Supporting Information

Host-Guest Feature of DPPP Bridged Arene-Ruthenium Clip Derived Molecular Rectangle

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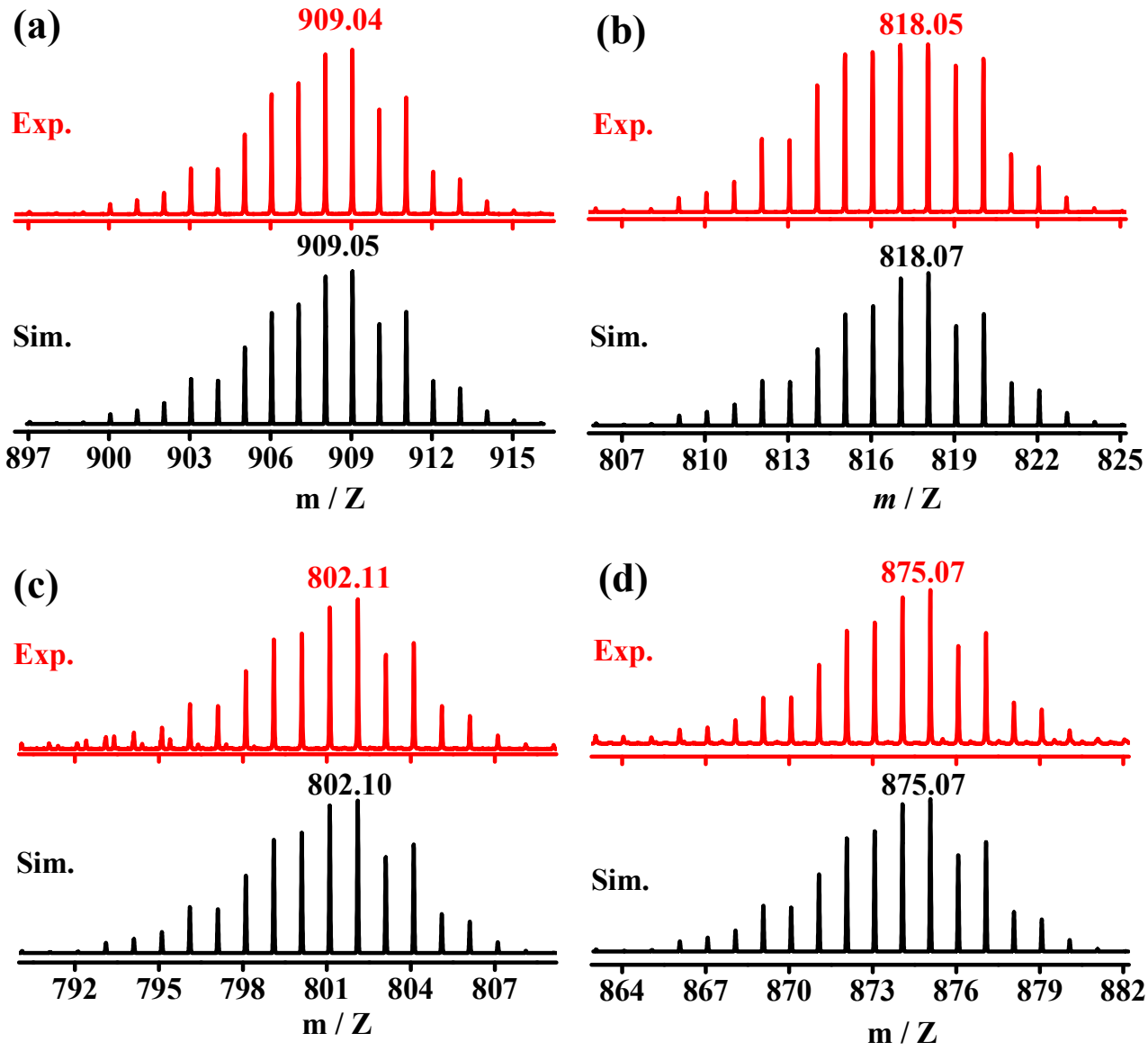


Figure S1. ESI Mass spectra of (a) $\{[\mathbf{1}\text{-}CF_3SO_3]\}^+$, (b) $\{[\mathbf{2}\text{-}SCN]\}^+$, (c) $\{[\mathbf{3}\text{-}N_3]\}^+$, (d) $\{[\mathbf{4}\text{-}NO_2]\}^+$ in CH_3CN.

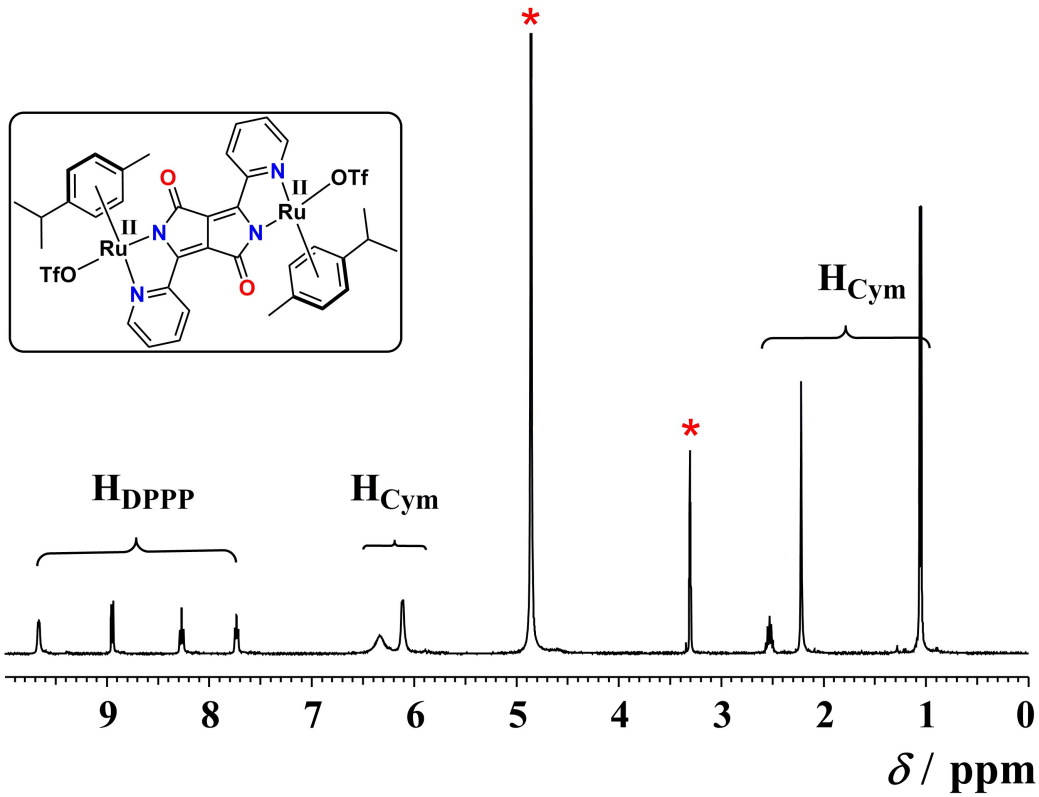


Figure S2a. ^{1}H NMR of **1** in CD_3OD (*CD_3OD).

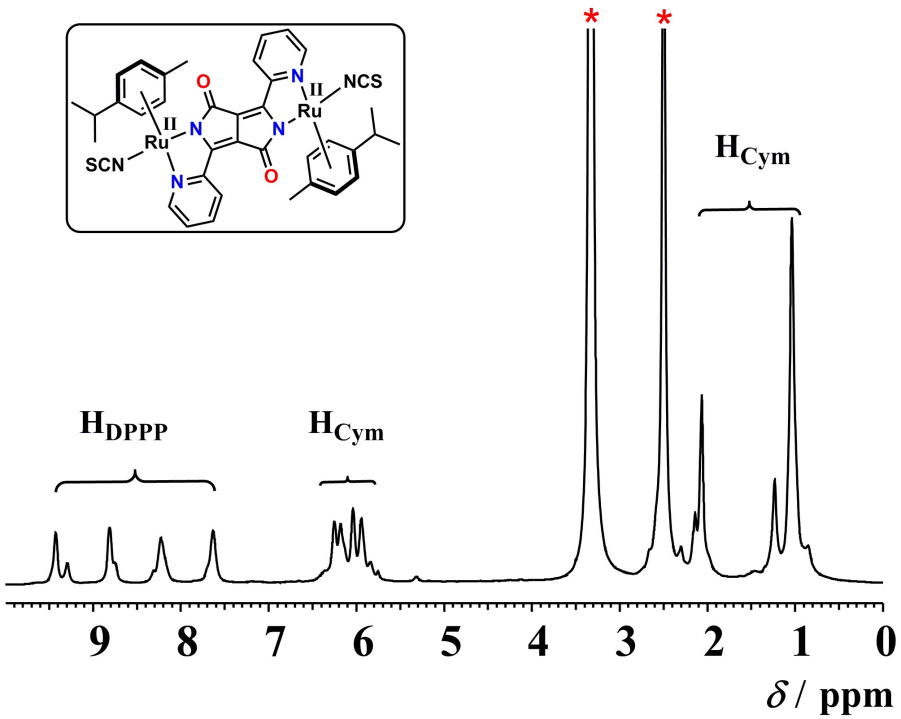


Figure S2b. ^{1}H NMR of **2** in $(CD_3)_2SO$ (*$(CD_3)_2SO$).

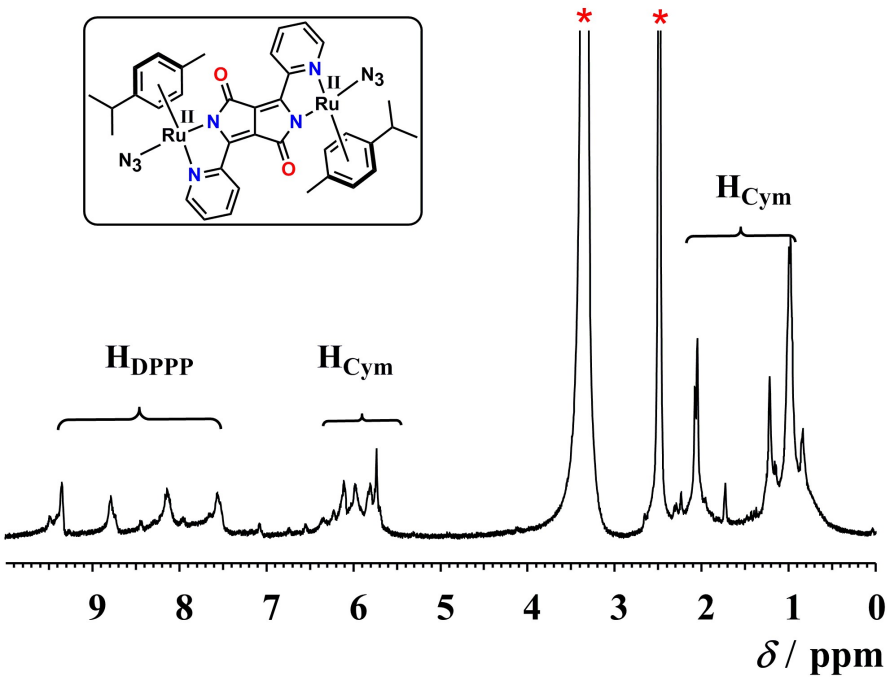


Figure S2c. ^{1}H NMR of **3** in $(CD_3)_2SO$ (*$(CD_3)_2SO$).

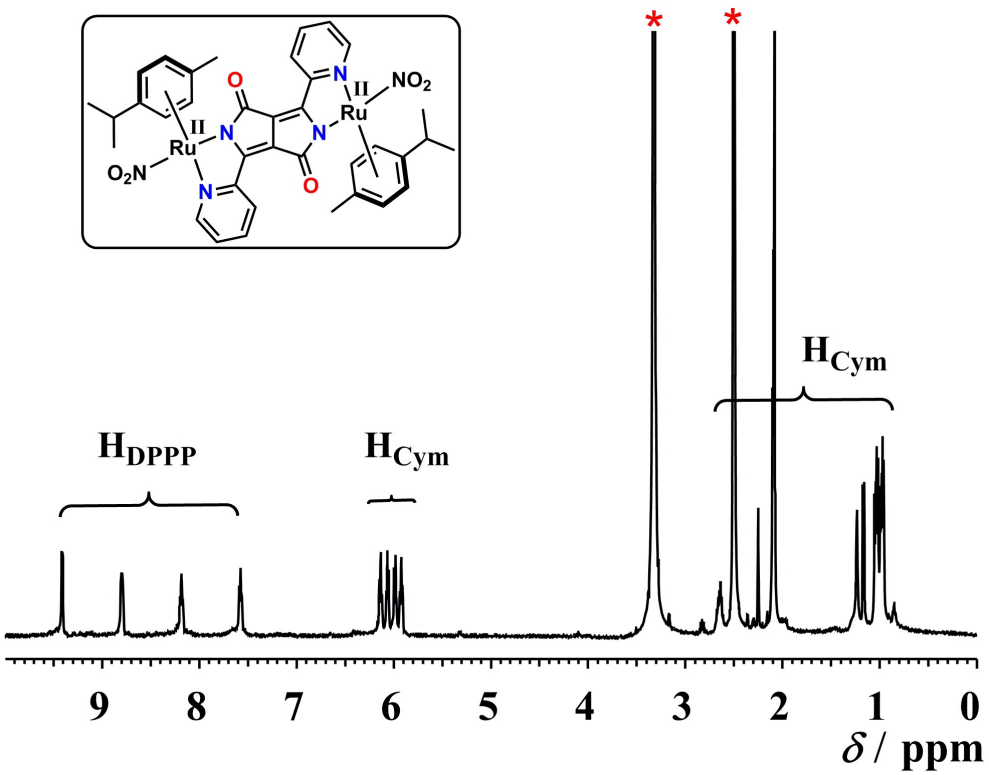


Figure S2d. ^{1}H NMR of **4** in $(CD_3)_2SO$ (*$(CD_3)_2SO$).

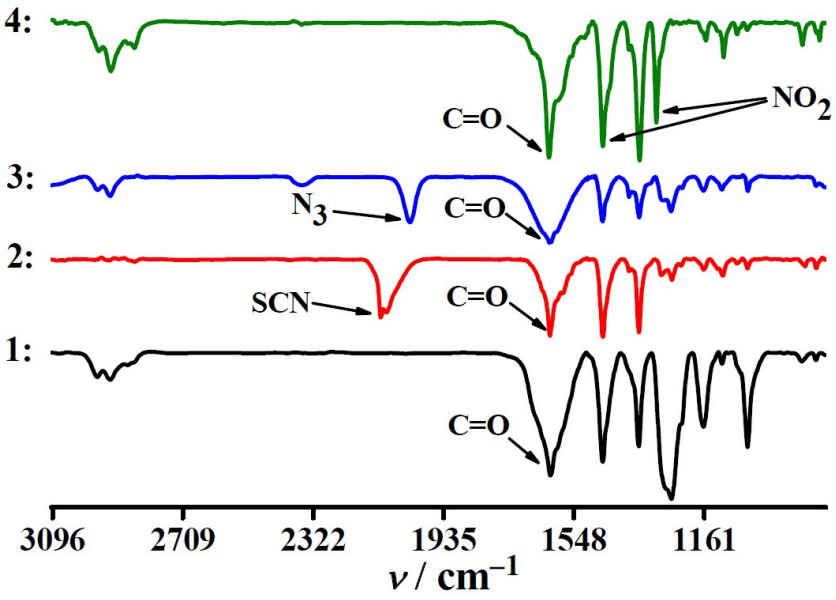


Figure S3. FT-IR spectra of **1-4** as KBr pellets.

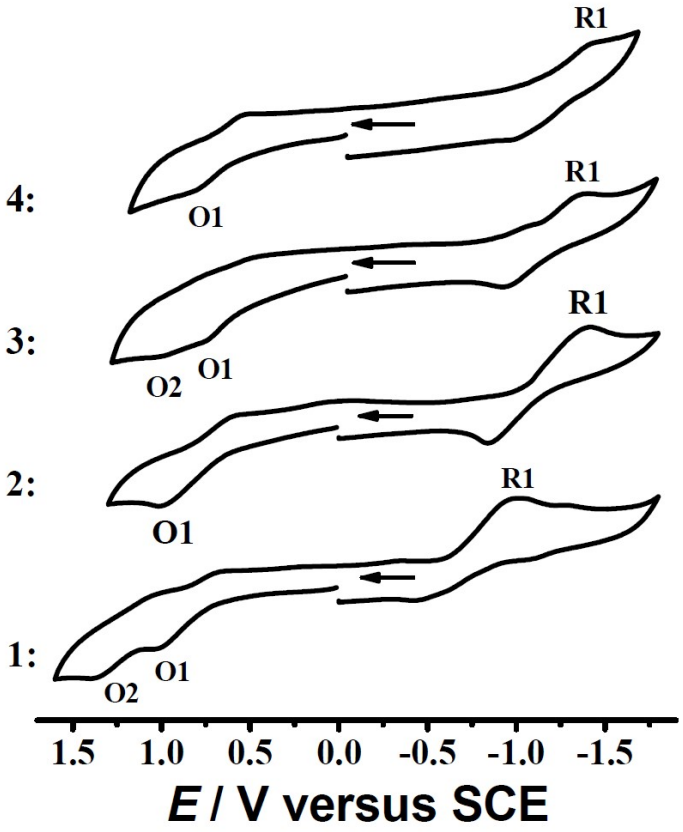


Figure S4. Cyclic voltammograms of **1-4** in CH_2Cl_2/0.1 M Et_4NClO_4 versus SCE. (Scan rate: 100 mV/s).

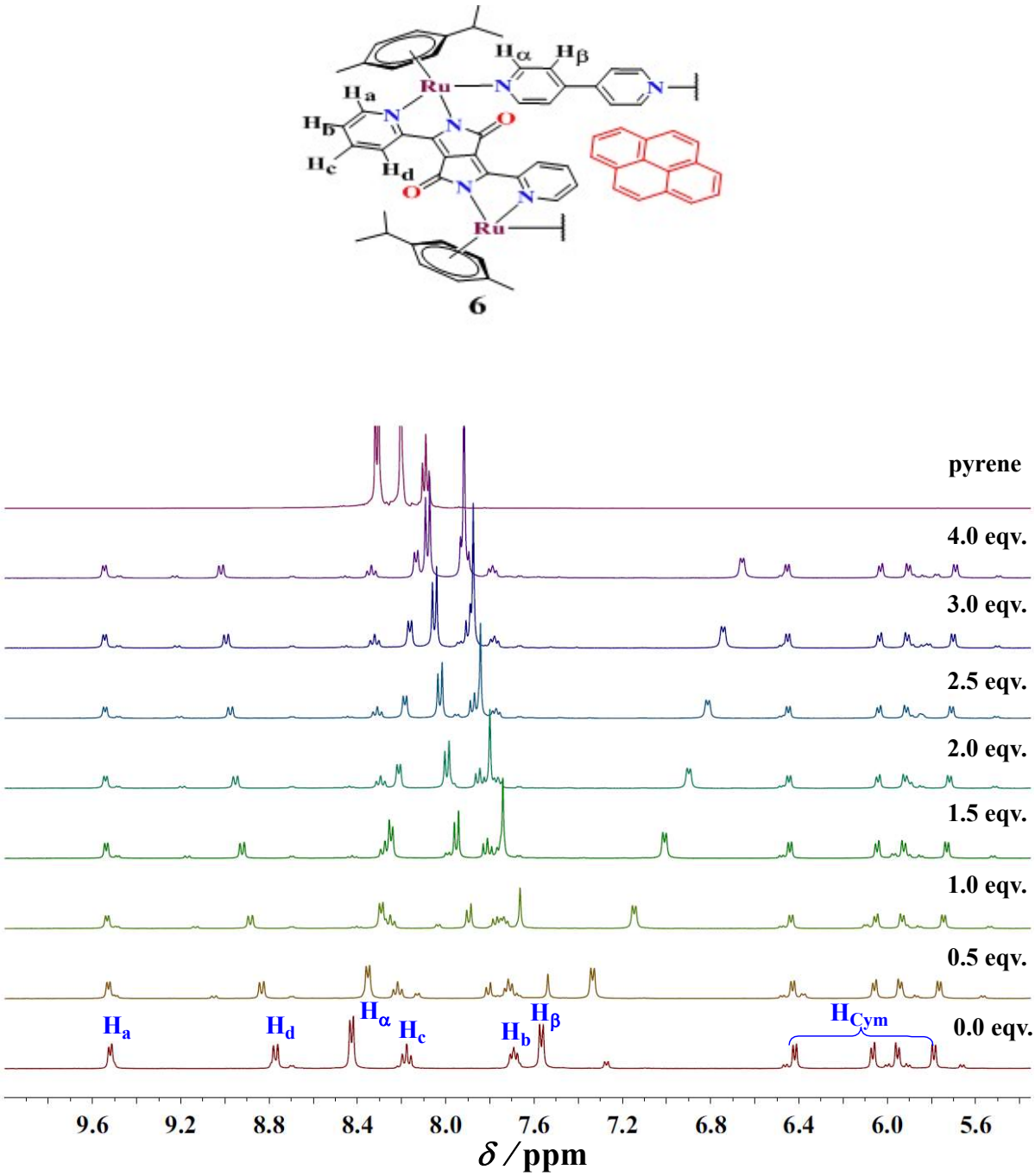


Figure S5. ^{1}H NMR spectral titration (400 MHz, CD_3CN, 298 K, δ, 10-5.5 ppm) of **5** (5 mM) with gradual addition of pyrene (0 to 4 equivalent).

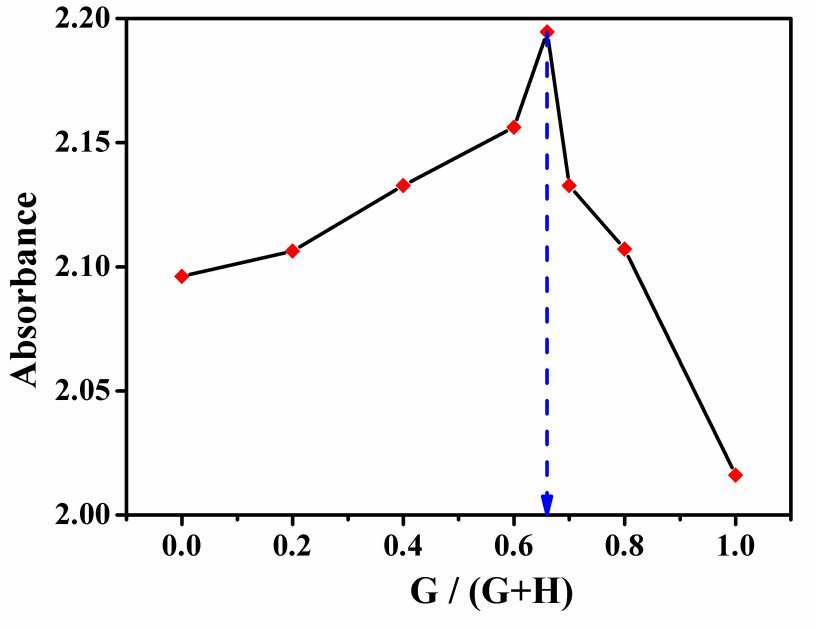
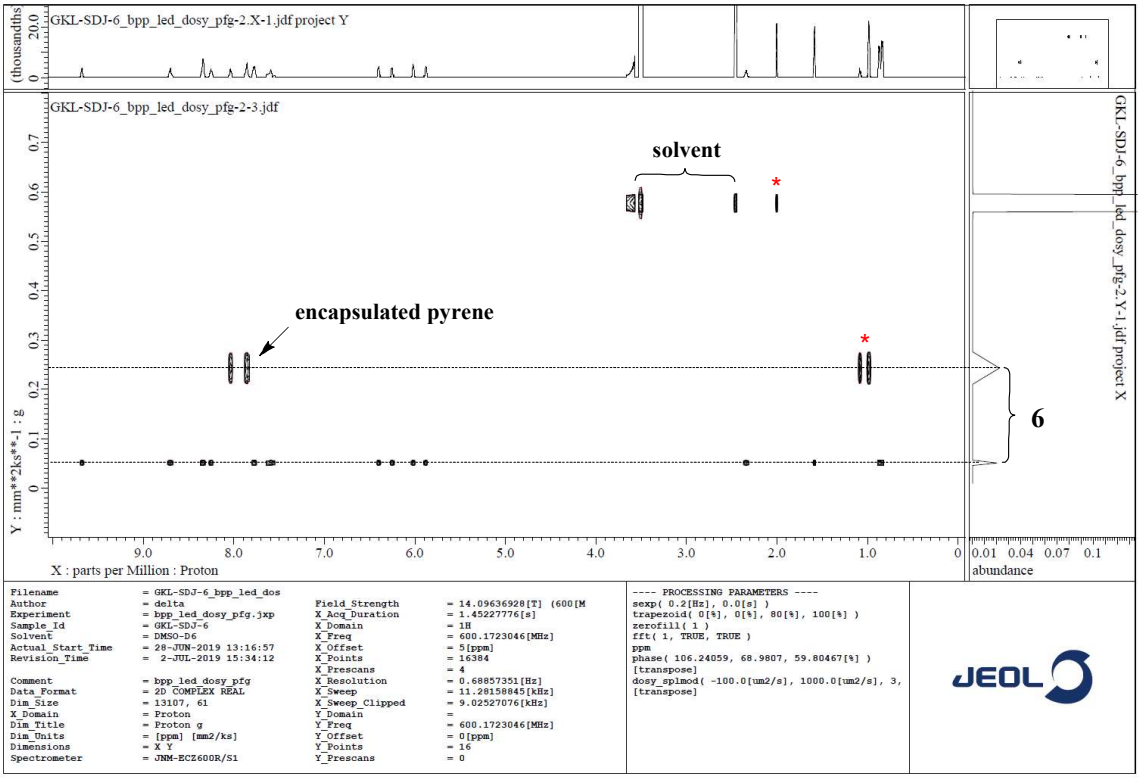


Figure S6. Job's plot (UV-visible titration) of **5** (30 μM) with pyrene (30 μM) in CH_3CN at λ_{max} = 240 nm (**G**: guest (pyrene) and **H**: host (**5**)).

(a)



(b)

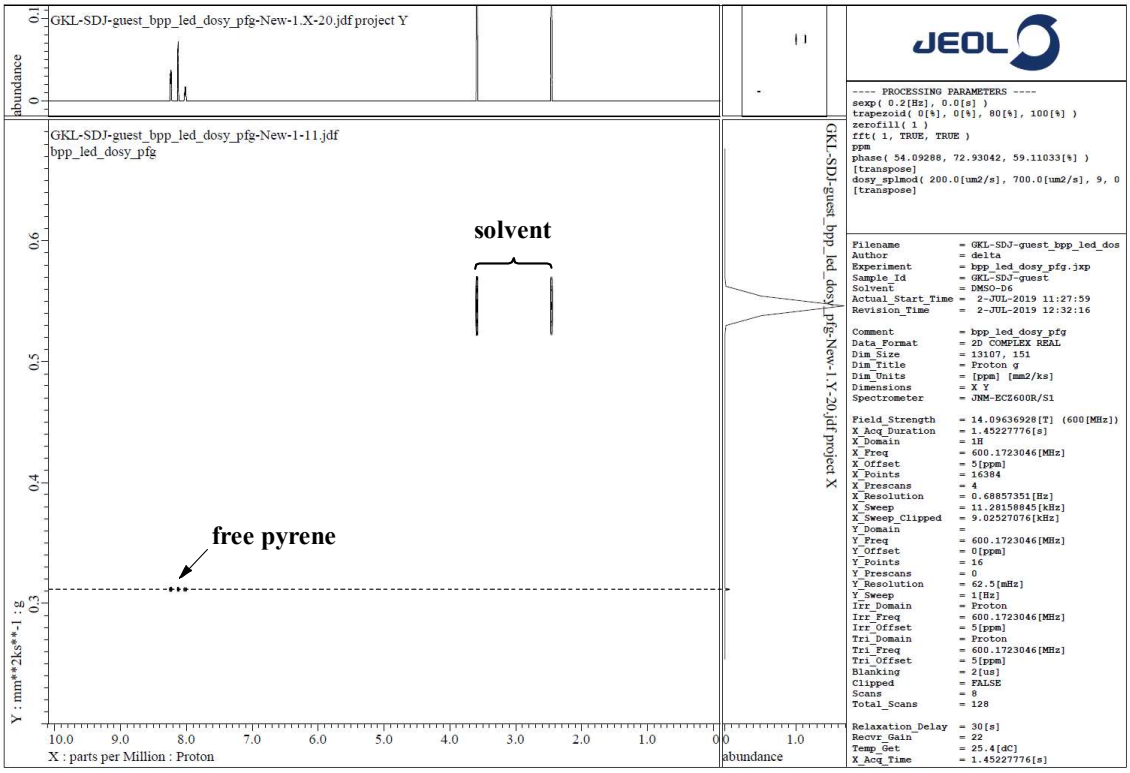


Figure S7. 2D-DOSY NMR of (a) **6** and (b) free pyrene ($(CD_3)_2SO$, 298 K, 600 HMz). (* indicates impurities).

Table S1. Selected Crystallographic Parameters

complex	**2**	**3**	**4**	**5**	**6**
empirical formula	$C_{38}H_{36}N_6O_2Ru_2S_2$	$C_{36}H_{36}N_{10}O_2Ru_2$	$C_{36}H_{36}N_6O_6Ru_2$	$C_{188}H_{174.7}F_{12}N_{24}O_{20}Ru_8S_4$	$C_{128}H_{112}F_{12}N_{14}O_{18}Ru_4S_4$
formula weight	874.99	842.89	850.85	4255.01	2866.81
radiation	MoK_α	MoK_α	MoK_α	MoK_α	MoK_α
crystal system	Triclinic	Triclinic	Triclinic	Triclinic	Monoclinic
space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$C2/c$
a (Å)	7.7034(5)	7.3000(4)	6.9284(13)	15.8946(3)	40.006(3)
b (Å)	9.2056(4)	14.4408(6)	8.1514(18)	20.2240(4)	10.0445(6)
c (Å)	12.8047(5)	16.8711(7)	15.609(3)	20.5704(4)	32.030(2)
α (deg)	81.621(4)	67.463(4)	89.603(19)	67.645(2)	90
β (deg)	77.670(4)	86.716(4)	78.565(17)	84.887(2)	108.099(8)
γ (deg)	84.089(4)	85.826(4)	83.400(18)	67.204(2)	90
V (Å^3)	875.19(8)	1637.50(14)	858.2(3)	5624.6(2)	12234.3(15)
Z	1	2	1	1	4
μ (mm^{-1})	1.027	0.974	0.936	0.627	0.643
T (K)	150(2)	150(2)	150(2)	150(2)	150(2)
ρ_{calcd} (g cm^{-3})	1.660	1.709	1.646	1.256	1.556
F (000)	442.0	852.0	430.0	2155.0	5824.0
θ range (deg)	2.242 to 25	2.477 to 24.996	2.516 to 25	1.572 to 26.371	2.251 to 31.25
data/restraints/ parameters	3076/0/229	5768/120/457	2953/102/229	22936/1172/1313	17846/694/880
R_1, wR_2 [$I > 2\sigma(I)$]	0.0479, 0.1003	0.0664, 0.1731	0.1319, 0.2350	0.1044, 0.3176	0.1169, 0.2642
R_1, wR_2(all data)	0.0585, 0.1053	0.0855, 0.2023	0.1994, 0.2804	0.1370, 0.3605	0.2849, 0.3865
GOF on F^2	1.063	0.961	1.140	0.889	1.017
largest diff. peak/hole, (e Å^{-3})	0.53/ –0.94	1.62/ – 1.94	1.02/ –1.80	2.00/–2.24	2.13/–1.20

Table S2. Selected Bond Angles (deg) for 2 and 3

bond angle (deg)	**2**	bond angle (deg)	**3**
N1–Ru1–N2	77.26(15)	N1–Ru1–N2	77.5(2)
N1–Ru1–N3	86.23(15)	N1–Ru1–N3	84.7(2)
N2–Ru1–N3	83.04(15)	N2–Ru1–N3	83.0(2)
Ru1–N3–C9	176.2(4)	Ru1–N3–N4	123.6(4)
N3–C9–S1	178.1(4)	N3–N4–N5	174.8(7)
N1–C1–O1	125.3(4)	N6–Ru2–N7	77.0(2)
		N6–Ru2–N8	85.6(2)
		N7–Ru2–N8	82.5(2)
		Ru2–N8–N9	122.4(5)
		N8–N9–N10	175.0(7)

Table S3. Selected Bond Lengths (Å) and Angles (deg)

bond (Å)	**4**	bond angle (deg)	**4**
Ru1-N1	2.089(13)	N1-Ru1-N2	77.7(5)
Ru1-N2	2.118(12)	N1-Ru1-N3	83.9(6)
Ru1-N3	2.116(15)	N2-Ru1-N3	87.4(5)
Ru1-C10	2.232(16)	Ru1-N3-O2	119.7(12)
Ru1-C11	2.243(16)	Ru1-N3-O3	119.0(12)
Ru1-C12	2.205(17)	O2-N3-O3	121.3(15)
Ru1-C13	2.215(15)		
Ru1-C14	2.201(16)		
Ru1-C15	2.196(15)		
N3-O2	1.238(16)		
N3-O3	1.229(16)		
C1-O1	1.198(18)		
Ru-Ru	8.452		

Table S4. Electrochemical Data

complexes	E°_{298}/V[a, b]		
	O2	O1	R1
1	1.21	0.86	–0.72
2	-	1.30	–1.13
3	0.91	0.64	–1.07
4	-	0.70	–1.14

[a]From cyclic voltammetry in CH_2Cl_2/0.1 M Bu_4NClO_4 at 100 mVs^{-1}. [b]Peak potentials of the irreversible responses in V versus SCE.