Electronic Supplementary Information (ESI)

for

Synthesis, Structure and Photophysical Properties of a Supramolecular Complex with Gold Dicyanide Donors Coordinated to Aza[5]helicene Viologen Acceptors

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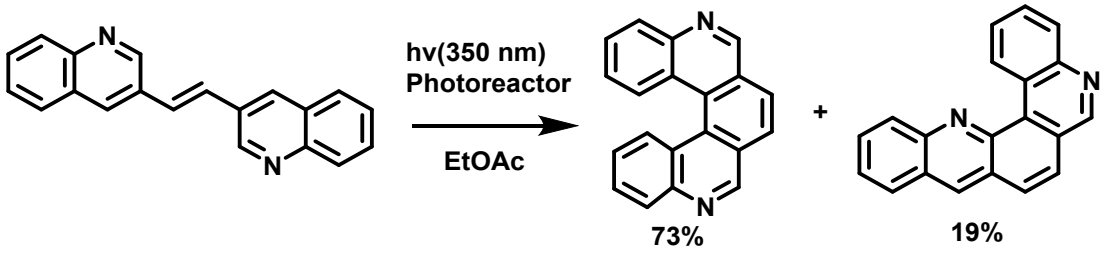
Synthesis details:



During the synthesis of 5,10-diaza[5]helicene **(5), s**ide-product- Benzo-[b]-1,8-diaza[4]-helicene (**6**) was also recovered. Yield: 0.11 g (19%) **^{1}H NMR (400 MHz, $CDCl_3$)** δ 11.37 (d, 1H, *J*=Hz), 9.37 (s, 1H), 8.75 (s,1H), 8.49 (d, 2H, *J*=8.7 Hz), 8.30 (d,2H, *J*=8.1 Hz), 8.09-7.98 (m, 2H), 7.93-7.83 (m, 4H), 7.67 (dd, 1H, *J*= 7.96, 6.92 Hz) ppm.

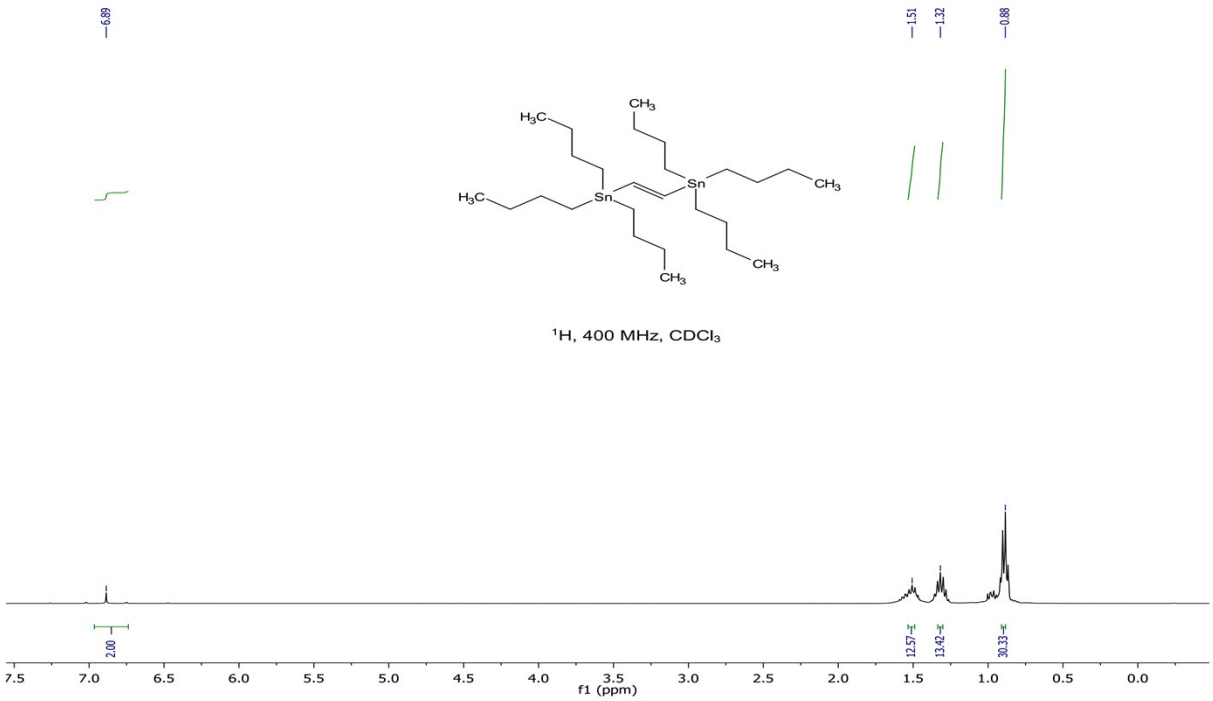


Figure S1. ^{1}H MNR spectrum of **2**.

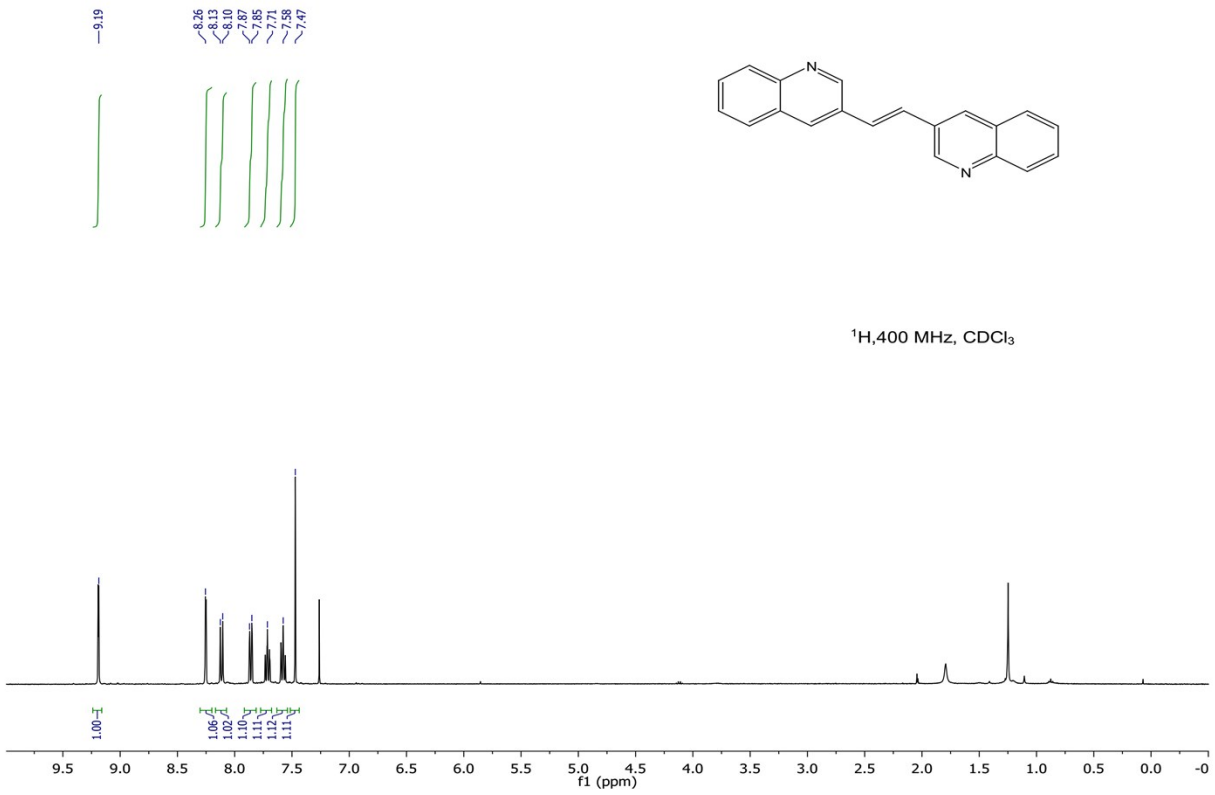


Figure S2. ^{1}H MNR spectrum of **4**.

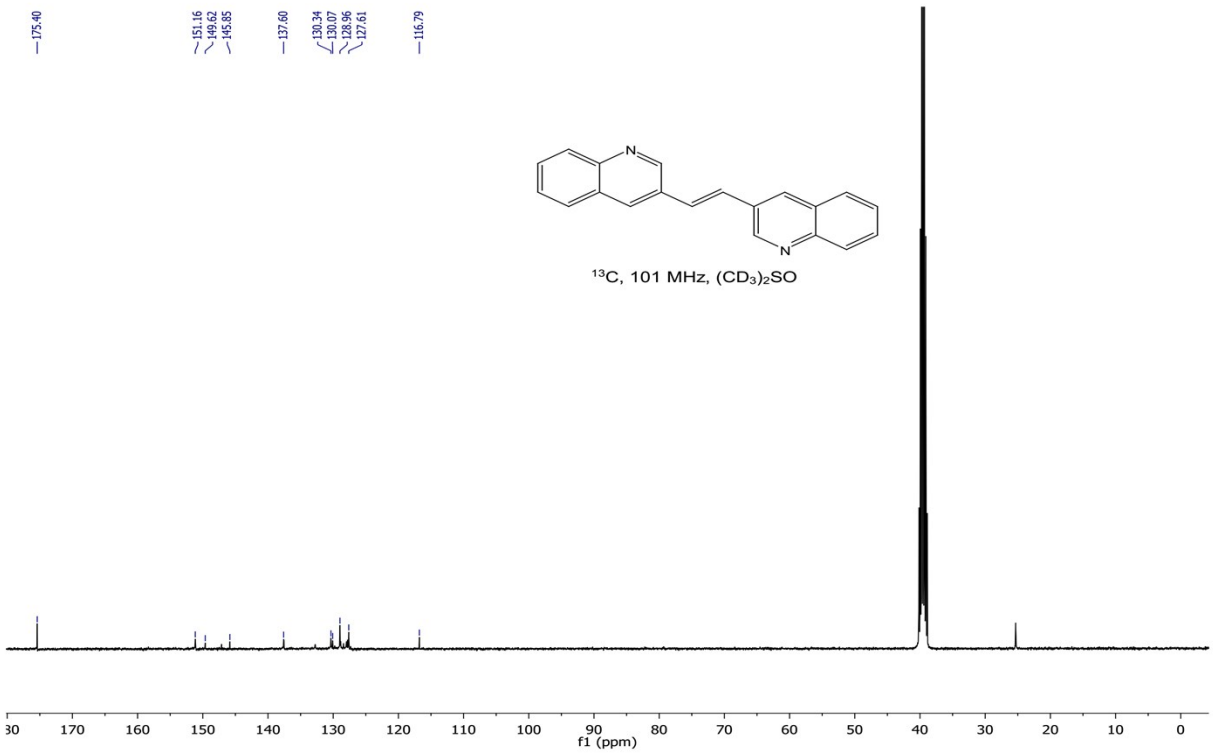


Figure S3. ^{13}C MNR spectrum of **4**.

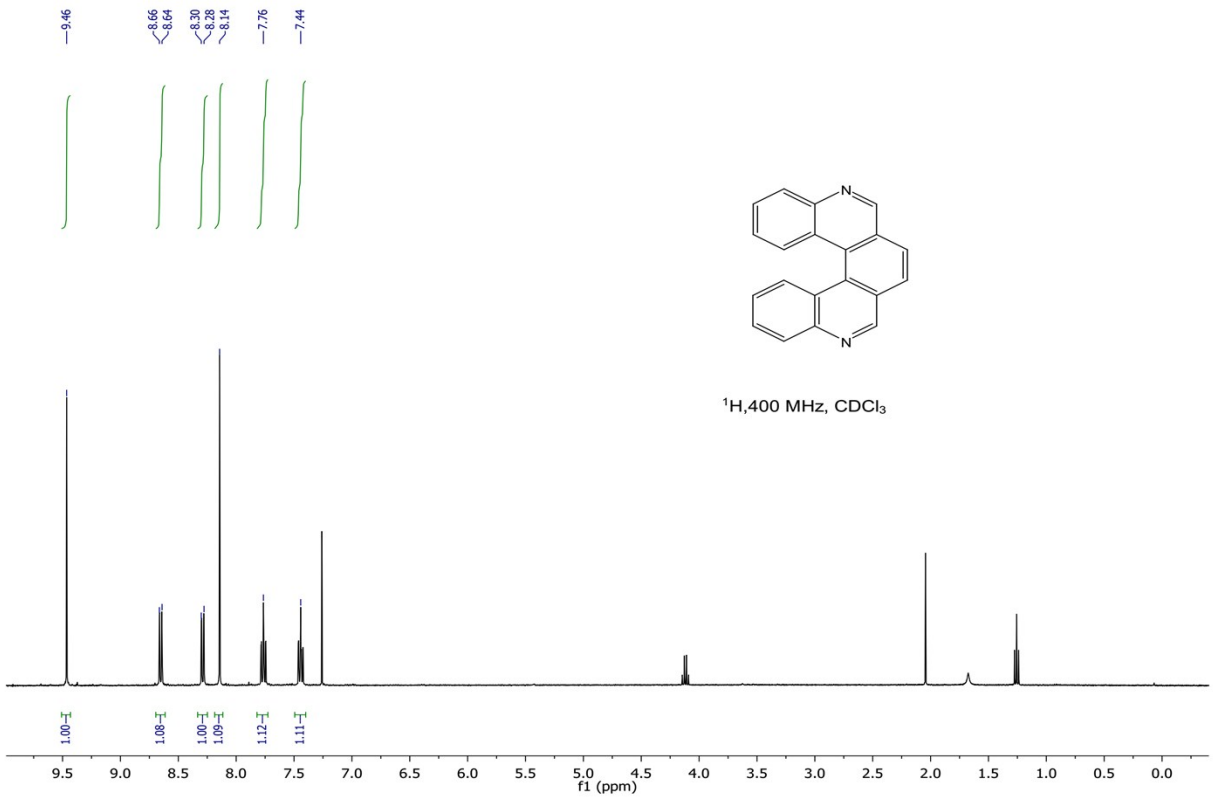


Figure S4. ^{1}H MNR spectrum of **5**.

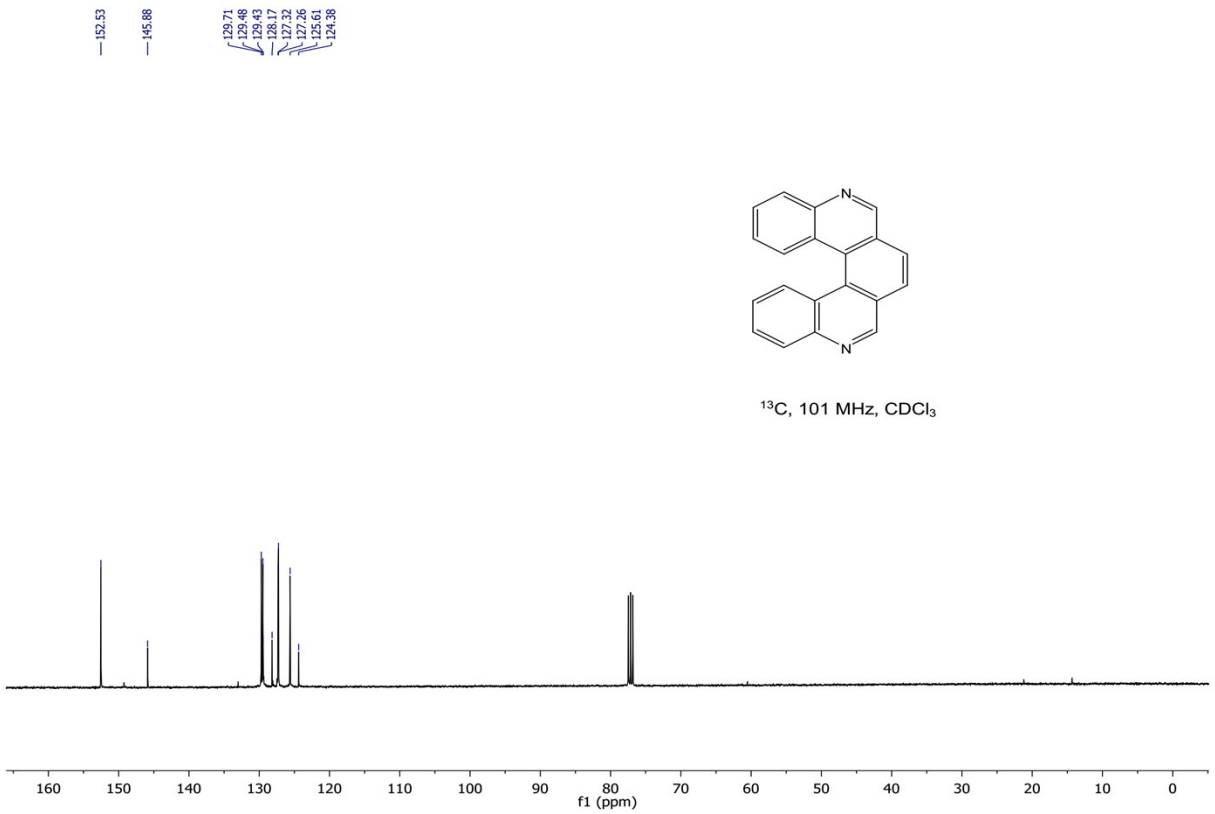


Figure S5. ^{13}C MNR spectrum of **5**.

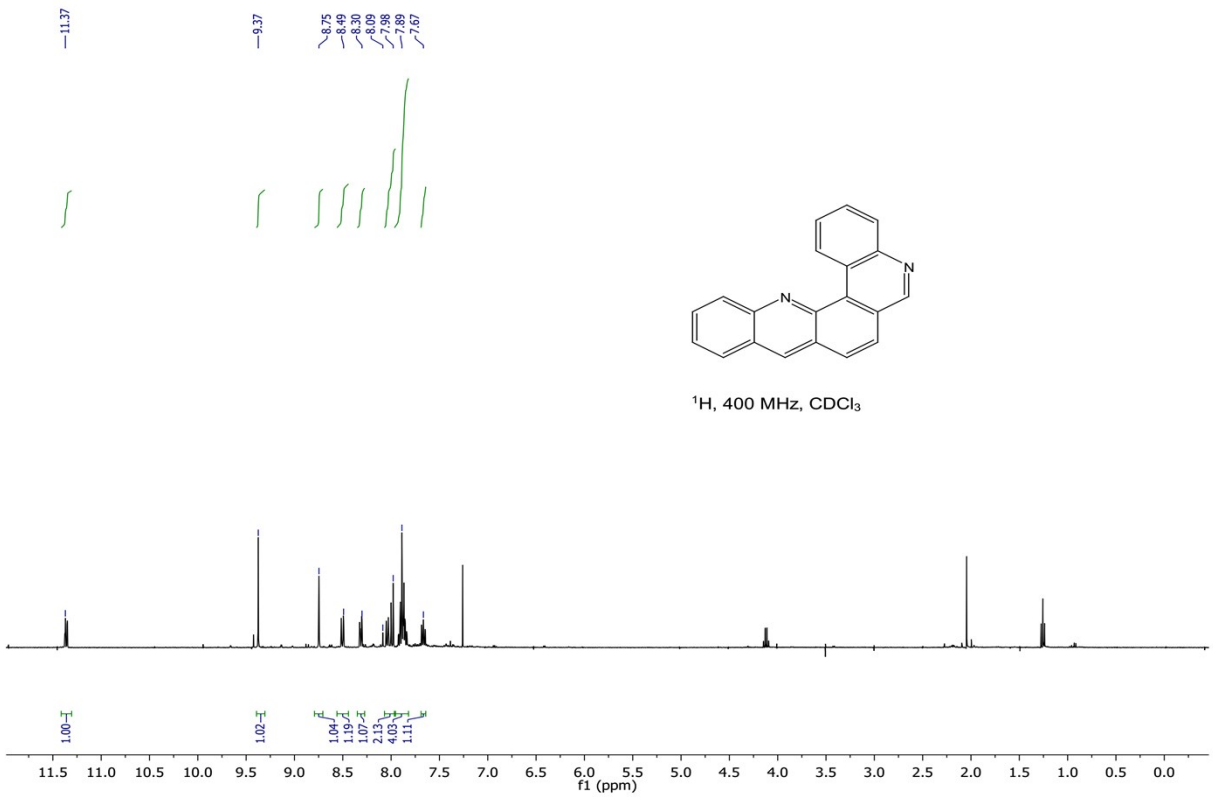


Figure S6. ^{1}H MNR spectrum of **6**.

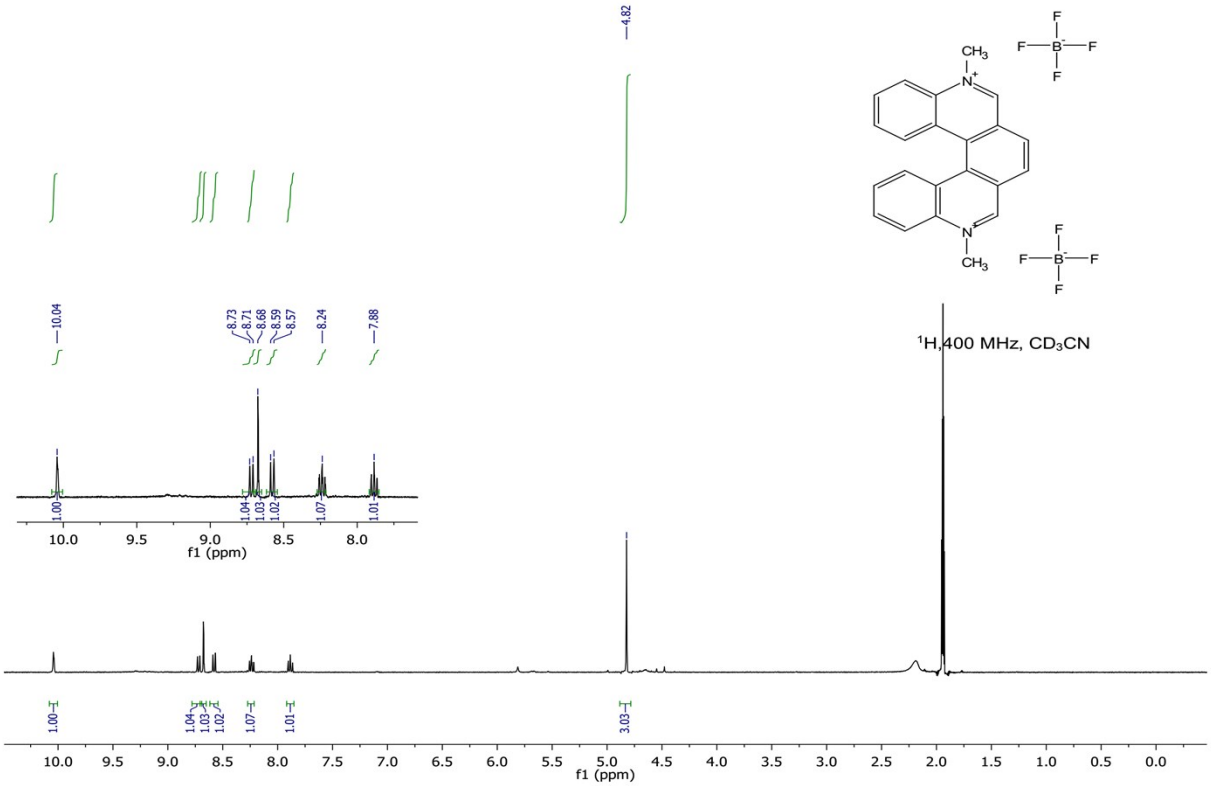


Figure S7. ^{1}H MNR spectrum of **7a**.

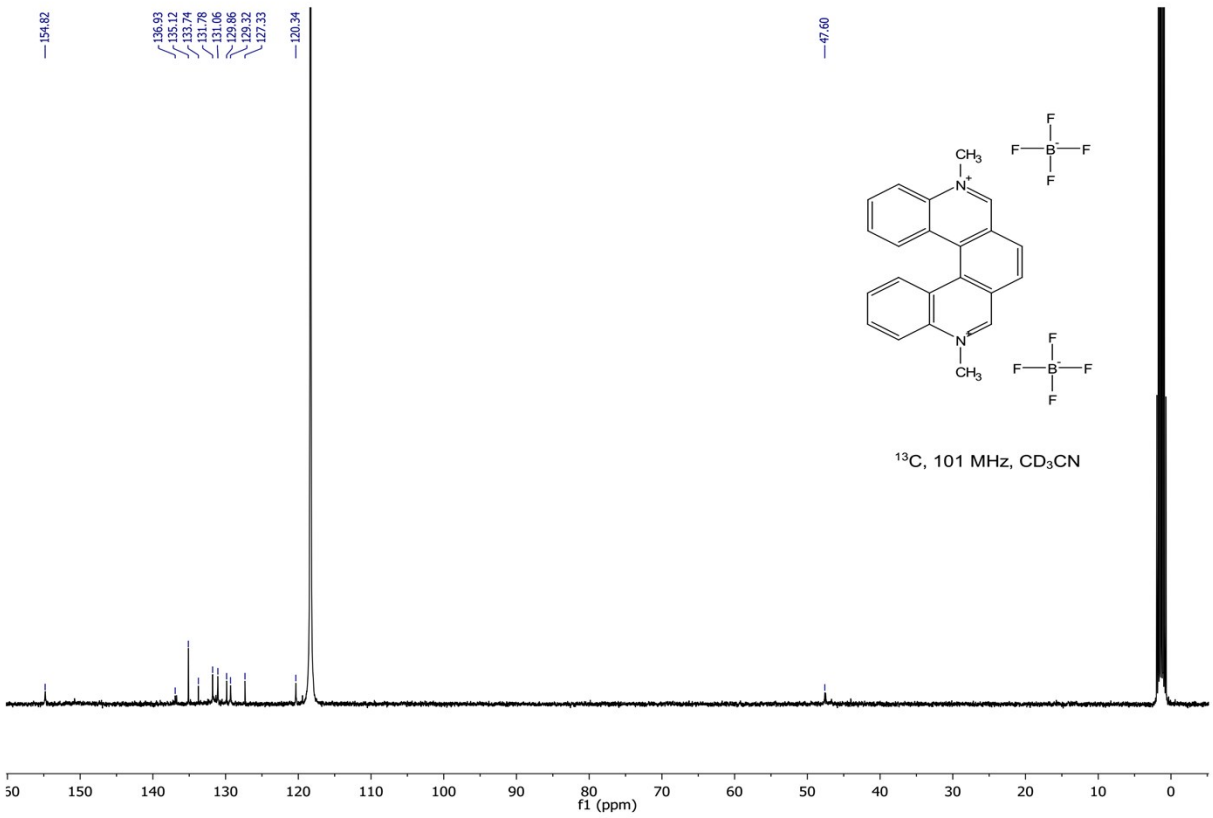


Figure S8. ^{13}C MNR spectrum of **7a**.

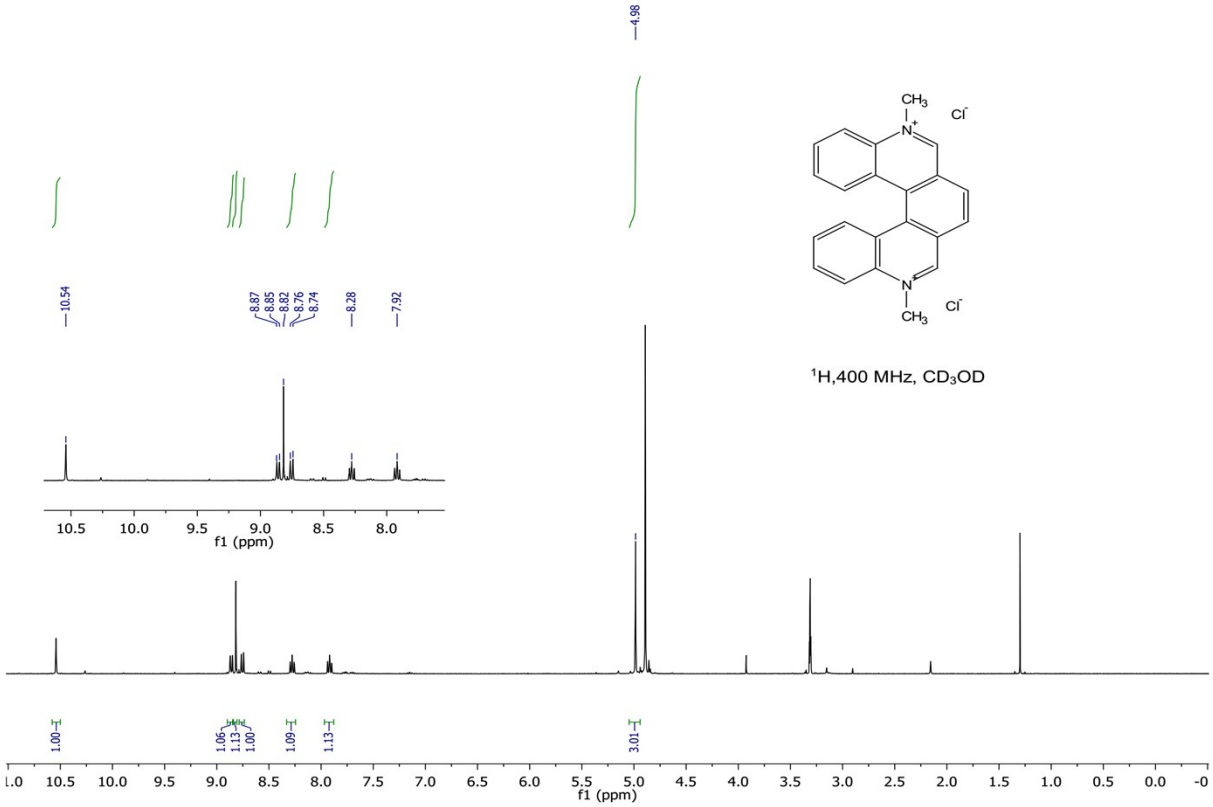


Figure S9. ^{1}H MNR spectrum of **7b**.

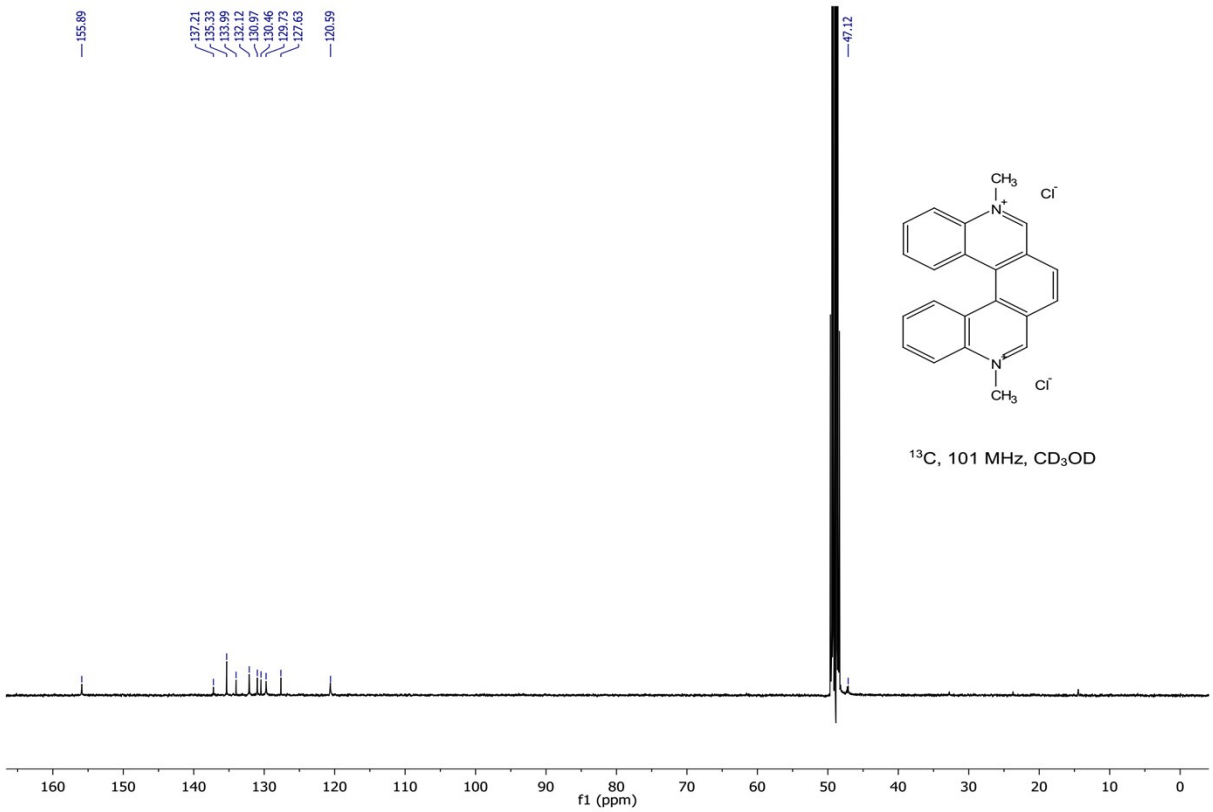


Figure S10. ^{13}C MNR spectrum of **7b**.

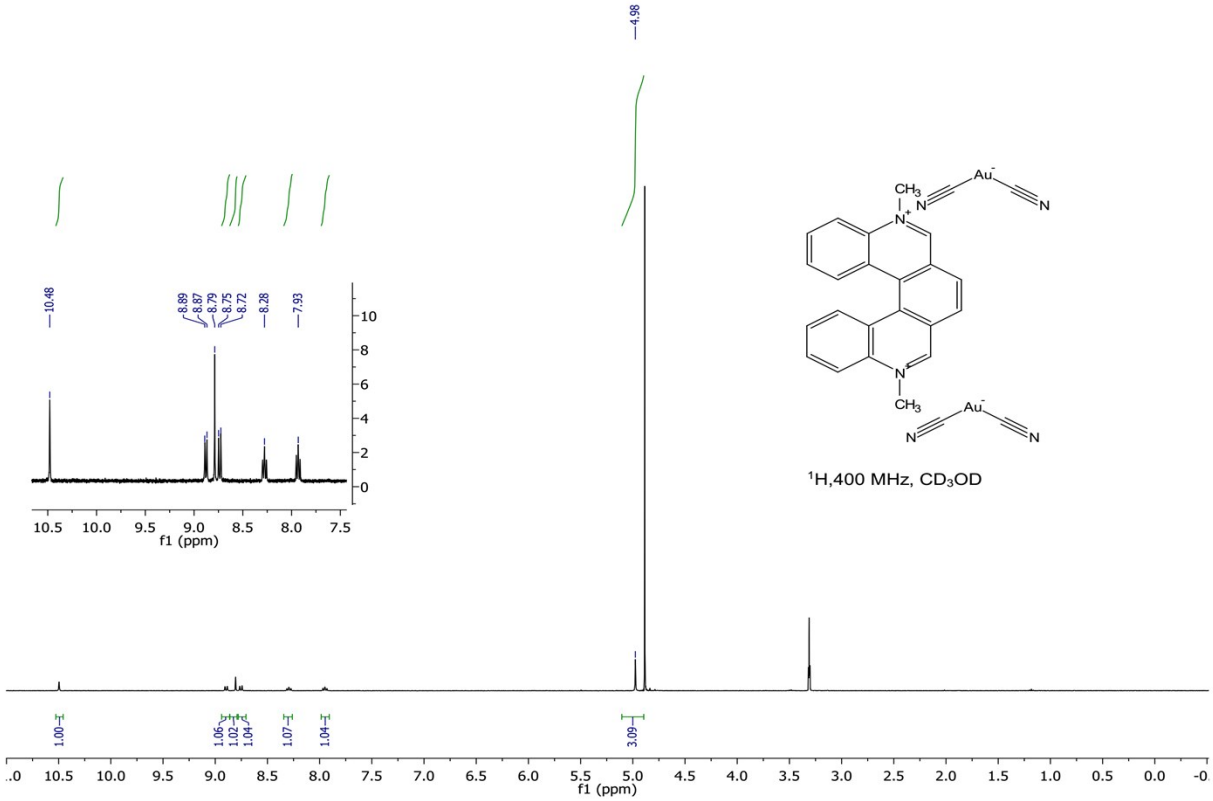


Figure S11. ^{1}H MNR spectrum of **8**.

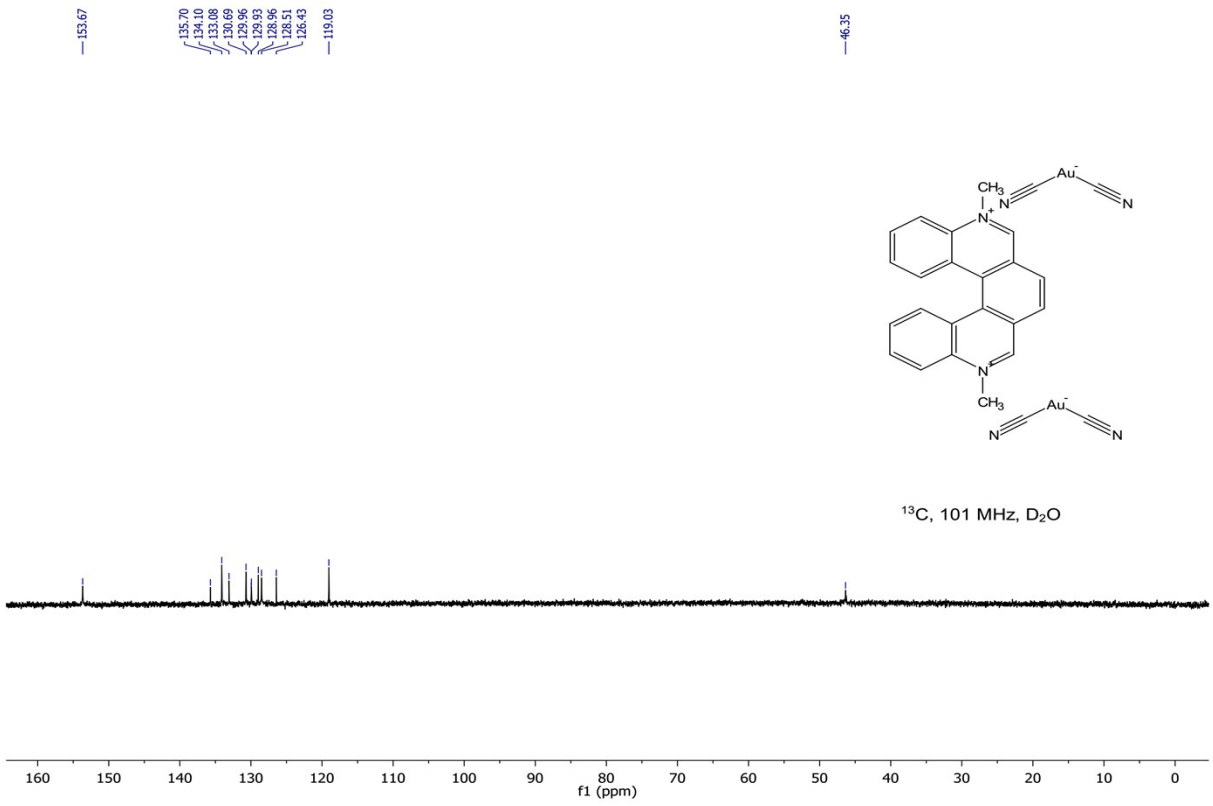


Figure S12. ^{13}C MNR spectrum of **8**.

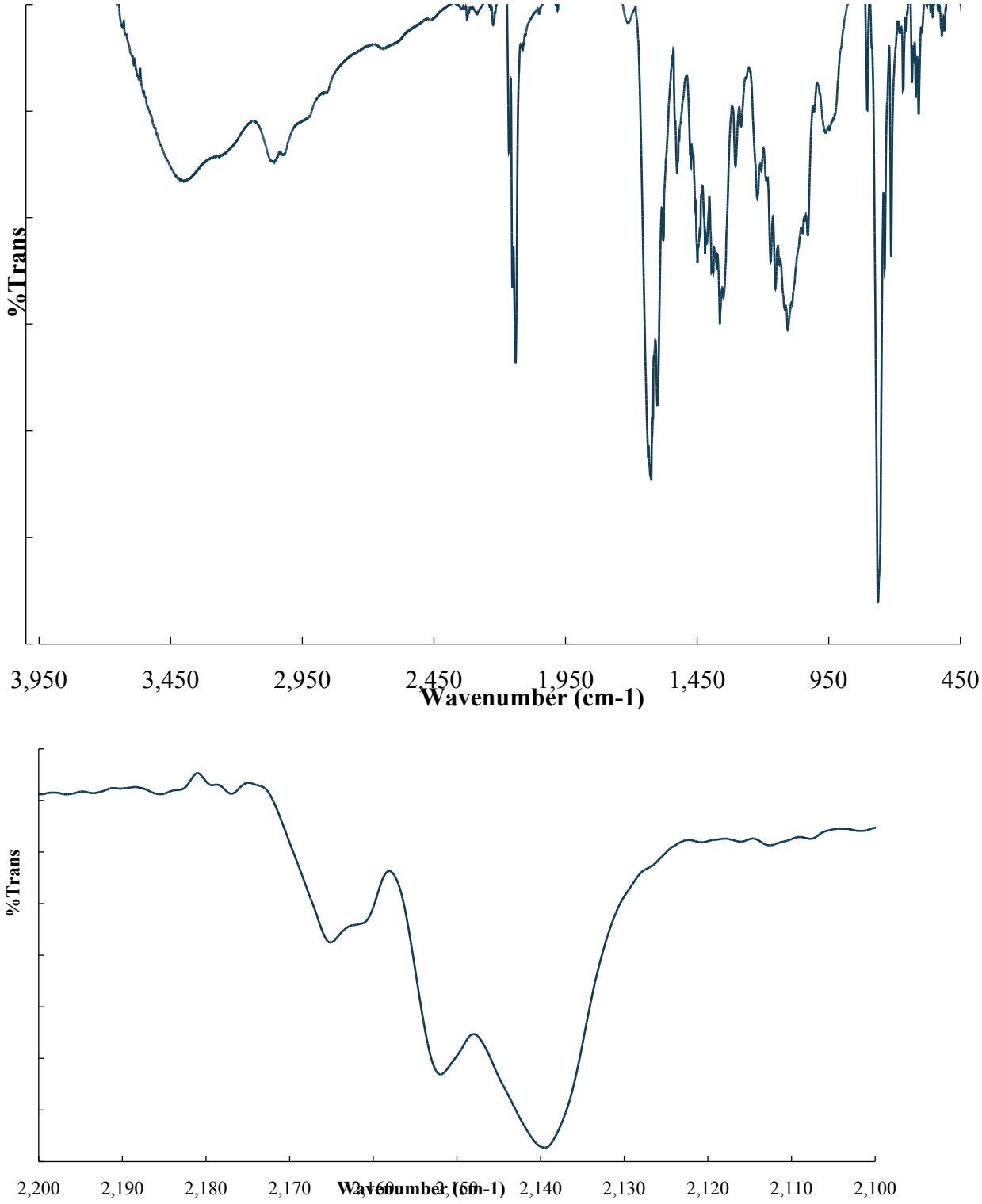


Figure S13. IR spectrum of microcrystalline Au heli-viologen (**8**) at 298 K.

Table S1. Select bond lengths of Au heli-viologen.

Au(1)-C(1)	2.0107(1)	C(9)-C(10)	1.4369(1)
Au(1)-C(2)	2.0068(1)	C(10)-C(11)	1.4131(1)
Au(2)-C(4)	1.9837(1)	C(10)-C(19)	1.3644(1)
Au(2)-C(3)	1.9433(1)	C(13)-C(18)	1.4101(1)
N(1)-C(1)	1.1318(1)	C(13)-C(14)	1.4156(1)
N(2)-C(2)	1.0913(1)	C(14)-C(15)	1.3473(1)
N(3)-C(3)	1.1708(1)	C(15)-C(16)	1.3870(1)
N(4)-C(4)	1.1198(1)	C(16)-C(17)	1.3998(1)
N(5)-C(5)	1.4637(1)	C(17)-C(18)	1.3923(1)
N(5)-C(6)	1.2860(1)	C(18)-C(19)	1.4561(1)
N(5)-C(26)	1.4028(1)	C(19)-C(20)	1.4407(1)
N(6)-C(11)	1.3096(1)	C(20)-C(21)	1.4663(1)
N(6)-C(12)	1.4724(1)	C(21)-C(26)	1.4320(1)
N(6)-C(13)	1.4031(1)	C(21)-C(22)	1.4159(1)
C(6)-C(7)	1.4320(1)	C(22)-C(23)	1.3267(1)
C(7)-C(8)	1.4136(1)	C(23)-C(24)	1.4234(1)
C(7)-C(20)	1.4379(1)	C(24)- (C25)	1.3774(1)
C(8)-C(9)	1.3398(1)	C(25)-C(26)	1.3754(1)

Table S2. Select bond angles of Au heli-viologen.

C(1)-Au(1)-C(2)	176.62(1)	N(6)-C(13)-C(14)	120.77(1)
C(3)-Au(2)-C(4)	177.67(1)	C(13)-C(14)-C(15)	120.78(1)
Au(1)-C(1)-N(1)	177.15(1)	C(14)-C(15)-C(16)	121.68(1)
Au(1)-C(2)-N(2)	175.42(1)	C(15)-C(16)-C(17)	117.87(1)
Au(2)-C(3)-N(3)	175.29(1)	C(16)-C(17)-C(18)	122.24(1)
Au(2)-C(4)-N(4)	176.96(1)	C(13)-C(18)-C(17)	117.82(1)
C(11)-N(6)-C(13)	119.08(1)	C(13)-C(18)-C(19)	118.40(1)
C(12)-N(6)-C(13)	119.16(1)	C(17)-C(18)-C(19)	118.40(1)
C(11)-N(6)-C(12)	121.62(1)	C(10)-C(19)-C(20)	116.99(1)
C(5)-N(5)-C(26)	118.65(1)	C(10)-C(19)-C(18)	116.94(1)
C(6)-N(5)-C(26)	122.98(1)	C(18)-C(19)-C(20)	125.97(1)
C(5)-N(5)-C(6)	117.87(1)	C(7)-C(20)-C(21)	116.80(1)
N(5)-C(6)-C(7)	123.13(1)	C(19)-C(20)-C(21)	126.22(1)
C(6)-C(7)-C(8)	120.84(1)	C(7)-C(20)-C(19)	116.64(1)
C(8)-C(7)-C(20)	121.99(1)	C(20)-C(21)-C(26)	119.32(1)
C(6)-C(7)-C(20)	117.14(1)	C(22)-C(21)-C(26)	116.97(1)
C(7)-C(8)-C(9)	119.55(1)	C(20)-C(21)-C(22)	122.64(1)
C(8)-C(9)-C(10)	118.18(1)	C(21)-C(22)-C(23)	121.43(1)
C(9)-C(10)-C(19)	124.38(1)	C(22)-C(23)-C(24)	120.64(1)
C(11)-C(10)-C(19)	120.09(1)	C(23)-C(24)-C(25)	119.77(1)
C(9)-C(10)-C(11)	115.47(1)	C(24)-C(25)-C(26)	119.63(1)
N(6)-C(11)-C(10)	122.91(1)	N(5)-C(26)-C(21)	117.72(1)
N(6)-C(13)-C(18)	120.16(1)	C(21)-C(26)-C(25)	120.78(1)
C(14)-C(13)-C(18)	118.99(1)	N(5)-C(26)-C(25)	121.41(1)

Table S3. DFT B3LYP/LANL2DZ select ground state parameters of Au heli-viologen with comparison to experimental values.

	Distance (Å) / Angle (°)	
	Experimental*	Calculated*
Au···Au	3.310	3.327
$N_{Au(CN)_2}\cdots N_{aza[5]helicene}$	3.216	3.088
Au-C	2.010	2.029
C-Au-C	176.6	166.8
N-C-Au	177.1	169.6

*Average distances

Figure S14. TD-DFT M06/CEP-31G calculated UV-vis of Au heli-viologen compared to experimental UV-Vis.

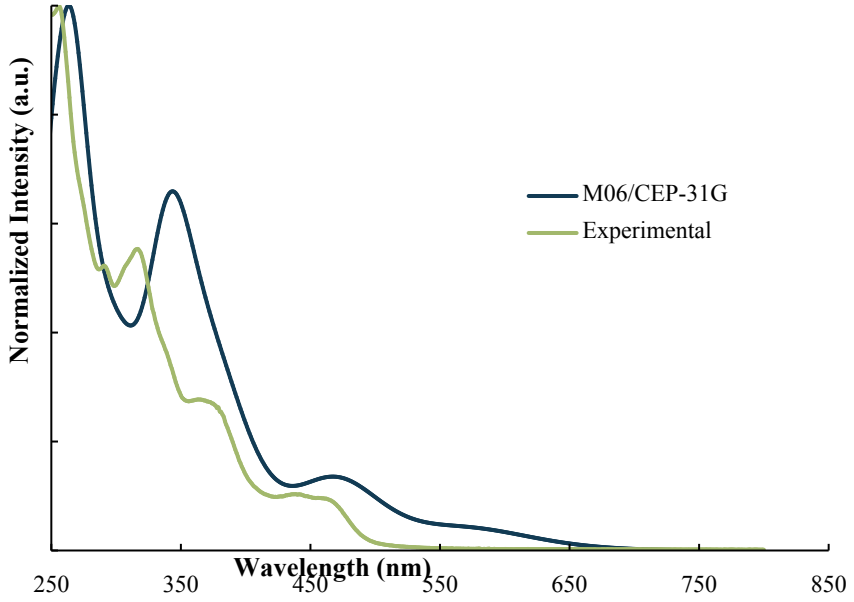


Table S4. TD-DFT calculated excited states of of Au heli-viologen with corresponding energy and f-oscillation.

Excited State Number	Excited State Energy	Excited State f-oscillation
7	428 nm	0.0078
8	425 nm	0.0067
9	423 nm	0.0014
10	421 nm	0.0000
11	421 nm	0.0069
12	420 nm	0.0027
13	406 nm	0.0004
14	404 nm	0.0009
15	401 nm	0.0028
16	399 nm	0.0132
17	392 nm	0.0011
18	390 nm	0.0083

Table S5. Calculated MO transitions of Au heli-viologen for excited state at 399 nm with percent contribution.

Orbital Transition	% Contribution
HOMO-9→LUMO+1	25%
HOMO-11→LUMO	21%
HOMO→LUMO+2	18%
HOMO→LUMO+3	16%
HOMO-9→LUMO	12%
HOMO-11→LUMO+1	8%

Figure S15. Isodensity representations of MO transitions of excited state at 399 nm for Au heli-viologen with percent contribution.