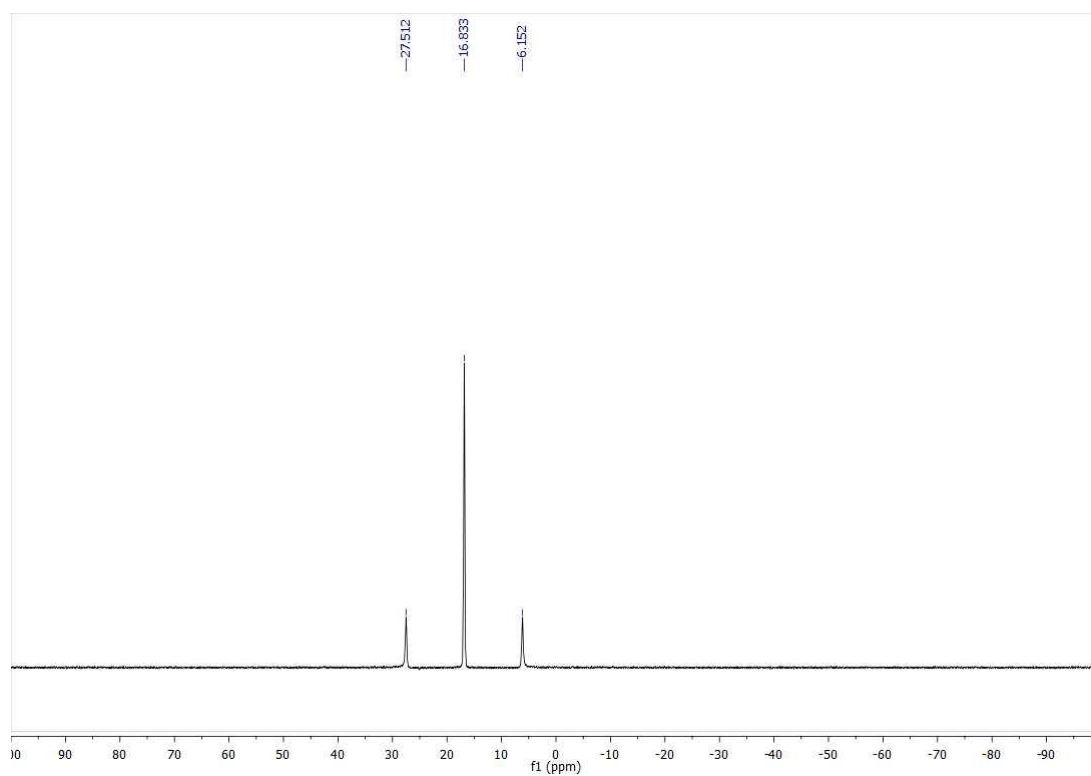


Figure S9. ^{31}P NMR spectrum (121 MHz, CDCl_3) of **3**.

Complex 4:

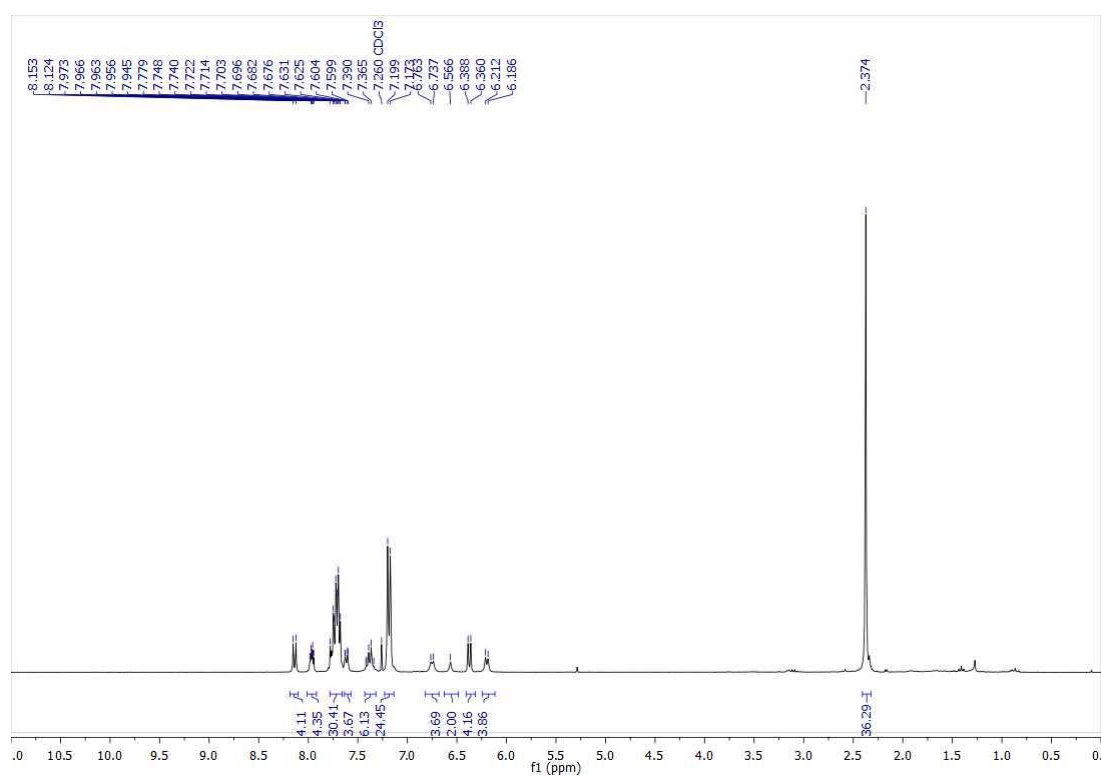
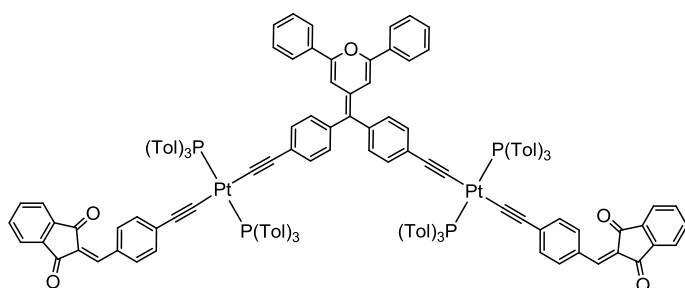


Figure S10. ^1H NMR spectrum (300 MHz, CDCl_3) of **4**.

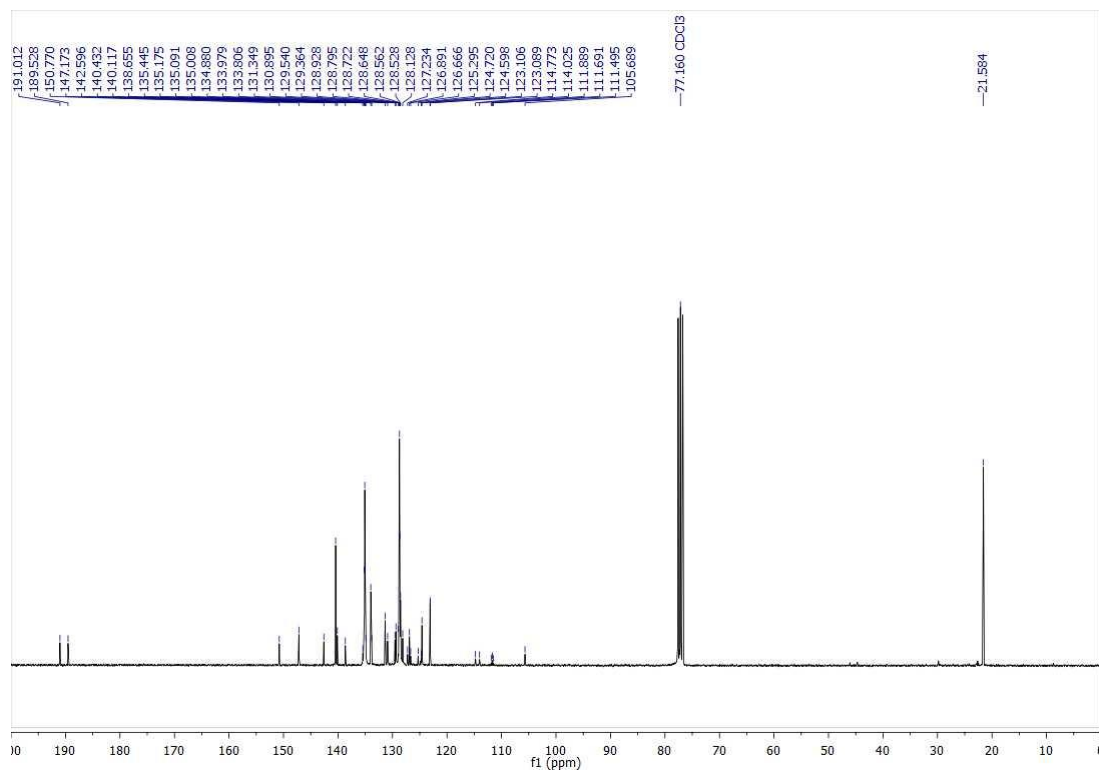


Figure S11. ^{13}C NMR spectrum (75 MHz, CDCl_3) of **4**.

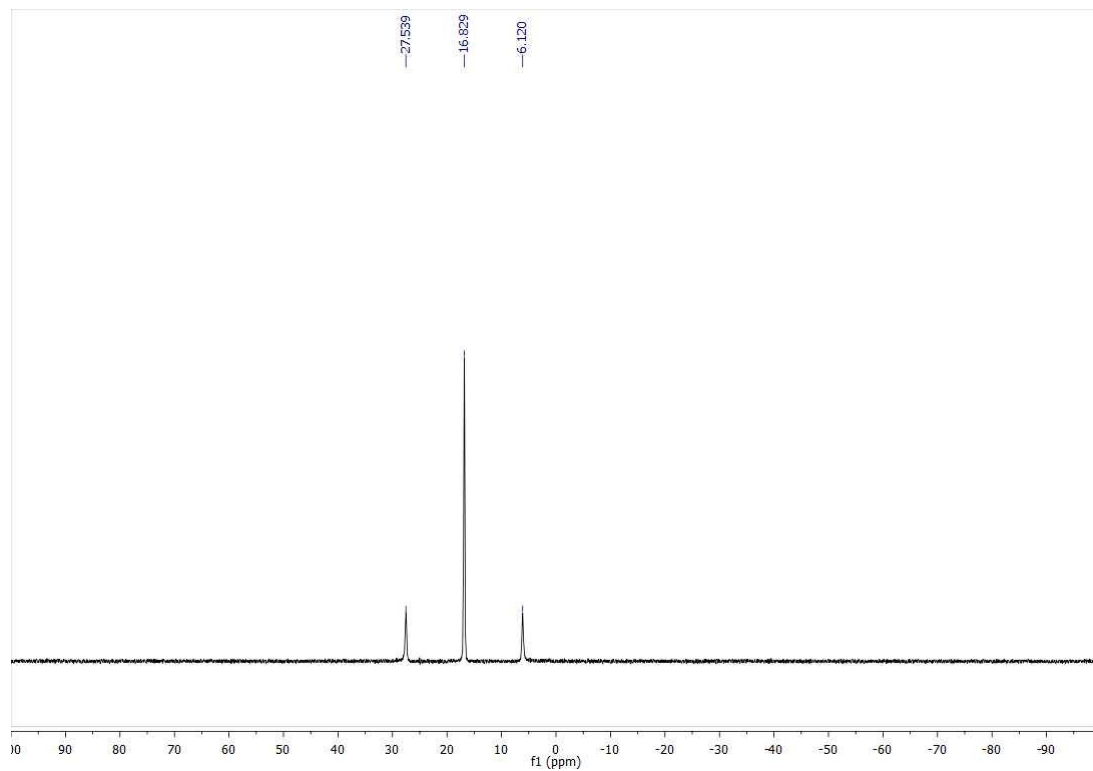


Figure S12. ^{31}P NMR spectrum (121 MHz, CDCl_3) of **4**.

Complex 5:

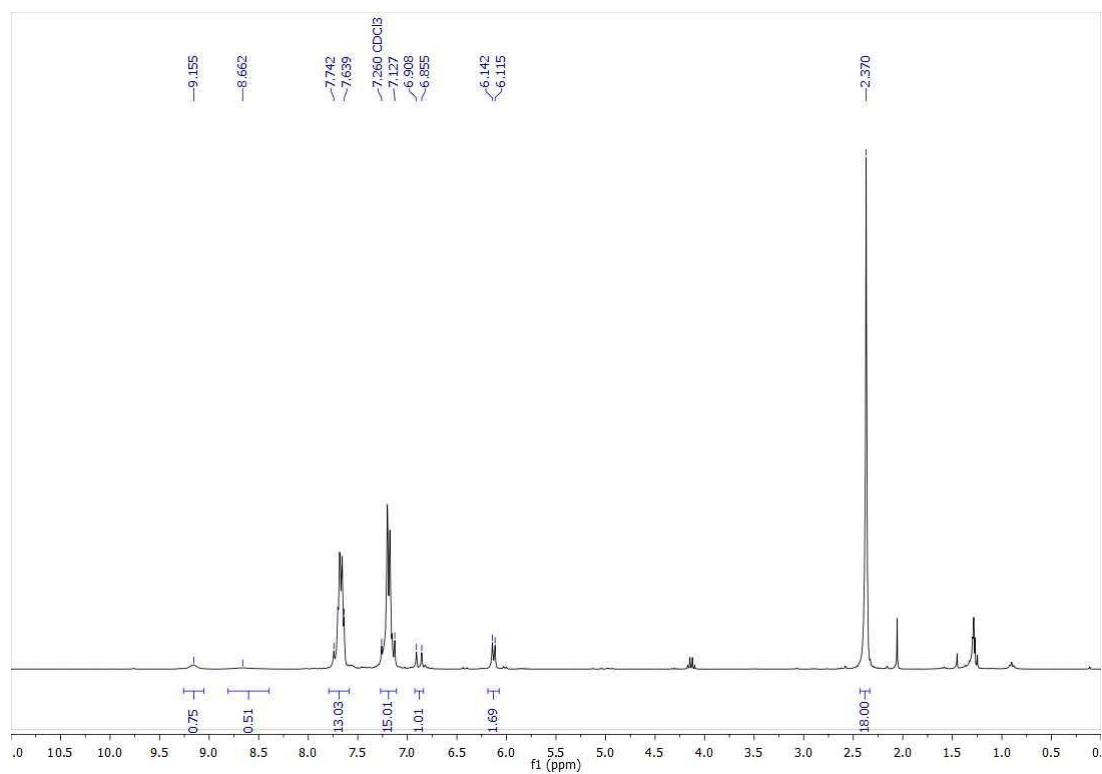
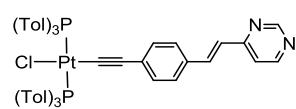


Figure S13. ^1H NMR spectrum (300 MHz, CDCl_3) of 5.

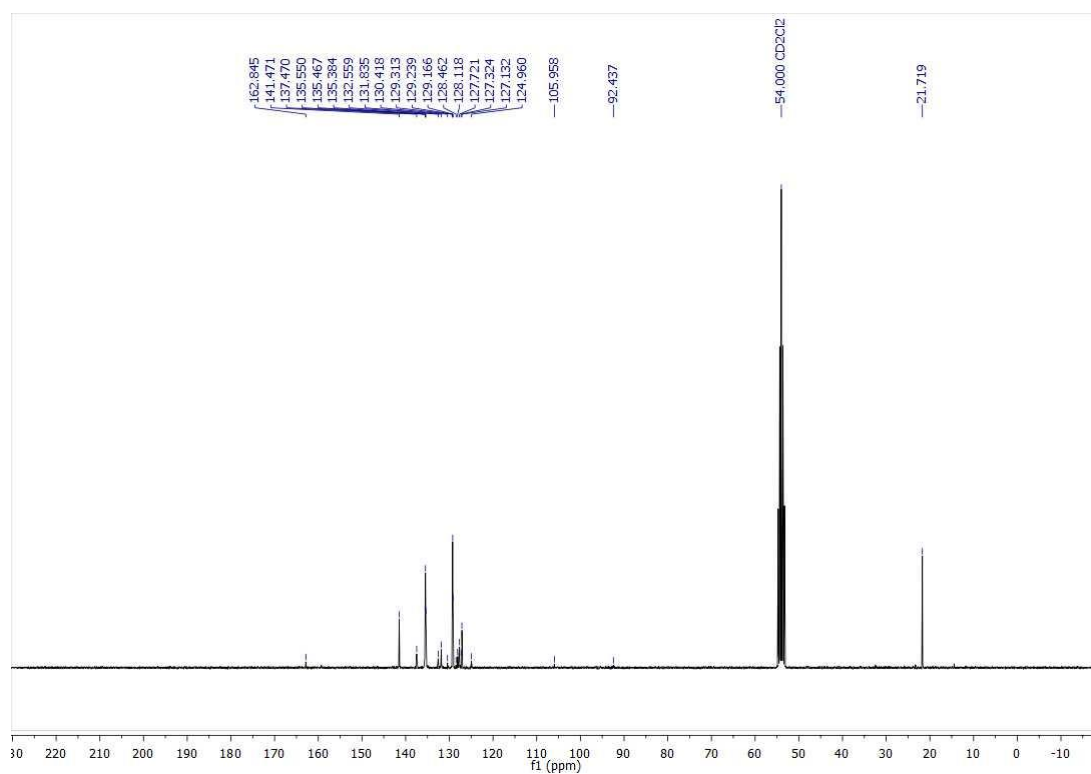


Figure S14. ¹³C NMR spectrum (75 MHz, CD₂Cl₂) of 5.

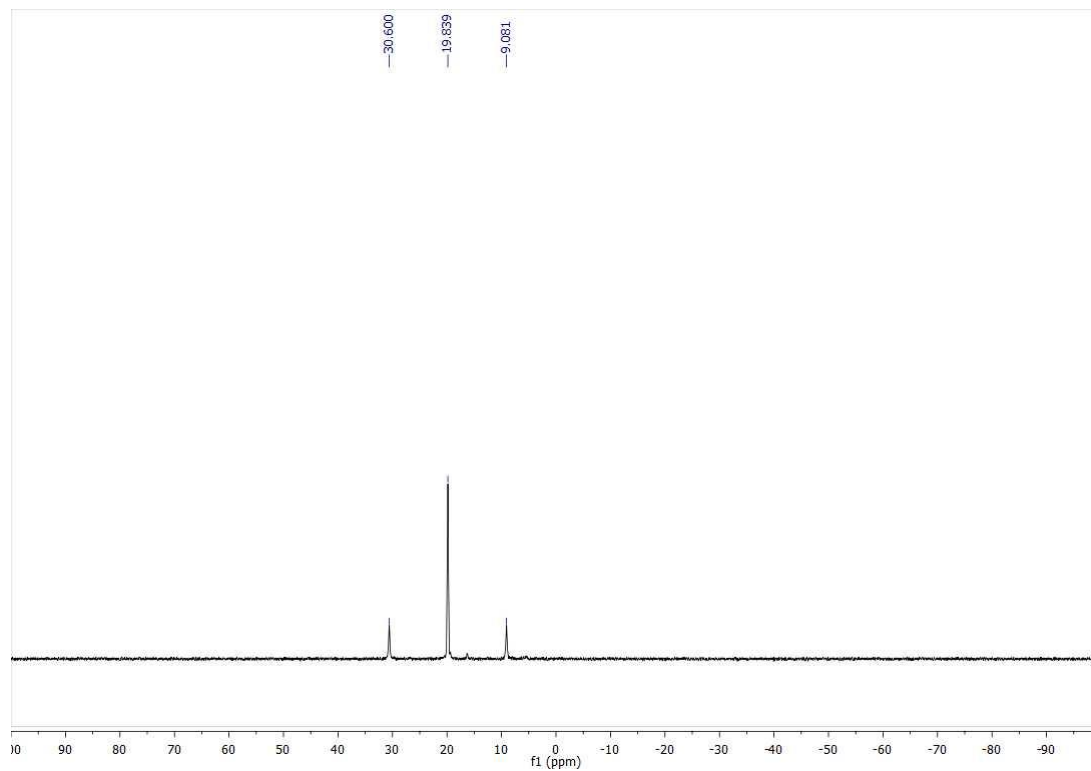


Figure S15. ³¹P NMR spectrum (121 MHz, CDCl₃) of 5.

Complex 6

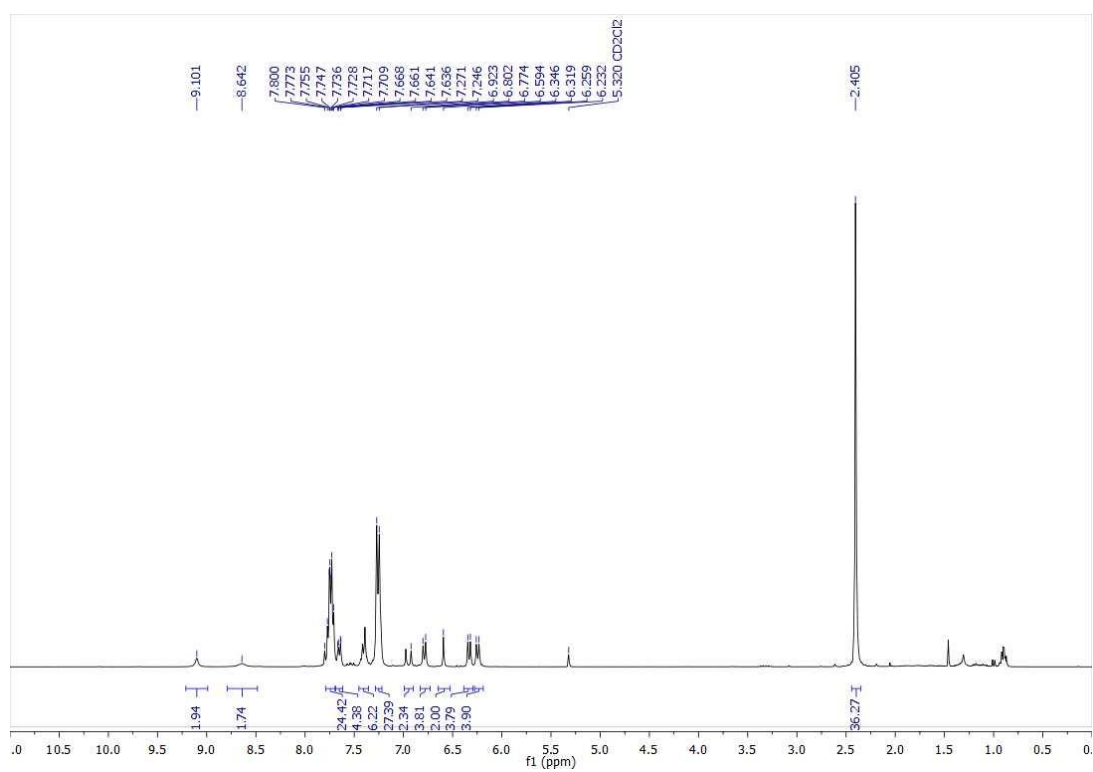
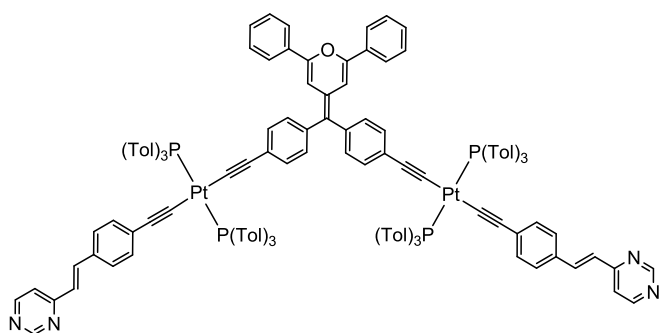


Figure S16. ¹H NMR spectrum (300 MHz, CD₂Cl₂) of **6**.

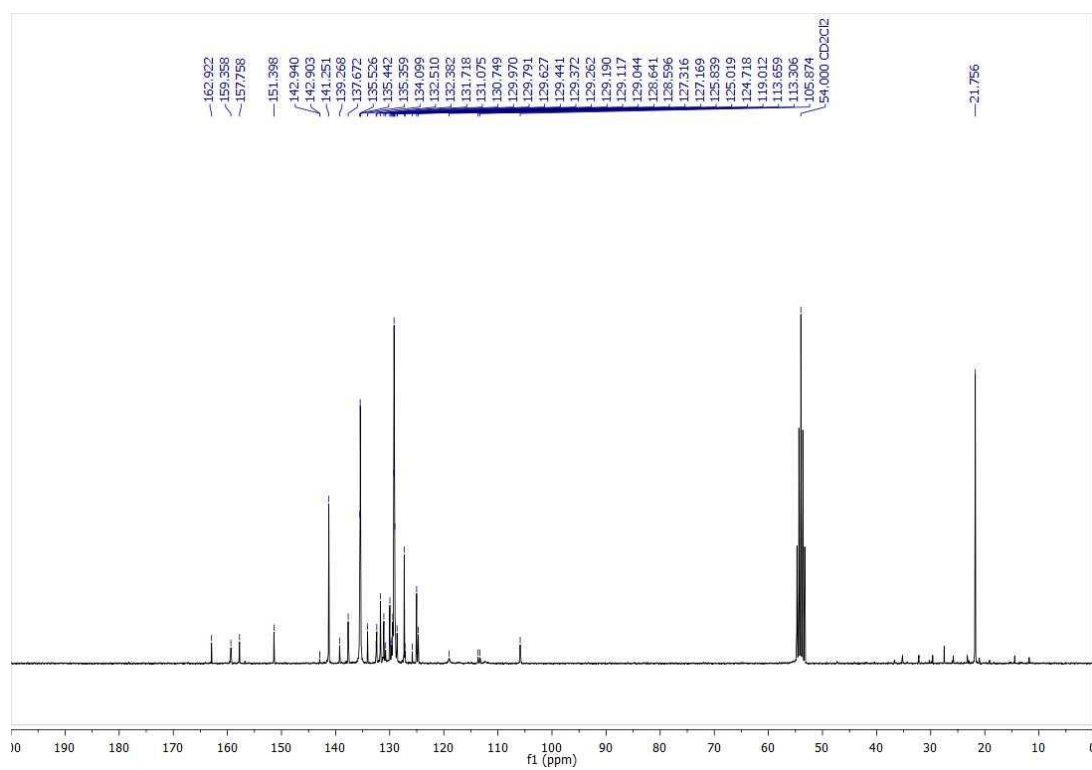


Figure S17. ¹³C NMR spectrum (75 MHz, CD₂Cl₂) of 6.

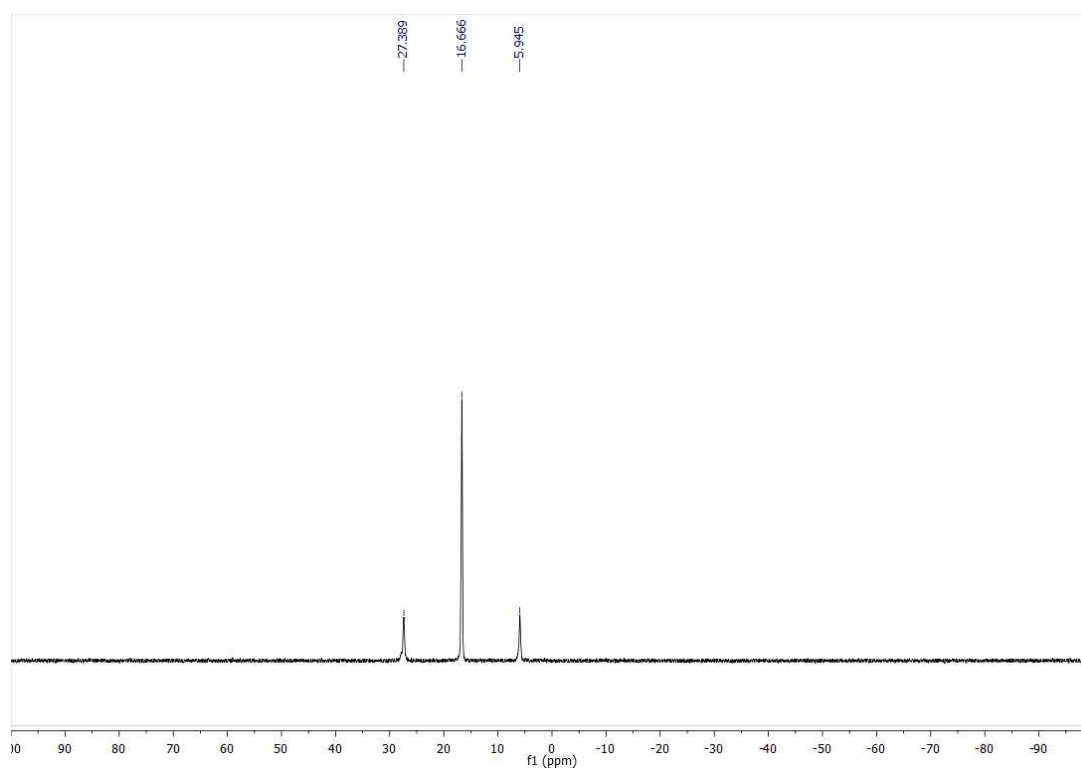


Figure S18. ³¹P NMR spectrum (121 MHz, CDCl₃) of 6.

Complex 7:

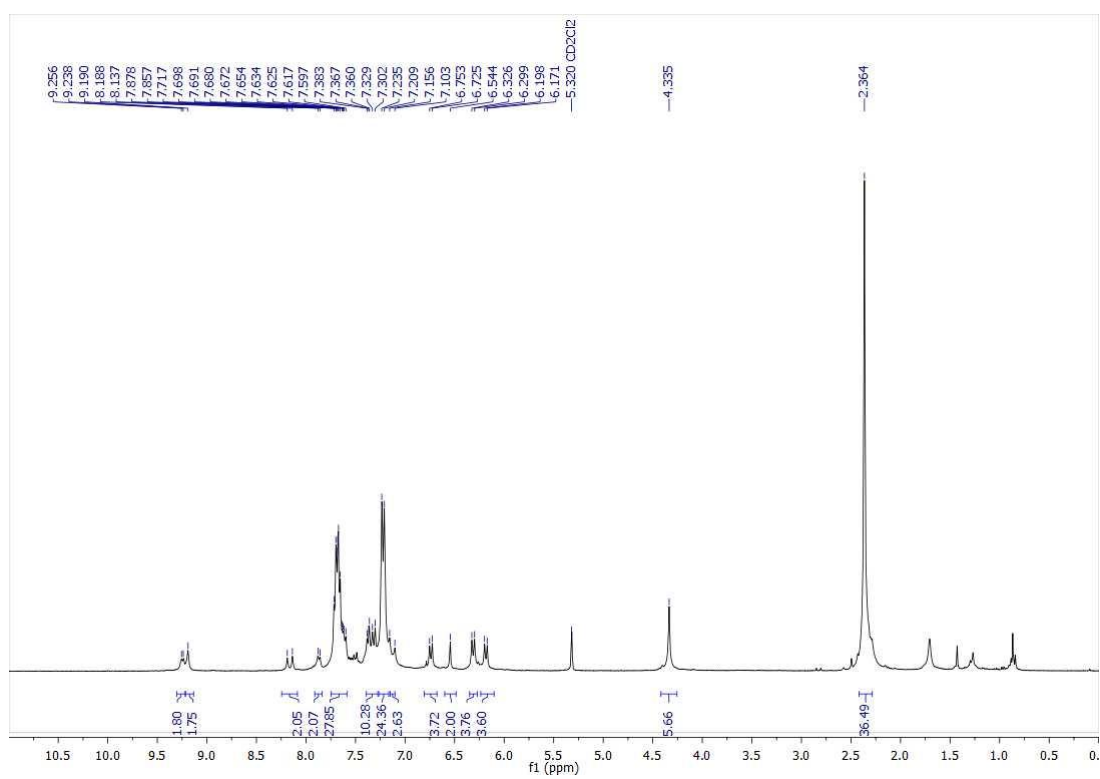
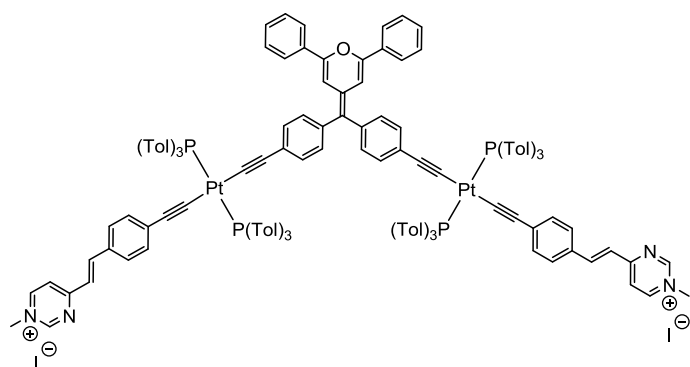


Figure S19. ^1H NMR spectrum (300 MHz, CD_2Cl_2) of **7**.

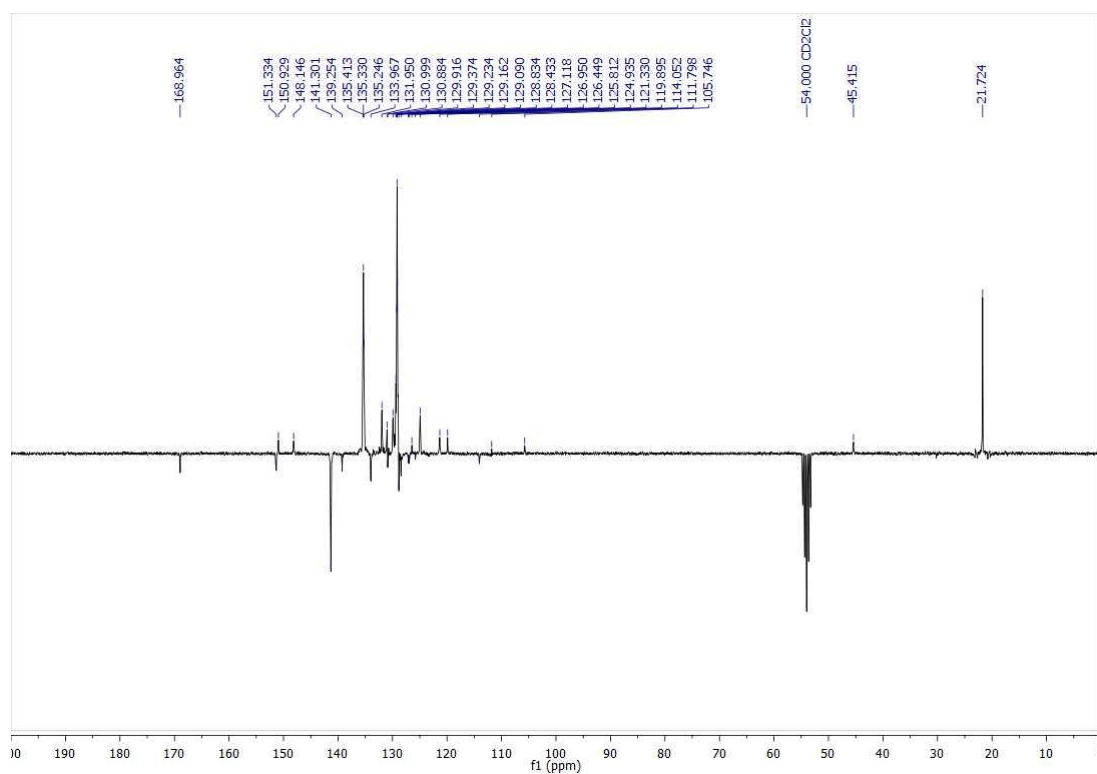


Figure S20. $^{13}\text{C}\{^1\text{H}\}$ and JMOD NMR spectrum of compound **7** (75 MHz, CD_2Cl_2) of **7**.

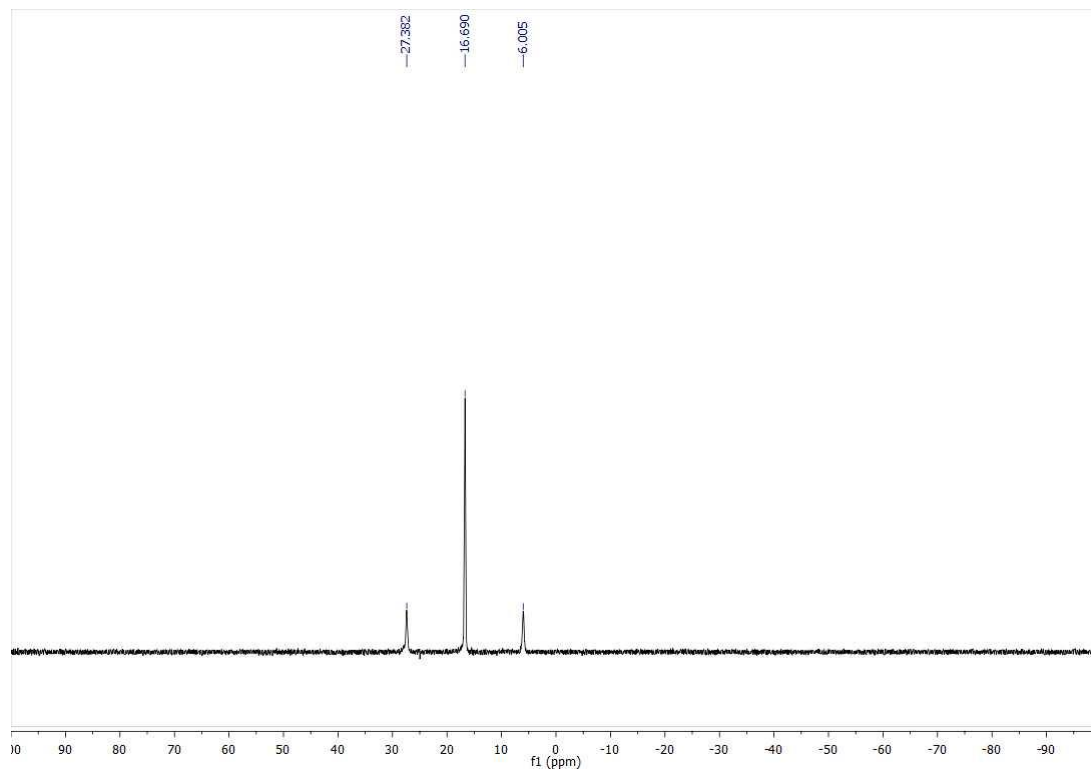


Figure S21. ^{31}P NMR spectrum (121 MHz, CD_2Cl_2) of **7**.

DOSY of complex 6:

DOSY experiments were performed on a 500 MHz Avance III HD Bruker spectrometer, fitted with a BBFO probehead. Temperature was carefully regulated at 298K. Gradients had previously been calibrated using a standard Gadolinium doped water sample, and their strength was found to be 4.975 G/cm. The pulse program ledbpgp2s (stimulated echo with eddy current compensation and bipolar gradients). Specific parameters were Δ 60ms and δ 2ms, gradients strength was varied from 2 to 95 % (16 steps). Since complex concentration was very low, 320 scans were used for each gradient step.

Complex 6 was analyzed in two different samples, meant to be representative of electrochemical conditions: solvent was CD₂Cl₂, complex concentration was 0.5 mM, and NBu₄PF₆ concentration was 0 or 0.1M respectively.

Data processing: Diffusion spectra were processed with both the dosy program to get a DOSY plot (see figure S22 and S23), and the Topspin T1/T2 package for a fitting of the diffusion decay on several relevant spectral regions. Calculated D for complex 6 were $7.8 \cdot 10^{-6} \text{ cm}^2/\text{s}$ ($\pm 0.1 \cdot 10^{-6}$) or $6.0 \cdot 10^{-6} \text{ cm}^2/\text{s}$ ($\pm 0.2 \cdot 10^{-6}$) for the sample with 0 or 0.1M NBu₄PF₆ respectively.

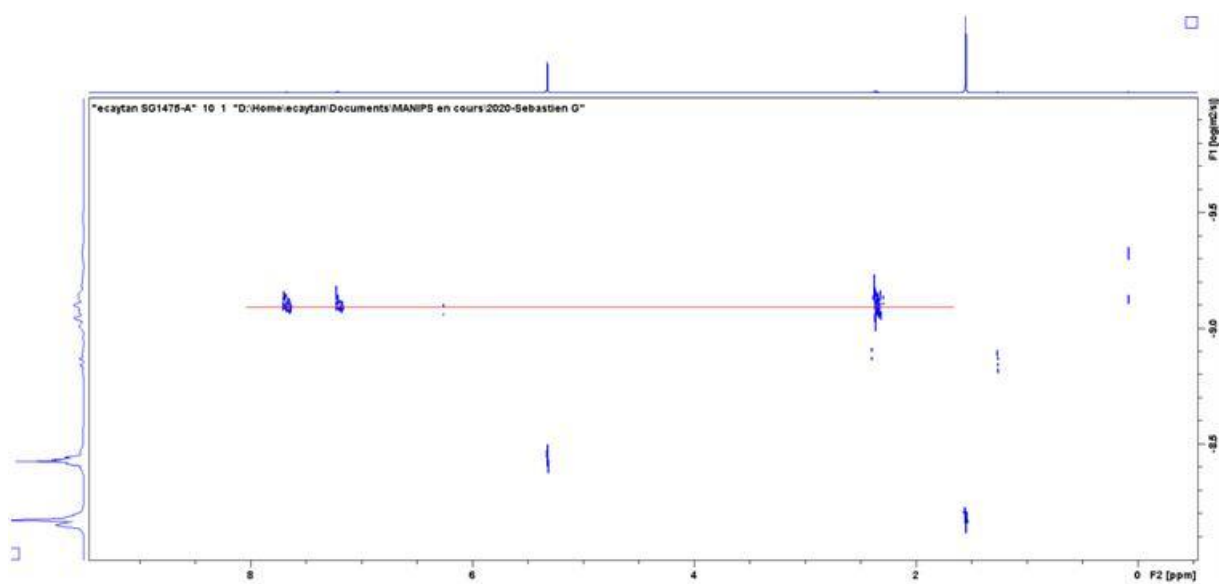


Figure S22. ^1H DOSY spectrum of complex **6** (0.5mM in CD_2Cl_2)

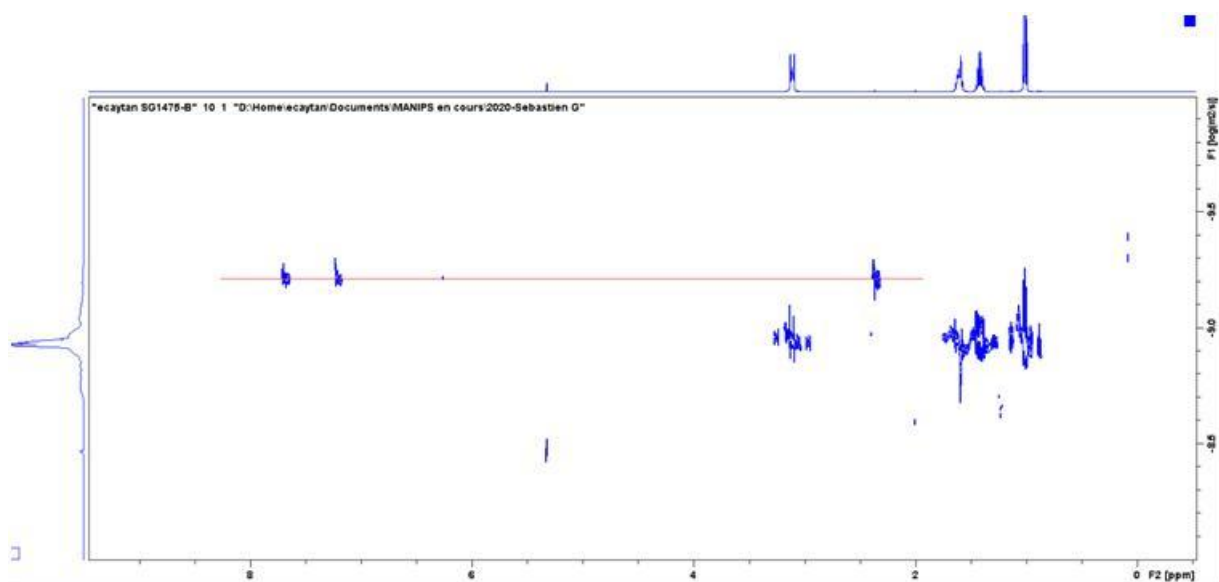


Figure S23. ^1H DOSY spectrum of complex **6** (0.5mM in CD_2Cl_2 + 0.1M NBu_4PF_6)

Cyclic voltammetry

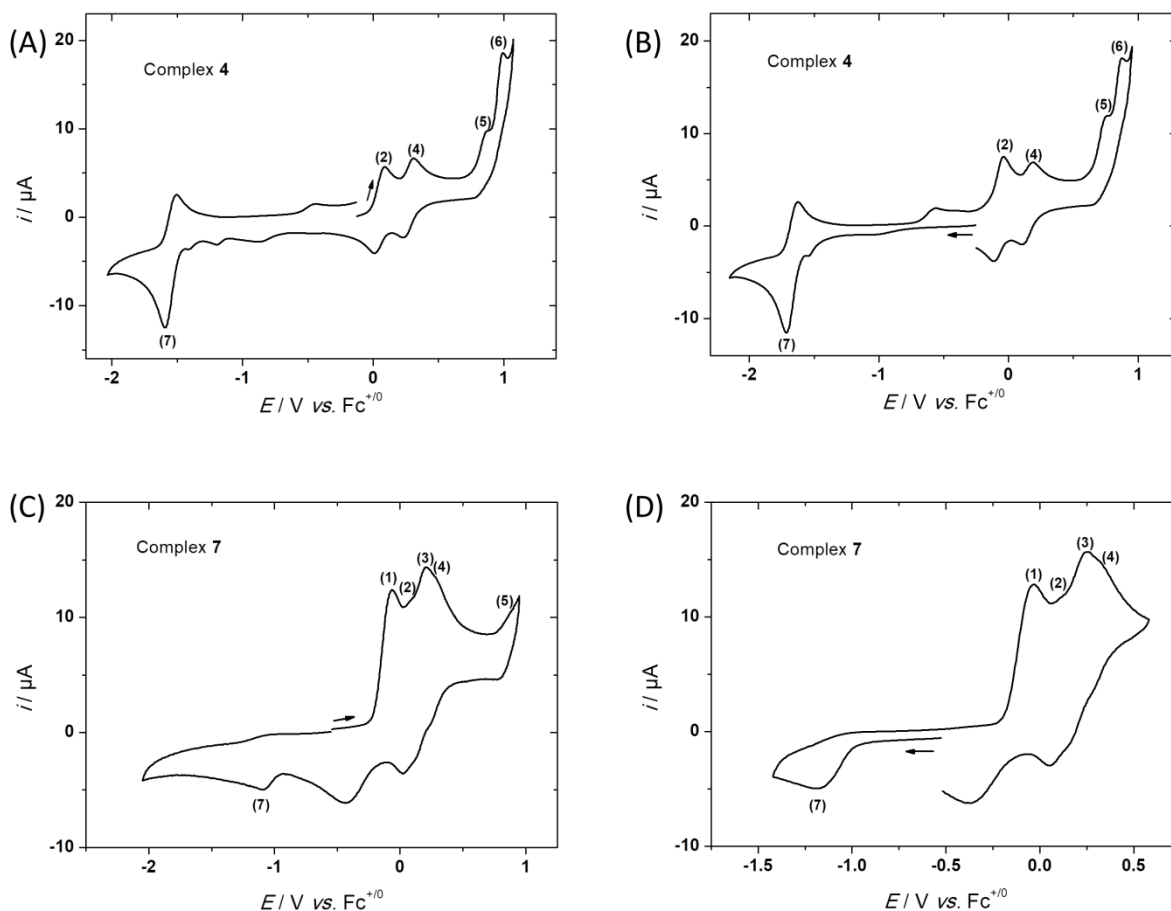


Figure S24. Cyclic voltammograms at a Pt working electrode of complex **4** ((A) and (B)), and complex **7** ((C) and (D)) in CH₂Cl₂/NBu₄PF₆ 0.1 M (E /V vs. Fc, $\nu = 0.1$ V s⁻¹). Concentration in complex: 0.5 mM. Arrows indicate the initial scanning direction. Panels (A) and (C): positive scan; Panels (B) and (D): negative scan. Numbers refer to the redox systems given in Table 2 and text.

Determination of the number of electron for the process (2) for complex 6

The Randles–Sevcik equation can be used assuming a simple electron-transfer mechanism for the process (2) for the complex **6** since the system is reversible:

$$i_p = 0.446n^{3/2}FACD^{1/2} \left[\frac{F}{RT} \right]^{1/2} \nu^{1/2}$$

where n = number of electrons, A = electrode surface area (cm²), D = diffusion coefficient (cm² s⁻¹), ν = scan rate (V s⁻¹) and C = concentration of the complex (M).

From the value of D determined by ^1H NMR DOSY (Figure S23, $D = 6 \times 10^{-6} \text{ cm}^2 \text{ s}^{-1}$), plots of $i_{\text{pa}}(2)$ versus $v^{1/2}$ ($0.01 \text{ V s}^{-1} < v < 1 \text{ V s}^{-1}$) (Figure S25) display a linear trend yielding $n = 0.82$, hence confirming the mono-electronic character of the reaction.

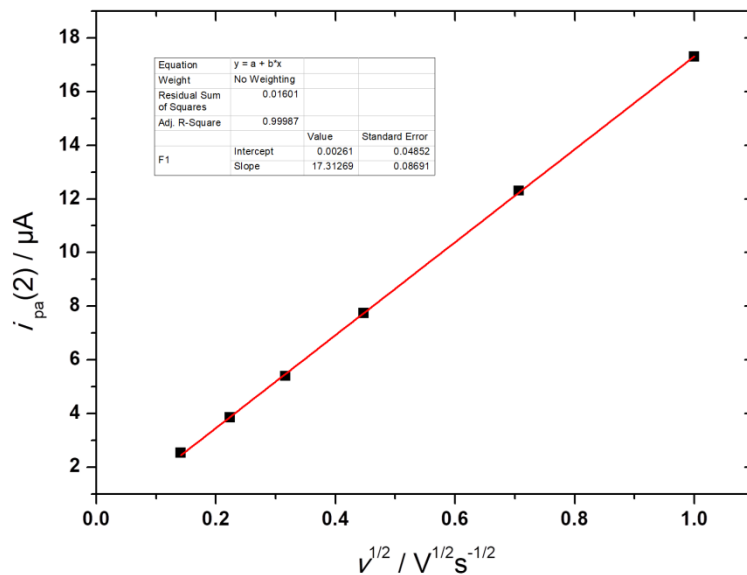


Figure S25. Plots of $i_{\text{pa}}(2)$ versus $v^{1/2}$ for $0.01 \text{ Vs}^{-1} < v < 1 \text{ Vs}^{-1}$ from CVs at a Pt electrode of complex **6** ($C = 0.5 \text{ mM}$) in $\text{CH}_2\text{Cl}_2/\text{NBu}_4\text{PF}_6$ 0.1 M .

Additional Theoretical Results

TD-DFT data

Table S1. Main TD-DFT data for 3, 4, 6, 7, SG1, SG2, RD1 and RD2. We report only relevant transitions with large f (>0.2).

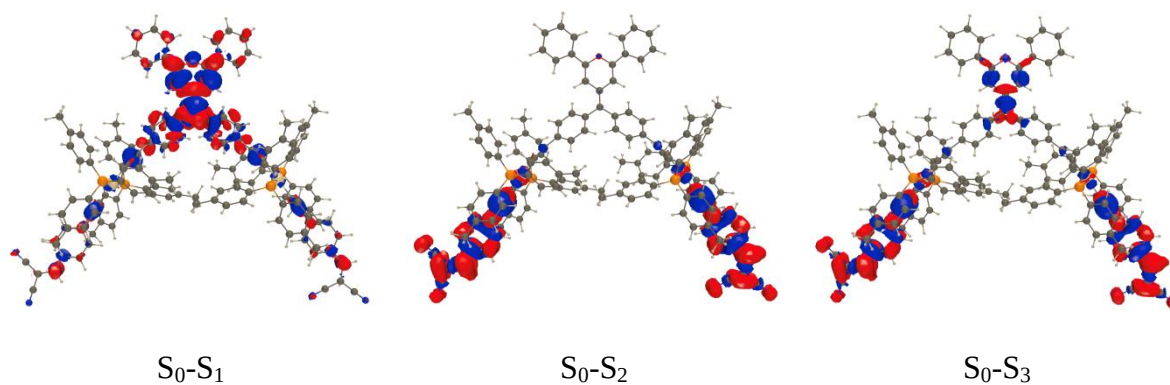
Complex	Excited-state	λ_{vert} [nm] ^a	f^b	$d^{\text{CT}}[\text{\AA}]/q^{\text{CT}}[\text{e}]^c$
3	S ₁	408	2.97	0.22 / 0.40
	S ₂	397	1.34	3.04 / 0.66
	S ₃	395	0.38	2.37 / 0.58
4	S ₁	412	3.61	2.16 / 0.61
	S ₂	411	1.58	3.03 / 0.70
6	S ₁	408	2.16	1.02 / 0.46
	S ₂	388	0.26	2.51 / 0.84
	S ₃	375	1.73	2.93 / 0.62
	S ₄	371	1.52	2.96 / 0.60
7	S ₁	473	1.90	4.64 / 0.80
	S ₂	472	2.39	4.64 / 0.79
	S ₅	403	1.16	0.12 / 0.47
SG1	S ₁	398	1.28	1.01 / 0.44
	S ₃	308	0.59	1.55 / 0.60
SG2	S ₁	405	1.53	1.23 / 0.46
	S ₃	322	0.87	1.81 / 0.61
RD1	S ₁	403	1.94	0.52 / 0.46
	S ₃	373	1.32	3.57 / 0.60
RD2	S ₁	477	2.12	6.26 / 0.82
	S ₃	398	1.11	3.29 / 0.51

^a Vertical transition wavelengths.
^b Corresponding oscillator strength.
^c ICT distance and charge according to Le Bahers' model.

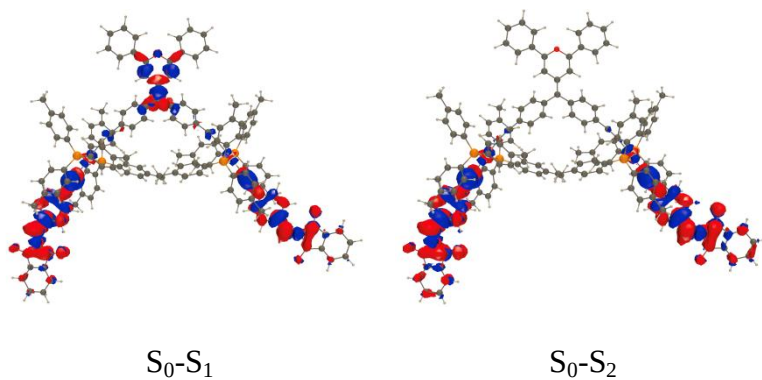
Density Difference Plots

Below are density difference plots showing the difference between the excited state and the ground state densities. The blue and red lobes indicate density decrease (donor) and increase (acceptor) upon absorption, respectively. The contour threshold is 4×10^{-4} au.

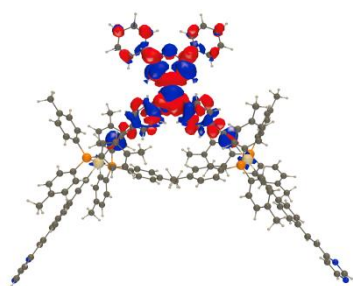
Molecule 3



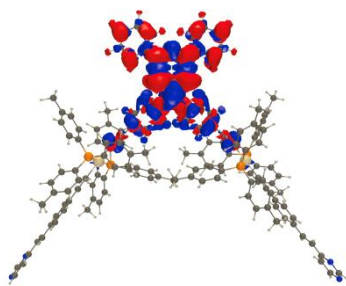
Molecule 4



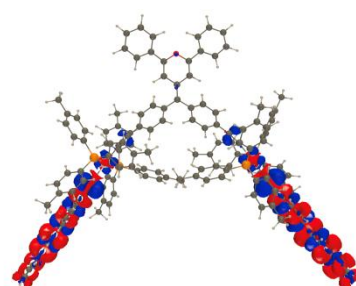
Molecule 6



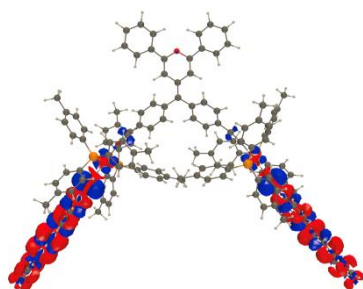
S_0-S_1



S_0-S_2

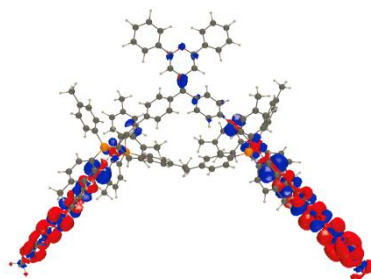


S_0-S_3

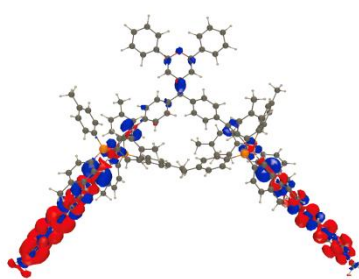


S_0-S_4

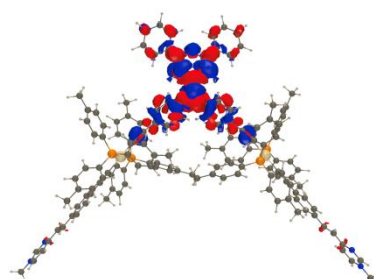
Molecule 7



S_0-S_1



S_0-S_2



S_0-S_5

Cartesian coordinates (Å)

3

Pt	-6.7695600	-0.4985940	-0.0970230
P	-7.4390950	-0.1094640	2.1369150
C	-8.5080590	-1.4134660	2.8583120
C	-8.0090800	-2.4142950	3.6982110
H	-6.9806600	-2.3690710	4.0614090
C	-8.8280130	-3.4848230	4.0794980
H	-8.4258040	-4.2622050	4.7320410
C	-10.1513800	-3.5777710	3.6323590
C	-10.6492060	-2.5543190	2.8062990
H	-11.6822350	-2.6070220	2.4544510
C	-9.8393320	-1.4929430	2.4137000
H	-10.2392620	-0.7264380	1.7449510
C	-11.0248190	-4.7453220	3.9975270
H	-11.9820290	-4.4112990	4.4193810
H	-11.2597020	-5.3449250	3.1057080
H	-10.5380580	-5.4032750	4.7273280
C	-8.3651000	1.4441690	2.4186630
C	-9.0330980	1.6608110	3.6372530
H	-9.0098840	0.8967590	4.4179870
C	-9.7316550	2.8472890	3.8516870
H	-10.2443880	3.0090270	4.8020910
C	-9.7886230	3.8429040	2.8604220
C	-9.1221360	3.6160490	1.6492920
H	-9.1552120	4.3772550	0.8676790
C	-8.4162030	2.4300450	1.4249960
H	-7.8967350	2.2689780	0.4770950
C	-10.5655560	5.1074900	3.0991050
H	-11.6462510	4.9099050	3.0805930
H	-10.3342940	5.5351760	4.0832620
H	-10.3502010	5.8634260	2.3347040
C	-5.9268540	-0.0338230	3.1726600
C	-4.9412140	-1.0144590	2.9678450
H	-5.1121810	-1.8161080	2.2427570
C	-3.7365890	-0.9594500	3.6667230
H	-2.9846460	-1.7353730	3.5064420
C	-3.4712430	0.0854780	4.5682810
C	-4.4589310	1.0601540	4.7635870
H	-4.2712650	1.8809950	5.4584650
C	-5.6761320	1.0054520	4.0759470
H	-6.4190030	1.7889920	4.2355350
C	-2.1444110	0.1744100	5.2695940
H	-2.2188810	0.7445220	6.2036150
H	-1.7443040	-0.8213210	5.5002380
H	-1.4046980	0.6825500	4.6332990
P	-5.8751980	-0.8217530	-2.2702860
C	-6.6814750	-2.1690580	-3.2199290
C	-6.4100770	-3.5013920	-2.8638510
H	-5.6399960	-3.7233520	-2.1207810
C	-7.1297030	-4.5438250	-3.4408250
H	-6.9093920	-5.5759220	-3.1577310
C	-8.1562390	-4.2899150	-4.3675040
C	-8.4157680	-2.9603820	-4.7214720
H	-9.2017580	-2.7413090	-5.4467800
C	-7.6882390	-1.9062720	-4.1553250
H	-7.9160110	-0.8787700	-4.4464720
C	-8.9634860	-5.4253270	-4.9320040

H	-8.3158240	-6.2210920	-5.3231470
H	-9.5912980	-5.8773710	-4.1497780
H	-9.6246390	-5.0905120	-5.7402320
C	-6.0697700	0.6878880	-3.2966940
C	-5.1106860	1.0914230	-4.2339730
H	-4.1911560	0.5183850	-4.3656000
C	-5.3163060	2.2450770	-4.9975330
H	-4.5587420	2.5521970	-5.7211510
C	-6.4775670	3.0153700	-4.8485900
C	-7.4346560	2.6013930	-3.9070880
H	-8.3456850	3.1887460	-3.7756500
C	-7.2327140	1.4591340	-3.1334730
H	-7.9821820	1.1645310	-2.3926640
C	-6.6873990	4.2693770	-5.6510290
H	-6.0424540	4.2926540	-6.5377120
H	-7.7307560	4.3633740	-5.9781670
H	-6.4561670	5.1594020	-5.0492850
C	-4.0872070	-1.2446560	-2.2957490
C	-3.2627580	-0.9399960	-1.2001810
H	-3.6909050	-0.4709950	-0.3115030
C	-1.8966620	-1.2151560	-1.2535220
H	-1.2656640	-0.9604000	-0.3979840
C	-1.3152530	-1.8034240	-2.3870150
C	-2.1464060	-2.1170280	-3.4720610
H	-1.7174060	-2.5806880	-4.3623080
C	-3.5157560	-1.8415650	-3.4312540
H	-4.1411500	-2.0996160	-4.2889440
C	0.1614180	-2.0824260	-2.4230680
H	0.4584450	-2.5724070	-3.3584990
H	0.7367320	-1.1489460	-2.3286170
H	0.4626010	-2.7308000	-1.5880610
C	-5.5482590	1.0987280	0.0528610
C	-4.6698420	1.9683270	0.0989460
C	-3.5372520	2.8412700	0.1136620
C	-2.4377460	2.5527970	0.9516410
H	-2.4981020	1.6895770	1.6196130
C	-1.2902080	3.3388510	0.9163350
H	-0.4450460	3.0884010	1.5612500
C	-1.1933890	4.4597290	0.0662160
C	-2.2978280	4.7479700	-0.7602280
H	-2.2336880	5.5839020	-1.4601230
C	-3.4455300	3.9575210	-0.7415170
H	-4.2774880	4.1790590	-1.4122850
C	0.0576170	5.2467470	0.0067040
C	0.0557150	6.6268810	0.0071150
C	-1.1202680	7.4269970	0.2985220
H	-2.0439470	6.9345250	0.5931270
C	-1.0898030	8.7812920	0.2967350
O	0.0516490	9.4769190	0.0078550
C	-2.2172720	9.6699360	0.6160820
C	-3.5382590	9.1845310	0.6430140
H	-3.7468510	8.1423070	0.3983480
C	-4.5992640	10.0323180	0.9574180
H	-5.6159020	9.6400830	0.9699710
C	-4.3647480	11.3834740	1.2444040
H	-5.1959480	12.0451210	1.4871030
C	-3.0568110	11.8768720	1.2097760
H	-2.8636400	12.9267710	1.4294570
C	-1.9914710	11.0294990	0.8963100
H	-0.9747500	11.4208140	0.8792570

C	5.6739390	1.1130420	-0.0426250
C	4.7937440	1.9808990	-0.0873560
C	3.6589380	2.8509960	-0.1015210
C	2.5601430	2.5599210	-0.9395600
H	2.6227150	1.6971140	-1.6078870
C	1.4104920	3.3428540	-0.9038350
H	0.5659540	3.0903510	-1.5487740
C	1.3107380	4.4631580	-0.0532730
C	2.4144750	4.7540090	0.7731940
H	2.3481120	5.5894690	1.4734460
C	3.5642930	3.9666260	0.7541200
H	4.3956320	4.1900910	1.4250150
C	1.2294150	7.4304910	-0.2838700
H	2.1545010	6.9408480	-0.5787840
C	1.1950430	8.7846980	-0.2814160
C	2.3199240	9.6767300	-0.6004710
C	3.6422970	9.1951530	-0.6279030
H	3.8539120	8.1533950	-0.3838370
C	4.7007860	10.0461590	-0.9421000
H	5.7185510	9.6568590	-0.9550830
C	4.4623220	11.3967840	-1.2283540
H	5.2915520	12.0609560	-1.4709010
C	3.1529780	11.8863870	-1.1932120
H	2.9567240	12.9358310	-1.4123340
C	2.0901540	11.0357830	-0.8799660
H	1.0723080	11.4241410	-0.8625380
Pt	6.8986180	-0.4820410	0.1035030
P	7.5618170	-0.0897180	-2.1316500
C	8.6283920	-1.3932550	-2.8574790
C	8.1239230	-2.3982050	-3.6892620
H	7.0926240	-2.3557480	-4.0444640
C	8.9407880	-3.4694260	-4.0725270
H	8.5341070	-4.2501930	-4.7181650
C	10.2677990	-3.5591920	-3.6355710
C	10.7711750	-2.5314630	-2.8183750
H	11.8072930	-2.5810370	-2.4752180
C	9.9632410	-1.4693730	-2.4233970
H	10.3677360	-0.6994870	-1.7613130
C	11.1381440	-4.7289390	-4.0010710
H	12.1019090	-4.3976130	-4.4098750
H	11.3586000	-5.3376360	-3.1116920
H	10.6550690	-5.3782530	-4.7409400
C	8.4863560	1.4645840	-2.4145320
C	9.1510560	1.6832160	-3.6346440
H	9.1269100	0.9197950	-4.4159570
C	9.8474260	2.8707780	-3.8497440
H	10.3576020	3.0341450	-4.8012620
C	9.9052470	3.8658210	-2.8578460
C	9.2424540	3.6368730	-1.6451660
H	9.2764540	4.3973680	-0.8629130
C	8.5386540	2.4496250	-1.4201760
H	8.0217660	2.2869930	-0.4711210
C	10.6776920	5.1326670	-3.0991620
H	10.4188330	5.5753690	-4.0697950
H	10.4850700	5.8775590	-2.3180730
H	11.7580980	4.9335640	-3.1151750
C	6.0466930	-0.0133810	-3.1631170
C	5.0608970	-0.9932380	-2.9552380
H	5.2327880	-1.7943060	-2.2297410
C	3.8549260	-0.9381880	-3.6517040

H	3.1030720	-1.7137380	-3.4892990
C	3.5882380	0.1060900	-4.5536420
C	4.5759940	1.0800840	-4.7518350
H	4.3873030	1.9004680	-5.4469670
C	5.7946660	1.0252300	-4.0667830
H	6.5375770	1.8082460	-4.2287090
C	2.2599520	0.1948610	-5.2521950
H	2.3315140	0.7683320	-6.1843720
H	1.8614370	-0.8008990	-5.4855450
H	1.5203820	0.6992210	-4.6127060
P	6.0065700	-0.8113390	2.2769830
C	6.8151000	-2.1595410	3.2234560
C	6.5464460	-3.4914270	2.8633270
H	5.7780720	-3.7127160	2.1182890
C	7.2667430	-4.5342600	3.4385820
H	7.0489360	-5.5659770	3.1522140
C	8.2911690	-4.2811270	4.3679200
C	8.5481990	-2.9521480	4.7256670
H	9.3324490	-2.7337910	5.4531210
C	7.8199120	-1.8975710	4.1611110
H	8.0453870	-0.8704500	4.4554320
C	9.0974080	-5.4174340	4.9320080
H	8.4489120	-6.2030160	5.3419280
H	9.7080600	-5.8844000	4.1450110
H	9.7737050	-5.0798010	5.7264540
C	6.1996420	0.6966990	3.3060990
C	5.2404620	1.0973250	4.2446300
H	4.3221030	0.5223870	4.3761460
C	5.4445380	2.2502770	5.0094830
H	4.6869940	2.5551020	5.7341000
C	6.6043130	3.0229960	4.8606840
C	7.5615780	2.6118360	3.9182470
H	8.4714970	3.2009400	3.7869780
C	7.3610780	1.4701400	3.1432340
H	8.1104940	1.1778740	2.4014110
C	6.8110020	4.2769300	5.6640550
H	6.1831960	4.2869340	6.5632410
H	7.8589920	4.3859910	5.9708990
H	6.5536090	5.1654910	5.0707840
C	4.2192200	-1.2369710	2.3031240
C	3.3928610	-0.9308320	1.2094080
H	3.8189820	-0.4586310	0.3214690
C	2.0273400	-1.2086720	1.2637090
H	1.3948460	-0.9528640	0.4095880
C	1.4484250	-1.8012050	2.3962620
C	2.2814800	-2.1160890	3.4794570
H	1.8545040	-2.5830230	4.3689580
C	3.6502520	-1.8379610	3.4377270
H	4.2771240	-2.0972570	4.2939520
C	-0.0275610	-2.0838110	2.4330790
H	-0.3230530	-2.5740080	3.3688780
H	-0.6054910	-1.1520270	2.3381530
H	-0.3271500	-2.7336580	1.5986160
C	8.0709470	-2.0925700	0.2542290
C	8.7951260	-3.0954940	0.3391740
C	-7.9377990	-2.1117310	-0.2507770
C	-8.6602730	-3.1158490	-0.3358270
C	9.6165680	-4.2474060	0.4301390
C	9.0449330	-5.5455430	0.4083520
C	11.0228340	-4.1339590	0.5426180

C	9.8362120	-6.6778090	0.4940440
H	7.9622840	-5.6373200	0.3172000
C	11.8125530	-5.2686570	0.6312780
H	11.4726190	-3.1411900	0.5611350
H	9.3577980	-7.6556210	0.4705280
H	12.8956790	-5.1667230	0.7201690
C	-9.4842220	-4.2661610	-0.4241050
C	-8.9240950	-5.5658260	-0.3999850
C	-10.8927460	-4.1415380	-0.5361750
C	-9.7399570	-6.6821560	-0.4831560
H	-7.8429830	-5.6728530	-0.3101170
C	-11.7056340	-5.2584320	-0.6230850
H	-11.3284090	-3.1422370	-0.5559660
H	-9.2950110	-7.6785790	-0.4605520
H	-12.7819470	-5.1188860	-0.7102980
C	11.2451450	-6.5668570	0.6093420
C	12.1557120	-7.6732250	0.7056210
H	13.2096600	-7.3928740	0.7833970
C	-11.1471360	-6.5614880	-0.5981980
C	-11.8970080	-7.7835820	-0.6799170
H	-11.2931290	-8.6942680	-0.6411440
C	11.9345960	-9.0312280	0.7175040
C	-13.2485840	-8.0120730	-0.7993880
C	-14.2569570	-6.9991380	-0.8721850
N	-15.1031770	-6.1913620	-0.9335550
C	10.6532440	-9.6626990	0.6312960
N	9.6176190	-10.2060240	0.5631910
C	-13.7272760	-9.3613980	-0.8600750
N	-14.1160060	-10.4651790	-0.9094390
C	13.0526050	-9.9211370	0.8248810
N	13.9680650	-10.6464840	0.9125320

4

Pt	6.6524970	0.1628580	0.0343710
P	7.1021520	0.3817420	-2.2758350
C	8.1714670	-0.9292210	-2.9849030
C	7.6618330	-2.0106870	-3.7102060
H	6.6077190	-2.0397330	-3.9920970
C	8.5031790	-3.0676290	-4.0807960
H	8.0924910	-3.9087230	-4.6428080
C	9.8597300	-3.0673510	-3.7353500
C	10.3663540	-1.9636590	-3.0260340
H	11.4243480	-1.9437600	-2.7541570
C	9.5355220	-0.9142110	-2.6454730
H	9.9458540	-0.0825160	-2.0667340
C	10.7586250	-4.2218710	-4.0790220
H	11.6838970	-3.8793510	-4.5609000
H	11.0531670	-4.7632200	-3.1676080
H	10.2641670	-4.9356060	-4.7488720
C	7.9072960	1.9427610	-2.7925830
C	8.4129550	2.0758450	-4.0985460
H	8.3299260	1.2462860	-4.8049770
C	9.0276650	3.2617330	-4.4941630
H	9.4146590	3.3582100	-5.5106960
C	9.1614410	4.3402100	-3.6015450
C	8.6592550	4.1956200	-2.3021450
H	8.7557690	5.0210700	-1.5945280

C	8.0369340	3.0106790	-1.8959420
H	7.6442070	2.9153610	-0.8805560
C	9.8416050	5.6065530	-4.0415680
H	10.9054360	5.4272500	-4.2488790
H	9.3956410	5.9926590	-4.9676570
H	9.7737850	6.3882840	-3.2758680
C	5.4946840	0.2814660	-3.1544870
C	4.6130410	-0.7488140	-2.7852190
H	4.9167990	-1.4830680	-2.0327820
C	3.3444180	-0.8299670	-3.3567900
H	2.6763170	-1.6449060	-3.0687650
C	2.9097710	0.1259930	-4.2906830
C	3.7941540	1.1525680	-4.6487910
H	3.4747360	1.9064560	-5.3709830
C	5.0746790	1.2334700	-4.0908070
H	5.7351730	2.0539580	-4.3770040
C	1.5169280	0.0708130	-4.8547130
H	1.4591240	0.5585450	-5.8354910
H	1.1656480	-0.9641010	-4.9595450
H	0.8091690	0.5883810	-4.1897340
P	5.9700460	-0.0053840	2.2959400
C	6.8741590	-1.2799730	3.2573190
C	6.5847390	-2.6343190	3.0183130
H	5.7495050	-2.9088060	2.3691130
C	7.3684230	-3.6325710	3.5899740
H	7.1344920	-4.6822330	3.3969460
C	8.4764310	-3.3121310	4.3939860
C	8.7527750	-1.9606250	4.6340820
H	9.6023050	-1.6899150	5.2641230
C	7.9627760	-0.9502270	4.0720470
H	8.2062080	0.0956030	4.2706310
C	9.3495390	-4.4025850	4.9489410
H	8.7522360	-5.1870860	5.4320490
H	9.9215280	-4.8848170	4.1424000
H	10.0669030	-4.0141560	5.6817980
C	6.2612000	1.5761630	3.1817220
C	5.4081920	2.0509500	4.1855860
H	4.5112080	1.4919530	4.4583420
C	5.6909220	3.2572780	4.8348820
H	5.0154020	3.6199950	5.6120860
C	6.8256980	4.0101460	4.5036500
C	7.6765470	3.5242670	3.4967180
H	8.5652140	4.0969320	3.2235860
C	7.3962230	2.3287280	2.8365580
H	8.0601610	1.9751820	2.0417620
C	7.1161190	5.3193760	5.1835290
H	6.5653270	5.4139840	6.1271040
H	8.1874310	5.4300510	5.3946840
H	6.8244720	6.1634300	4.5430330
C	4.1946500	-0.4177030	2.5305640
C	3.2619180	-0.1820050	1.5069600
H	3.5962610	0.2206600	0.5482030
C	1.9080450	-0.4408590	1.7197930
H	1.1921910	-0.2370380	0.9194600
C	1.4456010	-0.9464770	2.9445620
C	2.3843010	-1.1925920	3.9569600
H	2.0489540	-1.5901240	4.9167340
C	3.7424650	-0.9312930	3.7570040
H	4.4524340	-1.1342940	4.5621110
C	-0.0192620	-1.2172200	3.1489680

H	-0.2312350	-1.5561140	4.1702740
H	-0.6158170	-0.3136610	2.9571940
H	-0.3771940	-1.9904530	2.4542660
C	5.4085840	1.7414010	-0.1195850
C	4.5308270	2.6118980	-0.1610680
C	3.4053370	3.4935280	-0.1722080
C	2.2815260	3.1884300	-0.9710570
H	2.3151740	2.3020360	-1.6094230
C	1.1447250	3.9891690	-0.9349770
H	0.2807230	3.7266470	-1.5491490
C	1.0815610	5.1400680	-0.1225720
C	2.2094460	5.4444310	0.6653870
H	2.1721210	6.3047170	1.3371960
C	3.3476090	4.6400050	0.6453190
H	4.1995320	4.8754440	1.2857550
C	-0.1621240	5.9380270	-0.0611730
C	-0.1556880	7.3167300	-0.1101120
C	1.0176650	8.1023780	-0.4479030
H	1.9352300	7.5970090	-0.7399320
C	0.9904390	9.4559270	-0.4924780
O	-0.1447150	10.1646480	-0.2103090
C	2.1150970	10.3295890	-0.8594870
C	3.4346470	9.8402980	-0.8861010
H	3.6442950	8.8073360	-0.6056570
C	4.4930280	10.6734150	-1.2454080
H	5.5086700	10.2785620	-1.2569440
C	4.2573490	12.0137260	-1.5785860
H	5.0865410	12.6640350	-1.8562990
C	2.9509430	12.5112480	-1.5447570
H	2.7568980	13.5528590	-1.8002310
C	1.8882150	11.6784830	-1.1864450
H	0.8725340	12.0725530	-1.1703850
C	-5.7706570	1.8007620	0.1572130
C	-4.8816060	2.6601690	0.1912200
C	-3.7521450	3.5367410	0.1726600
C	-2.6492080	3.2884820	1.0181600
H	-2.7026830	2.4541570	1.7215710
C	-1.5049320	4.0764210	0.9442550
H	-0.6547840	3.8552690	1.5931940
C	-1.4160360	5.1603720	0.0470970
C	-2.5262900	5.4133070	-0.7825820
H	-2.4687910	6.2208460	-1.5156890
C	-3.6702690	4.6192500	-0.7261440
H	-4.5064400	4.8093860	-1.4014420
C	-1.3235540	8.1331730	0.1687790
H	-2.2459130	7.6557610	0.4912900
C	-1.2861330	9.4863100	0.1181110
C	-2.4043560	10.3927190	0.4196820
C	-3.7272320	9.9162900	0.4856090
H	-3.9448670	8.8664940	0.2853780
C	-4.7789520	10.7816720	0.7827780
H	-5.7972280	10.3958980	0.8260940
C	-4.5333190	12.1416570	1.0133570
H	-5.3573530	12.8169020	1.2426800
C	-3.2235970	12.6258500	0.9397610
H	-3.0216940	13.6823750	1.1154360
C	-2.1675450	11.7608970	0.6433580
H	-1.1492740	12.1455430	0.5956090
Pt	-7.0387390	0.2402150	0.0049930
P	-7.8117820	0.7097480	2.1910380

C	-8.9744880	-0.5344540	2.8730910
C	-8.5619900	-1.5392820	3.7542860
H	-7.5519170	-1.5301810	4.1684180
C	-9.4438810	-2.5672190	4.1110360
H	-9.1090250	-3.3480070	4.7967060
C	-10.7452250	-2.6141560	3.5970600
C	-11.1554330	-1.5882710	2.7271830
H	-12.1694810	-1.6062270	2.3209240
C	-10.2823280	-0.5689130	2.3594040
H	-10.6140450	0.1997920	1.6567580
C	-11.6819080	-3.7406860	3.9330660
H	-12.6677000	-3.3644660	4.2368740
H	-11.8401020	-4.3841100	3.0548360
H	-11.2876140	-4.3684460	4.7411690
C	-8.6850420	2.3065740	2.3988340
C	-9.4423060	2.5579790	3.5574080
H	-9.5234800	1.7947250	4.3349590
C	-10.0996320	3.7763500	3.7145390
H	-10.6836130	3.9636970	4.6180360
C	-10.0257750	4.7718440	2.7242090
C	-9.2724900	4.5104900	1.5726650
H	-9.2050440	5.2699450	0.7915660
C	-8.6069650	3.2917880	1.4061940
H	-8.0186690	3.1047310	0.5044230
C	-10.7534160	6.0748240	2.9048590
H	-10.4883000	6.5453080	3.8609060
H	-10.5222700	6.7813470	2.0990090
H	-11.8405890	5.9175630	2.9159340
C	-6.3689810	0.7314590	3.3262110
C	-5.3845610	-0.2581350	3.1595410
H	-5.5043320	-1.0195640	2.3826890
C	-4.2502680	-0.2684070	3.9694590
H	-3.4970290	-1.0478480	3.8336960
C	-4.0571170	0.7157030	4.9541930
C	-5.0417120	1.7002100	5.1104060
H	-4.9089980	2.4747750	5.8682460
C	-6.1882840	1.7119470	4.3085090
H	-6.9301400	2.5009250	4.4443410
C	-2.8086360	0.7268420	5.7919010
H	-2.9489450	1.2995170	6.7166240
H	-2.4955100	-0.2910490	6.0577940
H	-1.9762460	1.1883610	5.2412470
P	-6.0308130	-0.2192120	-2.0938300
C	-6.8385560	-1.5749340	-3.0295800
C	-6.6429830	-2.9025880	-2.6121200
H	-5.9162680	-3.1286760	-1.8278290
C	-7.3869600	-3.9340570	-3.1773960
H	-7.2283790	-4.9625720	-2.8443060
C	-8.3642600	-3.6718390	-4.1534820
C	-8.5482470	-2.3474760	-4.5688420
H	-9.2963450	-2.1228820	-5.3316470
C	-7.7947690	-1.3051710	-4.0147460
H	-7.9666560	-0.2799300	-4.3499550
C	-9.1992680	-4.7934960	-4.7045980
H	-8.5708190	-5.6033180	-5.0986630
H	-9.8260340	-5.2307950	-3.9131510
H	-9.8611630	-4.4496360	-5.5084590
C	-6.0820250	1.2286370	-3.2216590
C	-5.1427690	1.4097310	-4.2463920
H	-4.3144370	0.7092310	-4.3672970

C	-5.2509630	2.4995560	-5.1133740
H	-4.5114590	2.6332680	-5.9054580
C	-6.2960850	3.4269290	-4.9851450
C	-7.2349160	3.2341120	-3.9599460
H	-8.0569560	3.9433110	-3.8449310
C	-7.1279810	2.1534210	-3.0827790
H	-7.8598080	2.0250160	-2.2801030
C	-6.3894460	4.6133890	-5.9039080
H	-5.9751600	4.3871070	-6.8941980
H	-7.4280660	4.9438790	-6.0284170
H	-5.8219800	5.4631120	-5.4990710
C	-4.2679590	-0.7297140	-1.9711490
C	-3.5087800	-0.4003630	-0.8363720
H	-3.9716930	0.1516110	-0.0155860
C	-2.1640630	-0.7626090	-0.7610050
H	-1.5880310	-0.4981810	0.1294000
C	-1.5378060	-1.4590010	-1.8057430
C	-2.3029440	-1.7911860	-2.9332750
H	-1.8391210	-2.3404380	-3.7551380
C	-3.6512880	-1.4346430	-3.0180400
H	-4.2268320	-1.7224170	-3.9007840
C	-0.0842500	-1.8295570	-1.7095540
H	0.2129380	-2.5112420	-2.5163900
H	0.5515310	-0.9325500	-1.7712390
H	0.1407010	-2.3152910	-0.7500060
C	-8.2584750	-1.3357800	-0.1620000
C	-9.0041410	-2.3210300	-0.2584400
C	7.8504480	-1.4304140	0.1871010
C	8.5975770	-2.4164160	0.2630990
C	-9.8482570	-3.4582810	-0.3619120
C	-9.3135420	-4.7663600	-0.2558360
C	-11.2407860	-3.3163140	-0.5711420
C	-10.1266030	-5.8849040	-0.3499460
H	-8.2408240	-4.8780960	-0.0915850
C	-12.0520310	-4.4360170	-0.6683850
H	-11.6622330	-2.3142650	-0.6564410
H	-9.7043290	-6.8853040	-0.2634240
H	-13.1245750	-4.3124990	-0.8312320
C	9.4600710	-3.5419710	0.3395610
C	8.9367950	-4.8530190	0.4418850
C	10.8674170	-3.3792710	0.3119140
C	9.7890340	-5.9439250	0.5097650
H	7.8550410	-4.9890850	0.4621650
C	11.7184340	-4.4710150	0.3836700
H	11.2732430	-2.3695760	0.2355780
H	9.3720500	-6.9501500	0.5857400
H	12.7987770	-4.3329460	0.3632700
C	-11.5211930	-5.7459170	-0.5595190
C	-12.4509710	-6.8387610	-0.6687200
H	-13.4896510	-6.5203830	-0.8295780
C	11.1974290	-5.7850460	0.4835090
C	11.9913010	-6.9828830	0.5609380
H	11.3960640	-7.9027620	0.6353580
C	-12.3447770	-8.2034040	-0.6159290
C	-11.2158960	-9.1436530	-0.4251990
C	-13.5848880	-9.0124820	-0.7720380
C	-11.8040580	-10.5141780	-0.4673300
C	-13.1856410	-10.4406430	-0.6704640
C	-11.1561840	-11.7394270	-0.3346300
C	-13.9711560	-11.5876150	-0.7491960

C	-11.9379150	-12.8987590	-0.4120670
H	-10.0789170	-11.7875910	-0.1759850
C	-13.3275550	-12.8241750	-0.6169140
H	-15.0472060	-11.5193050	-0.9081520
H	-11.4678040	-13.8767310	-0.3128200
H	-13.9067600	-13.7453780	-0.6725510
C	13.3346810	-7.2502570	0.5639200
C	14.5531670	-6.4111070	0.4869100
C	13.7700980	-8.6707030	0.6633190
C	15.7102770	-7.3512390	0.5439220
C	15.2564120	-8.6698900	0.6468760
C	17.0701470	-7.0546650	0.5067910
C	16.1434930	-9.7408880	0.7166200
C	17.9701730	-8.1252190	0.5765640
H	17.4153350	-6.0240210	0.4262820
C	17.5130630	-9.4514710	0.6801640
H	15.7791750	-10.7649180	0.7967320
H	19.0425510	-7.9338830	0.5507090
H	18.2398960	-10.2615320	0.7324620
O	-10.0210890	-8.9173840	-0.2621180
O	-14.7216700	-8.5930420	-0.9495860
O	14.6661200	-5.1929720	0.3937100
O	13.0511200	-9.6587980	0.7434920

6

Pt	-6.8450700	-0.1924340	-0.0013480
P	-7.2114520	0.1517650	2.3060440
C	-8.2477730	-1.0736320	3.1981050
C	-7.7542740	-1.9154010	4.1996110
H	-6.7097600	-1.8516240	4.5097410
C	-8.6027050	-2.8425610	4.8202990
H	-8.2056740	-3.4946070	5.6007490
C	-9.9505620	-2.9436430	4.4581130
C	-10.4377950	-2.0874120	3.4533160
H	-11.4859060	-2.1573110	3.1539190
C	-9.6002050	-1.1706860	2.8253120
H	-9.9960670	-0.5255760	2.0370570
C	-10.8645650	-3.9489380	5.1015250
H	-11.7419610	-3.4605450	5.5463370
H	-11.2419520	-4.6645730	4.3565700
H	-10.3530670	-4.5163610	5.8882110
C	-7.9873890	1.7511610	2.7491690
C	-8.3706170	2.0037190	4.0788520
H	-8.1978180	1.2499340	4.8513600
C	-8.9780730	3.2113830	4.4148260
H	-9.2700290	3.4018420	5.4497140
C	-9.2279930	4.1920540	3.4379150
C	-8.8502210	3.9271970	2.1157550
H	-9.0402680	4.6743830	1.3430620
C	-8.2340300	2.7200460	1.7692300
H	-7.9382050	2.5282820	0.7346180
C	-9.8915020	5.4861510	3.8189190
H	-10.8845060	5.3059470	4.2522960
H	-9.3036590	6.0205260	4.5773180
H	-10.0128230	6.1478770	2.9532530
C	-5.5618240	0.1071100	3.1071030
C	-4.7487910	-1.0108260	2.8573060

H	-5.1364960	-1.8484220	2.2697700
C	-3.4400210	-1.0524130	3.3379670
H	-2.8244710	-1.9337820	3.1448400
C	-2.9008320	0.0251170	4.0600240
C	-3.7211010	1.1357510	4.3052850
H	-3.3197530	1.9842820	4.8632250
C	-5.0377180	1.1812900	3.8362080
H	-5.6458960	2.0682840	4.0231380
C	-1.4681670	0.0105250	4.5167150
H	-1.3484300	0.5136490	5.4844370
H	-1.0825580	-1.0135030	4.6072450
H	-0.8266580	0.5398970	3.7953820
P	-6.1950320	-0.4375150	-2.2625120
C	-7.0463760	-1.7394800	-3.2383420
C	-6.8364040	-3.0817430	-2.8749200
H	-6.1623740	-3.3242180	-2.0499200
C	-7.4855410	-4.1045700	-3.5596900
H	-7.3176610	-5.1436390	-3.2676110
C	-8.3737780	-3.8213970	-4.6137650
C	-8.5832420	-2.4827990	-4.9633480
H	-9.2673340	-2.2409730	-5.7790990
C	-7.9261860	-1.4468480	-4.2852410
H	-8.1025130	-0.4122230	-4.5853900
C	-9.0816980	-4.9405740	-5.3251690
H	-8.3649750	-5.6254170	-5.7983490
H	-9.6745910	-5.5390640	-4.6185870
H	-9.7567890	-4.5635270	-6.1026610
C	-6.5108170	1.1282210	-3.1659000
C	-5.5756860	1.7178740	-4.0228040
H	-4.6056190	1.2460910	-4.1899030
C	-5.8714080	2.9306410	-4.6572430
H	-5.1304310	3.3850130	-5.3178160
C	-7.0991260	3.5731720	-4.4555270
C	-8.0318520	2.9721560	-3.5915430
H	-8.9928320	3.4609530	-3.4178940
C	-7.7415910	1.7713550	-2.9477570
H	-8.4712450	1.3287500	-2.2628380
C	-7.4196330	4.8794610	-5.1276080
H	-6.6264080	5.1812040	-5.8218750
H	-8.3605000	4.8138300	-5.6902160
H	-7.5446630	5.6814470	-4.3873470
C	-4.4119070	-0.8192770	-2.5014960
C	-3.4756420	-0.5735720	-1.4839920
H	-3.8091340	-0.1801070	-0.5211970
C	-2.1192740	-0.8087620	-1.7088200
H	-1.3998330	-0.5941300	-0.9142480
C	-1.6586880	-1.3012930	-2.9394370
C	-2.6007720	-1.5571500	-3.9462200
H	-2.2660660	-1.9436310	-4.9107460
C	-3.9613220	-1.3183300	-3.7343980
H	-4.6741050	-1.5234700	-4.5367640
C	-0.1913850	-1.5479090	-3.1555950
H	0.0192040	-1.8791250	-4.1796540
H	0.3917750	-0.6353160	-2.9644330
H	0.1831460	-2.3187290	-2.4666790
C	-5.6075820	1.4005830	0.0598220
C	-4.7270970	2.2695350	0.0723660
C	-3.5872880	3.1320910	0.0878400
C	-2.4721530	2.7984410	0.8884280
H	-2.5244590	1.9032460	1.5145090

C	-1.3226740	3.5811480	0.8701480
H	-0.4681630	3.2968160	1.4881030
C	-1.2346680	4.7407210	0.0717920
C	-2.3518050	5.0698280	-0.7221670
H	-2.2956350	5.9348370	-1.3864770
C	-3.5040780	4.2855430	-0.7172550
H	-4.3476510	4.5439830	-1.3596290
C	0.0195110	5.5223850	0.0325050
C	0.0309790	6.9019330	0.0692410
C	-1.1357690	7.7084680	0.3793430
H	-2.0647240	7.2203290	0.6643190
C	-1.0896820	9.0619850	0.4086290
O	0.0595200	9.7511360	0.1351680
C	-2.2071250	9.9556470	0.7484390
C	-3.5336380	9.4849610	0.7626320
H	-3.7538660	8.4514160	0.4925040
C	-4.5851840	10.3371030	1.0964610
H	-5.6062720	9.9563890	1.0987350
C	-4.3355180	11.6782650	1.4158180
H	-5.1593490	12.3434410	1.6735460
C	-3.0219890	12.1573240	1.3939250
H	-2.8170500	13.1994230	1.6386890
C	-1.9660840	11.3054720	1.0612400
H	-0.9448920	11.6853230	1.0543560
C	5.5877990	1.3218590	-0.0490860
C	4.7113690	2.1946730	-0.0630050
C	3.5905410	3.0822220	-0.0743200
C	2.5116080	2.8396310	-0.9528010
H	2.5796810	1.9988220	-1.6480290
C	1.3738910	3.6396640	-0.9218000
H	0.5426300	3.4220520	-1.5961850
C	1.2677870	4.7306180	-0.0350950
C	2.3542480	4.9783840	0.8268180
H	2.2823840	5.7930260	1.5507920
C	3.4916350	4.1727670	0.8125970
H	4.3087910	4.3618430	1.5108870
C	1.2157530	7.6983080	-0.1956860
H	2.1371290	7.2038240	-0.4943660
C	1.1970200	9.0524240	-0.1629930
C	2.3334840	9.9386950	-0.4559640
C	3.6502150	9.4423470	-0.4923830
H	3.8489840	8.3922810	-0.2748680
C	4.7196160	10.2883540	-0.7820950
H	5.7326630	9.8872460	-0.8024200
C	4.4980990	11.6485590	-1.0346200
H	5.3358490	12.3087010	-1.2581590
C	3.1945310	12.1526130	-0.9903770
H	3.0112970	13.2095340	-1.1833080
C	2.1207930	11.3070890	-0.7014350
H	1.1076360	11.7070960	-0.6766970
Pt	6.8432840	-0.2574740	-0.0014490
P	7.6099700	0.4211580	-2.1263850
C	8.7342940	-0.7188150	-3.0240670
C	8.3468530	-1.4279350	-4.1652950
H	7.3518930	-1.2872080	-4.5915330
C	9.2399160	-2.3180310	-4.7774760
H	8.9261080	-2.8649720	-5.6687030
C	10.5279430	-2.5140060	-4.2669540
C	10.9075260	-1.7942350	-3.1189700
H	11.9063110	-1.9418780	-2.7021360

C	10.0242120	-0.9154390	-2.4995250
H	10.3352480	-0.3782670	-1.6003120
C	11.4893880	-3.4771280	-4.9056730
H	12.4104340	-2.9681120	-5.2203340
H	11.7862270	-4.2611200	-4.1939660
H	11.0510160	-3.9638960	-5.7850580
C	8.5247230	2.0091710	-2.1300580
C	9.2146590	2.4288220	-3.2818590
H	9.2104700	1.8061990	-4.1800420
C	9.9120180	3.6348750	-3.2806110
H	10.4425330	3.9547280	-4.1799150
C	9.9475150	4.4492580	-2.1345770
C	9.2624870	4.0198480	-0.9910540
H	9.2815410	4.6364140	-0.0905410
C	8.5562020	2.8125640	-0.9833660
H	8.0249780	2.4913930	-0.0836870
C	10.7169070	5.7407440	-2.1479940
H	10.3939680	6.3833070	-2.9778480
H	10.5871140	6.2978220	-1.2126530
H	11.7908420	5.5553290	-2.2858960
C	6.1436920	0.6408510	-3.2078020
C	5.1825180	-0.3839100	-3.2203030
H	5.3530200	-1.2973240	-2.6422700
C	4.0026090	-0.2359700	-3.9481890
H	3.2667850	-1.0432410	-3.9530650
C	3.7409600	0.9434100	-4.6665710
C	4.7065140	1.9589470	-4.6494740
H	4.5209510	2.8829160	-5.2006540
C	5.8970530	1.8144010	-3.9290670
H	6.6204160	2.6316220	-3.9170870
C	2.4401250	1.1256400	-5.3980980
H	2.5410750	1.8340970	-6.2293730
H	2.0647210	0.1739630	-5.7954100
H	1.6689900	1.5230580	-4.7215030
P	5.8193430	-0.8079660	2.0621190
C	6.5300520	-2.2177300	3.0001650
C	6.4343310	-3.5020300	2.4351400
H	5.9224310	-3.6409480	1.4799240
C	6.9914000	-4.5988750	3.0856900
H	6.9134350	-5.5917700	2.6370170
C	7.6731940	-4.4477370	4.3072970
C	7.7691080	-3.1655140	4.8593040
H	8.2912940	-3.0264850	5.8079350
C	7.2034360	-2.0566080	4.2153080
H	7.2872250	-1.0693100	4.6734010
C	8.2916070	-5.6417210	4.9795130
H	7.5404410	-6.4172090	5.1812740
H	9.0560630	-6.0991540	4.3348550
H	8.7668610	-5.3705940	5.9298310
C	5.9035460	0.6247050	3.2051240
C	4.8053170	1.0817960	3.9408770
H	3.8387830	0.5814160	3.8585320
C	4.9334580	2.2007950	4.7725960
H	4.0667780	2.5528300	5.3353700
C	6.1526260	2.8792990	4.8913420
C	7.2503330	2.4122260	4.1467080
H	8.2079980	2.9315600	4.2222060
C	7.1285610	1.3065850	3.3079380
H	7.9879650	0.9702940	2.7197870
C	6.2944340	4.0869260	5.7758330

H	5.3795880	4.2761730	6.3498860
H	7.1242190	3.9626900	6.4843800
H	6.5125700	4.9848480	5.1816800
C	4.0424140	-1.2521030	1.9056370
C	3.3255810	-0.9540220	0.7362500
H	3.8285350	-0.4560710	-0.0955410
C	1.9720770	-1.2793930	0.6409080
H	1.4274300	-1.0416430	-0.2765510
C	1.2979490	-1.9049460	1.7002250
C	2.0224590	-2.2057270	2.8637290
H	1.5189440	-2.7001380	3.6970950
C	3.3783470	-1.8865600	2.9683000
H	3.9226260	-2.1407280	3.8811310
C	-0.1646710	-2.2324950	1.5868520
H	-0.4828710	-2.9345770	2.3679410
H	-0.7770340	-1.3216340	1.6839600
H	-0.4013670	-2.6754080	0.6096040
C	8.0541700	-1.8500680	0.0473000
C	8.7954890	-2.8414640	0.0688360
C	-8.0410920	-1.7946800	-0.0581410
C	-8.7885870	-2.7810930	-0.0866500
C	9.6445840	-3.9863200	0.0919110
C	10.0132990	-4.6408700	-1.1030580
C	10.1383420	-4.4987920	1.3158000
C	10.8386420	-5.7604000	-1.0695540
H	9.6357920	-4.2538530	-2.0524340
C	10.9667150	-5.6125510	1.3414250
H	9.8567470	-3.9951640	2.2435200
H	11.1114790	-6.2595780	-2.0021310
H	11.3335790	-5.9783720	2.3016260
C	-9.6565420	-3.9109100	-0.1297860
C	-9.8892190	-4.6956000	1.0200510
C	-10.3103470	-4.2734050	-1.3320380
C	-10.7399640	-5.7952140	0.9640040
H	-9.3879930	-4.4242630	1.9522130
C	-11.1632240	-5.3675780	-1.3790810
H	-10.1321350	-3.6685040	-2.2244400
H	-10.9074200	-6.3960110	1.8608630
H	-11.6554490	-5.6160810	-2.3205250
C	11.3344060	-6.2698930	0.1472760
C	12.1963600	-7.4438850	0.1136650
H	12.3902540	-7.8390960	-0.8885220
C	-11.3964170	-6.1544500	-0.2302540
C	-12.2791400	-7.3134170	-0.2220580
H	-12.3521010	-7.8253100	0.7426410
C	12.7592170	-8.0675440	1.1760470
H	12.5912100	-7.7034890	2.1921080
C	-12.9938890	-7.7953140	-1.2667290
H	-12.9500120	-7.3116560	-2.2451360
C	13.6194670	-9.2448320	1.1030070
N	14.0822200	-9.7064490	2.2869620
C	13.9743040	-9.8948470	-0.0943530
C	14.8710580	-10.7811880	2.2486360
C	14.8031630	-11.0043280	0.0030910
H	13.6220200	-9.5556470	-1.0669170
N	15.2691920	-11.4711490	1.1745110
H	15.2372820	-11.1424400	3.2147000
H	15.1090870	-11.5455280	-0.8956530
C	-13.8711670	-8.9613420	-1.2211590
N	-14.4965430	-9.2692060	-2.3800970

C	-14.0868720	-9.7474140	-0.0732830
C	-15.3045400	-10.3301980	-2.3661990
C	-14.9529710	-10.8259890	-0.1918960
H	-13.6024660	-9.5335220	0.8778480
N	-15.5798620	-11.1406980	-1.3387560
H	-15.8031750	-10.5662060	-3.3114740
H	-15.1555480	-11.4684710	0.6685720

7

Pt	6.9145390	-0.0621630	-0.0885620
P	7.2827570	0.3063860	-2.3951180
C	8.3349800	-0.9074570	-3.2844880
C	7.8392390	-1.7810690	-4.2572790
H	6.7878830	-1.7446260	-4.5480100
C	8.6942610	-2.7032340	-4.8763170
H	8.2952950	-3.3784510	-5.6357550
C	10.0513480	-2.7678710	-4.5414640
C	10.5397130	-1.8830250	-3.5622150
H	11.5952200	-1.9236610	-3.2839720
C	9.6958780	-0.9709530	-2.9355760
H	10.0947130	-0.3013150	-2.1695990
C	10.9757590	-3.7588470	-5.1924730
H	11.7978530	-3.2499140	-5.7136550
H	11.4346250	-4.4180710	-4.4413870
H	10.4483900	-4.3869300	-5.9203290
C	8.0558370	1.9154960	-2.8060580
C	8.5003650	2.1697230	-4.1155800
H	8.3872040	1.4074540	-4.8905290
C	9.0971850	3.3896690	-4.4286050
H	9.4412150	3.5781440	-5.4475560
C	9.2702900	4.3826100	-3.4486670
C	8.8339980	4.1148210	-2.1442740
H	8.9701900	4.8697420	-1.3676380
C	8.2301570	2.8961660	-1.8208500
H	7.8902450	2.7036890	-0.8000240
C	9.8957580	5.7024120	-3.8043550
H	10.7349910	5.5719050	-4.4991990
H	9.1646150	6.3560880	-4.3001160
H	10.2600200	6.2286130	-2.9139340
C	5.6456320	0.2643610	-3.2213170
C	4.8056310	-0.8286530	-2.9509950
H	5.1618060	-1.6471330	-2.3181980
C	3.5116000	-0.8690160	-3.4695700
H	2.8741370	-1.7305620	-3.2582640
C	3.0142420	0.1866020	-4.2524610
C	3.8608850	1.2722610	-4.5169300
H	3.4921240	2.1029090	-5.1219330
C	5.1635490	1.3157730	-4.0096530
H	5.7925800	2.1837040	-4.2152700
C	1.5973170	0.1749840	-4.7560560
H	1.5042130	0.7124740	-5.7078770
H	1.2262060	-0.8485610	-4.8966700
H	0.9272060	0.6700620	-4.0367030
P	6.2534090	-0.3214240	2.1713390
C	7.1765630	-1.5632390	3.1606730
C	7.0495140	-2.9191340	2.8095790
H	6.3893300	-3.2105920	1.9890990

C	7.7625350	-3.8937990	3.5012630
H	7.6574830	-4.9439720	3.2195150
C	8.6334760	-3.5468740	4.5507070
C	8.7609230	-2.1946940	4.8873520
H	9.4300890	-1.9036670	5.6993430
C	8.0395070	-1.2075200	4.2021790
H	8.1524320	-0.1612680	4.4923360
C	9.4067610	-4.6136980	5.2745910
H	8.7318420	-5.3085680	5.7926670
H	10.0012900	-5.2128210	4.5699850
H	10.0885440	-4.1849120	6.0187080
C	6.4560110	1.2623700	3.0738900
C	5.4880570	1.7678370	3.9483580
H	4.5591180	1.2208660	4.1195570
C	5.6973960	2.9913050	4.5953650
H	4.9318520	3.3793020	5.2699880
C	6.8703910	3.7284910	4.3893610
C	7.8369020	3.2109640	3.5089320
H	8.7564580	3.7730990	3.3332830
C	7.6318650	1.9994090	2.8520610
H	8.3859060	1.6213390	2.1550560
C	7.0921890	5.0508900	5.0695240
H	6.3441750	5.2334580	5.8502200
H	8.0883610	5.0987260	5.5285300
H	7.0318170	5.8766450	4.3472330
C	4.4960050	-0.8189050	2.3821100
C	3.5626110	-0.6284450	1.3500440
H	3.8848800	-0.2029830	0.3972970
C	2.2222750	-0.9597830	1.5477100
H	1.5039910	-0.7936030	0.7408570
C	1.7752050	-1.4919090	2.7668650
C	2.7149710	-1.6907570	3.7886120
H	2.3911040	-2.1078690	4.7439920
C	4.0595790	-1.3581090	3.6031100
H	4.7706610	-1.5224720	4.4162090
C	0.3232680	-1.8322900	2.9573180
H	0.1351670	-2.2778330	3.9416200
H	-0.3036040	-0.9335610	2.8656890
H	-0.0182260	-2.5408380	2.1895510
C	5.6077230	1.4709430	-0.1593560
C	4.7077330	2.3188600	-0.1689920
C	3.5669790	3.1801910	-0.1721060
C	2.4370250	2.8435780	-0.9494530
H	2.4753100	1.9443480	-1.5702000
C	1.2903340	3.6301430	-0.9152270
H	0.4226470	3.3437050	-1.5135300
C	1.2225830	4.7968490	-0.1258660
C	2.3558810	5.1306720	0.6423010
H	2.3156220	6.0038570	1.2970390
C	3.5043010	4.3411920	0.6238330
H	4.3613840	4.6016850	1.2473370
C	-0.0288570	5.5826160	-0.0651060
C	-0.0360430	6.9606940	-0.1372240
C	1.1255700	7.7507920	-0.5033350
H	2.0430850	7.2494900	-0.8022600
C	1.0868100	9.1033960	-0.5659870
O	-0.0501570	9.8068060	-0.2796230
C	2.2004130	9.9799810	-0.9584020
C	3.5243760	9.5027030	-0.9811100
H	3.7451910	8.4786000	-0.6772880

C	4.5726470	10.3376780	-1.3650830
H	5.5921500	9.9528060	-1.3731030
C	4.3218790	11.6677900	-1.7268010
H	5.1431110	12.3197840	-2.0235370
C	3.0109860	12.1536970	-1.6961880
H	2.8056830	13.1875740	-1.9732660
C	1.9583730	11.3190840	-1.3132640
H	0.9389880	11.7036460	-1.2994820
C	-5.6101270	1.4171260	0.3248840
C	-4.7168650	2.2720790	0.3131160
C	-3.5925930	3.1535610	0.2604650
C	-2.4721960	2.9238960	1.0879480
H	-2.5055950	2.0972720	1.8016490
C	-1.3368480	3.7211400	0.9843860
H	-0.4736290	3.5154470	1.6208940
C	-1.2732860	4.7951190	0.0730490
C	-2.4006870	5.0289120	-0.7390820
H	-2.3640620	5.8284460	-1.4821770
C	-3.5366980	4.2264110	-0.6518610
H	-4.3884830	4.4034200	-1.3112950
C	-1.2068730	7.7716440	0.1444790
H	-2.1208660	7.2921150	0.4869040
C	-1.1814990	9.1243000	0.0730350
C	-2.3034160	10.0258710	0.3753390
C	-3.6212860	9.5394950	0.4645100
H	-3.8326020	8.4851480	0.2820480
C	-4.6764850	10.4005000	0.7621050
H	-5.6909510	10.0072120	0.8235210
C	-4.4393080	11.7656180	0.9699480
H	-5.2660260	12.4374240	1.1996590
C	-3.1347170	12.2594800	0.8730840
H	-2.9395920	13.3200590	1.0309310
C	-2.0751720	11.3990340	0.5761230
H	-1.0608900	11.7914200	0.5099180
Pt	-6.8993400	-0.1297870	0.2215760
P	-7.5593310	0.3805820	2.4334770
C	-8.6944260	-0.8004590	3.2622320
C	-8.2999080	-1.6118890	4.3304190
H	-7.2891080	-1.5381560	4.7357170
C	-9.2061230	-2.5184860	4.8974680
H	-8.8869710	-3.1444280	5.7330350
C	-10.5147530	-2.6289700	4.4145230
C	-10.9008690	-1.8073390	3.3393250
H	-11.9168250	-1.8851170	2.9456800
C	-10.0048220	-0.9114540	2.7640520
H	-10.3231760	-0.2914370	1.9224180
C	-11.4926640	-3.6046620	5.0076950
H	-12.3858920	-3.0895550	5.3860930
H	-11.8364720	-4.3230780	4.2494040
H	-11.0487060	-4.1702320	5.8355620
C	-8.4104170	1.9924170	2.6258130
C	-9.0678510	2.3044490	3.8293050
H	-9.0790350	1.5837120	4.6506330
C	-9.7113610	3.5314380	3.9792100
H	-10.2147610	3.7671290	4.9190560
C	-9.7241460	4.4740370	2.9362520
C	-9.0686620	4.1526310	1.7405040
H	-9.0664170	4.8721670	0.9196190
C	-8.4170000	2.9259170	1.5810580
H	-7.9042540	2.6938130	0.6442730

C	-10.4451030	5.7824530	3.1033780
H	-10.2386780	6.2272910	4.0852830
H	-10.1568920	6.5033030	2.3290930
H	-11.5324990	5.6384500	3.0374960
C	-6.0485530	0.4425030	3.4724930
C	-5.1239730	-0.6081450	3.3475380
H	-5.3424940	-1.4496260	2.6828850
C	-3.9214100	-0.5766860	4.0525550
H	-3.2135350	-1.4023460	3.9502740
C	-3.6013430	0.5091690	4.8853710
C	-4.5302840	1.5518530	5.0034350
H	-4.2991060	2.4042890	5.6451710
C	-5.7428590	1.5240840	4.3066110
H	-6.4381220	2.3598020	4.4037390
C	-2.2794980	0.5680080	5.5992190
H	-2.3445720	1.1633500	6.5181670
H	-1.9176770	-0.4349760	5.8586300
H	-1.5158350	1.0351330	4.9604190
P	-5.9882060	-0.4935130	-1.9370920
C	-6.7713870	-1.8025390	-2.9605870
C	-6.6508000	-3.1371180	-2.5336580
H	-6.0776060	-3.3724520	-1.6335430
C	-7.2589730	-4.1623540	-3.2518490
H	-7.1593740	-5.1953840	-2.9110350
C	-8.0161200	-3.8886920	-4.4059680
C	-8.1393890	-2.5571400	-4.8179410
H	-8.7213090	-2.3224930	-5.7113560
C	-7.5235310	-1.5192710	-4.1051960
H	-7.6294990	-0.4909060	-4.4556590
C	-8.6775270	-5.0094070	-5.1586500
H	-7.9345490	-5.7241590	-5.5378080
H	-9.3565200	-5.5736150	-4.5032520
H	-9.2574170	-4.6372940	-6.0116100
C	-6.1132680	1.0401250	-2.9349310
C	-5.0558140	1.5424610	-3.7002340
H	-4.0966190	1.0223830	-3.7259110
C	-5.2132050	2.7335260	-4.4192150
H	-4.3774860	3.1205260	-5.0052770
C	-6.4215950	3.4407240	-4.3938370
C	-7.4770810	2.9289260	-3.6180540
H	-8.4240480	3.4713350	-3.5786160
C	-7.3262040	1.7494590	-2.8921550
H	-8.1516510	1.3785620	-2.2766590
C	-6.5974940	4.7191940	-5.1652170
H	-5.6734370	5.0112360	-5.6780320
H	-7.3876170	4.6165030	-5.9214040
H	-6.8948020	5.5423870	-4.5018770
C	-4.2159580	-0.9788450	-1.9095050
C	-3.4538190	-0.8470470	-0.7384550
H	-3.9155220	-0.4434170	0.1649960
C	-2.1088300	-1.2180080	-0.7306370
H	-1.5281560	-1.1115690	0.1890420
C	-1.4881680	-1.7252390	-1.8817940
C	-2.2573210	-1.8590900	-3.0480020
H	-1.7955590	-2.2587370	-3.9532140
C	-3.6056810	-1.4945320	-3.0649110
H	-4.1867380	-1.6222780	-3.9815030
C	-0.0335730	-2.1036900	-1.8586410
H	0.2354700	-2.7315090	-2.7173200
H	0.6016850	-1.2047670	-1.8890460

H	0.2221780	-2.6473500	-0.9388430
C	-8.1406590	-1.6876770	0.0872800
C	-8.9134940	-2.6532090	0.0010480
C	8.1884770	-1.5971560	-0.0154500
C	8.9809650	-2.5494660	0.0276020
C	-9.8097270	-3.7471960	-0.1068600
C	-10.2028150	-4.4821540	1.0368600
C	-10.3373510	-4.1246850	-1.3696580
C	-11.0896560	-5.5415950	0.9185680
H	-9.7963690	-4.1975240	2.0096820
C	-11.2257500	-5.1795730	-1.4809740
H	-10.0303030	-3.5588030	-2.2519660
H	-11.3881640	-6.1024800	1.8066120
H	-11.6191460	-5.4404250	-2.4640300
C	9.8894400	-3.6371680	0.0780880
C	10.1262170	-4.4381620	-1.0643110
C	10.5822600	-3.9456000	1.2782120
C	11.0179060	-5.4981700	-1.0043730
H	9.5934250	-4.2049690	-1.9885680
C	11.4757900	-5.0008530	1.3305020
H	10.3965340	-3.3277870	2.1594160
H	11.1916680	-6.1122460	-1.8904040
H	11.9962340	-5.2104590	2.2656320
C	-11.6251910	-5.9128710	-0.3366500
C	-12.5543720	-7.0114360	-0.3889110
H	-12.7657340	-7.4774650	0.5779930
C	11.7153310	-5.8031170	0.1877800
C	12.6337570	-6.9116240	0.1808740
H	12.7045320	-7.4399330	-0.7744710
C	-13.1787470	-7.5030500	-1.5026250
H	-12.9965400	-7.0694240	-2.4866370
C	13.4014110	-7.3487440	1.2258130
H	13.3659420	-6.8531790	2.1967720
C	-14.1078420	-8.5927790	-1.4994010
N	-14.6247190	-8.9361080	-2.7148790
C	-14.5128640	-9.3124470	-0.3411730
C	-15.4841910	-9.9173390	-2.7805160
C	-15.4171040	-10.3289790	-0.4841880
H	-14.1335630	-9.0842770	0.6509540
N	-15.9143150	-10.6378260	-1.7155900
H	-15.9034860	-10.1997660	-3.7478800
H	-15.7797730	-10.9275790	0.3495390
C	14.2995430	-8.4622600	1.1592450
N	14.9759830	-8.7528820	2.3083500
C	14.5203730	-9.2570200	0.0003060
C	15.8070990	-9.7607350	2.3132550
C	15.4046390	-10.2975060	0.0777840
H	14.0137700	-9.0690720	-0.9420880
N	16.0575180	-10.5585940	1.2459680
H	16.3533810	-10.0015250	3.2273600
H	15.6298740	-10.9526980	-0.7619060
C	-16.8826490	-11.7317090	-1.8646040
H	-17.7386510	-11.5494110	-1.2085360
H	-17.2239140	-11.7706260	-2.9017660
H	-16.4061950	-12.6806660	-1.6006570
C	17.0011190	-11.6811310	1.3250840
H	17.7880570	-11.5474540	0.5770830
H	17.4481250	-11.7047580	2.3214080
H	16.4684390	-12.6192730	1.1424740