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Supporting Information

for

Design and synthesis of an axially chiral platinum(II) complex and its CPL properties in PMMA matrix

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Spectroscopic details and theoretical calculations

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1. Spectroscopic details

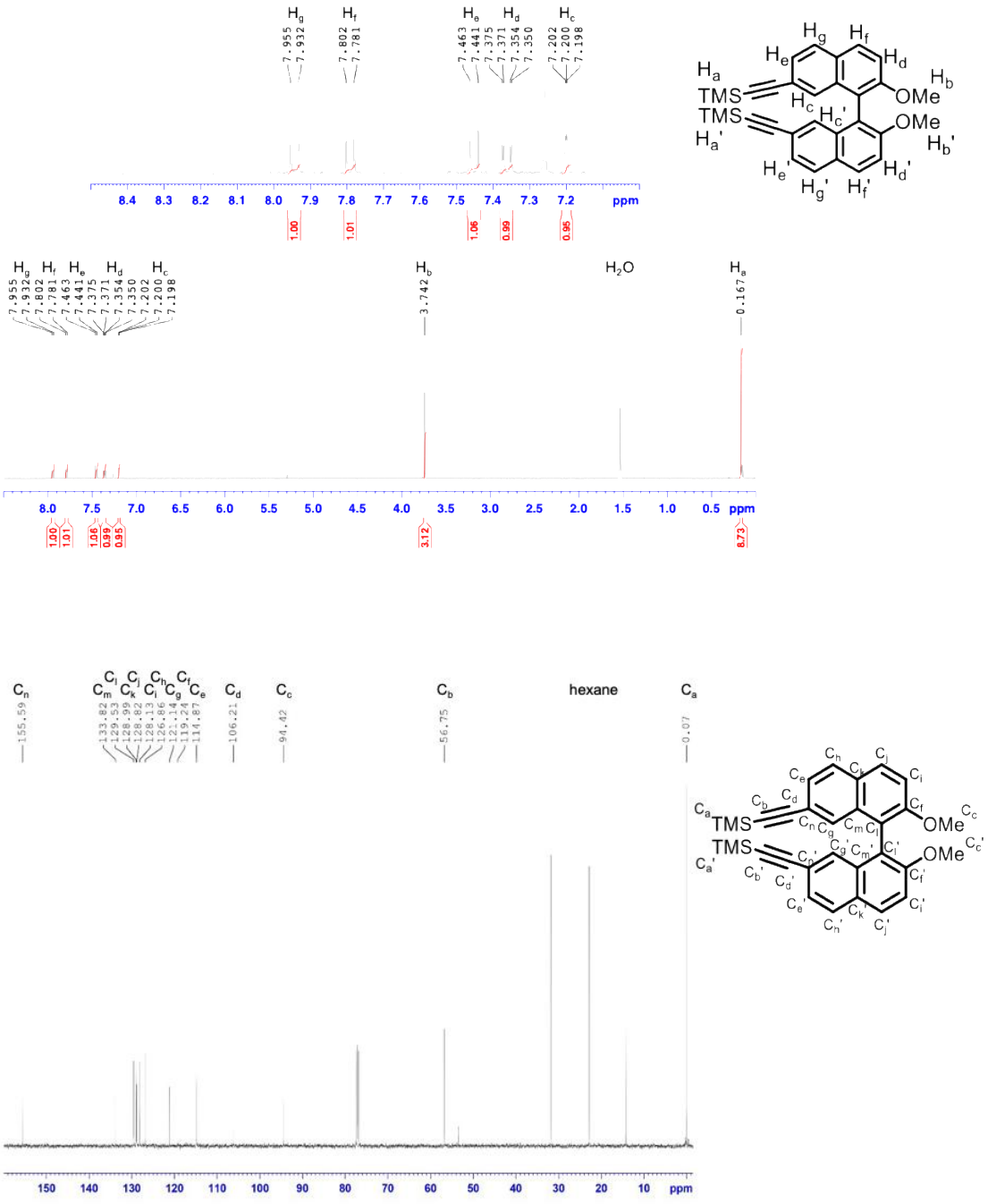

Figure S1: ^{1}H (top) and ^{13}C NMR spectra (bottom) of ***S*-2**

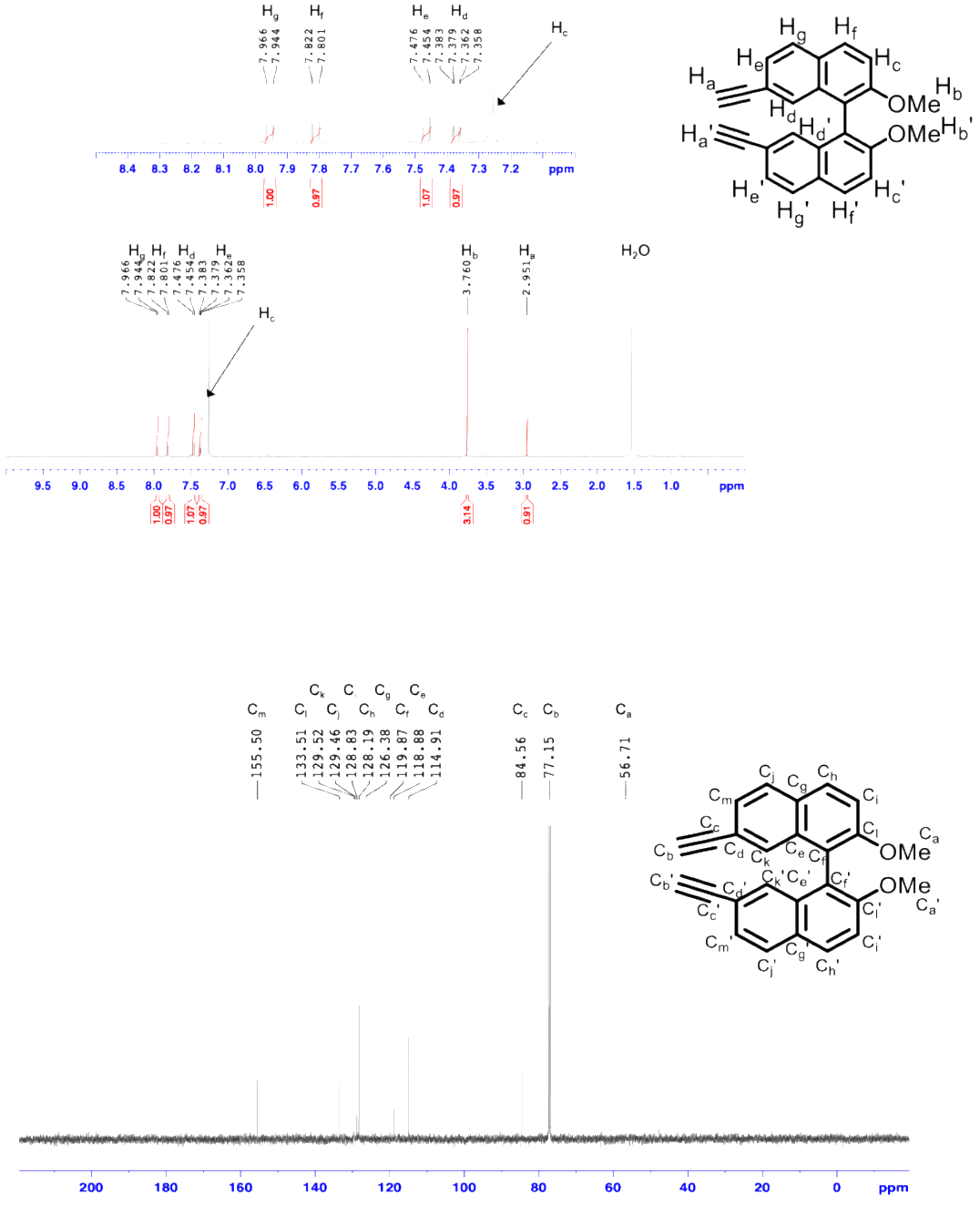

Figure S2: ^{1}H (top) and ^{13}C NMR spectra (bottom) of ***S*-3**

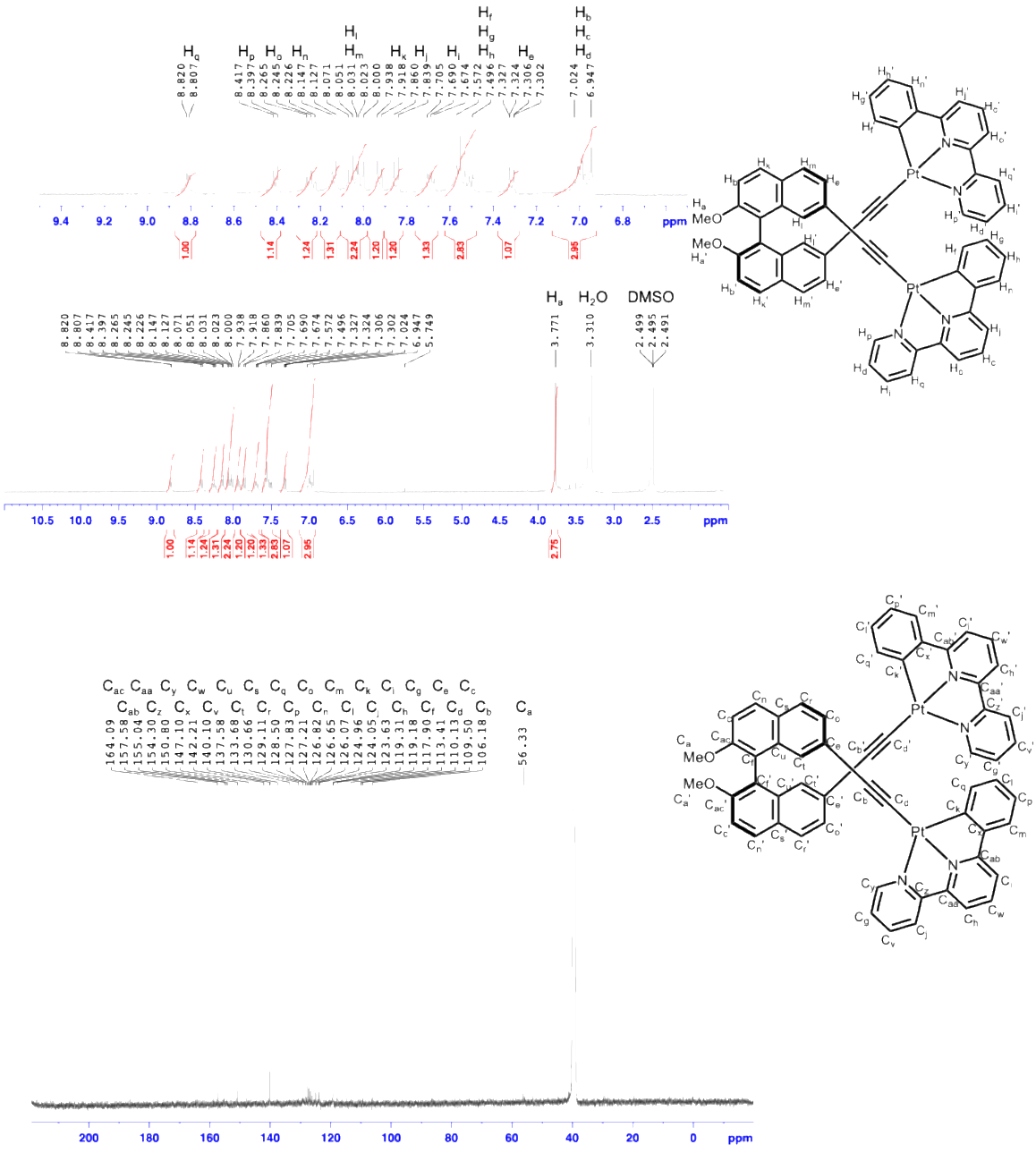

Figure S3: ^{1}H (top) and ^{13}C NMR spectra (bottom) of ***R*-Pt**

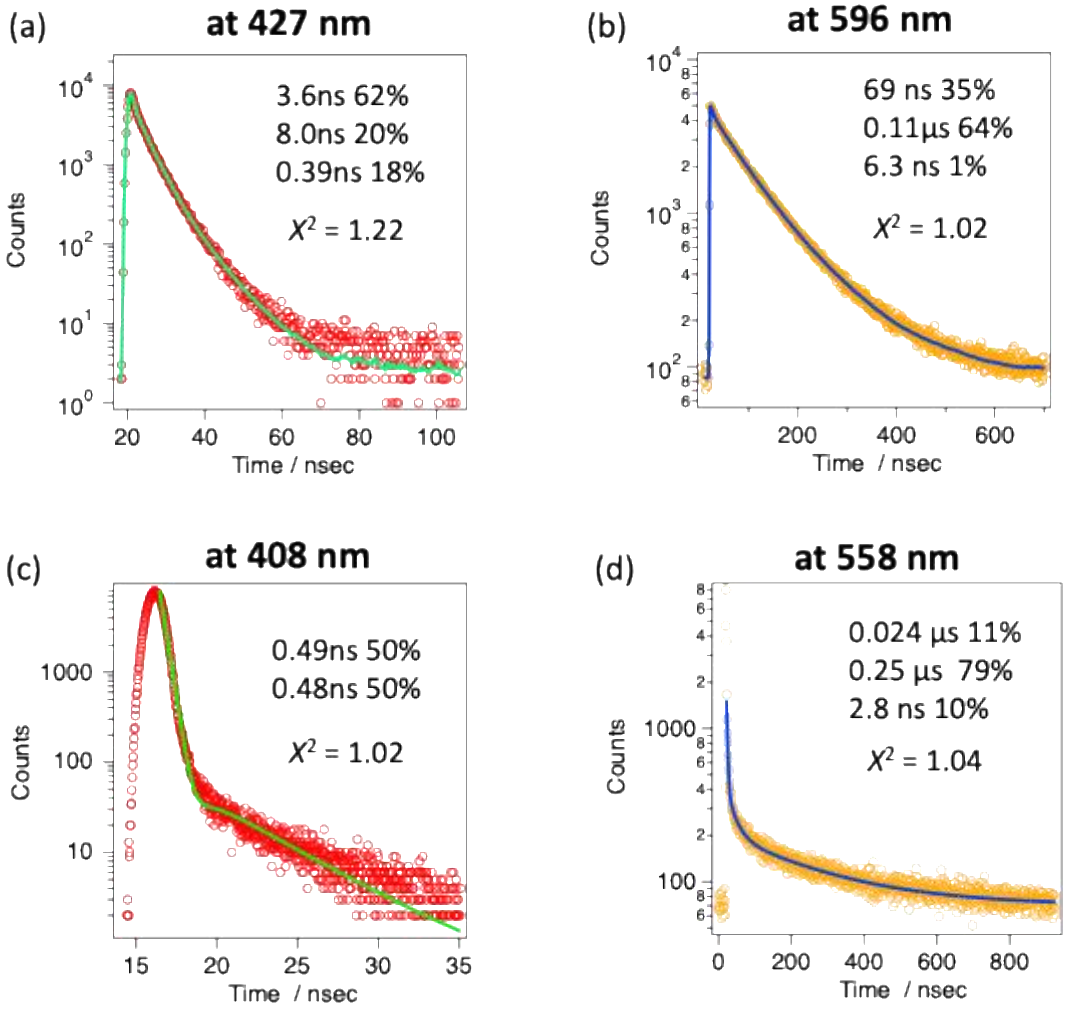

Figure S4: (a) Emission lifetime of dichloromethane solution at 427 nm, **(**b) at 596 nm (λ_{ex} = 370 nm). **(**c) Emission life time of PMMA matrix at 408 nm **(d)** at 558 nm.

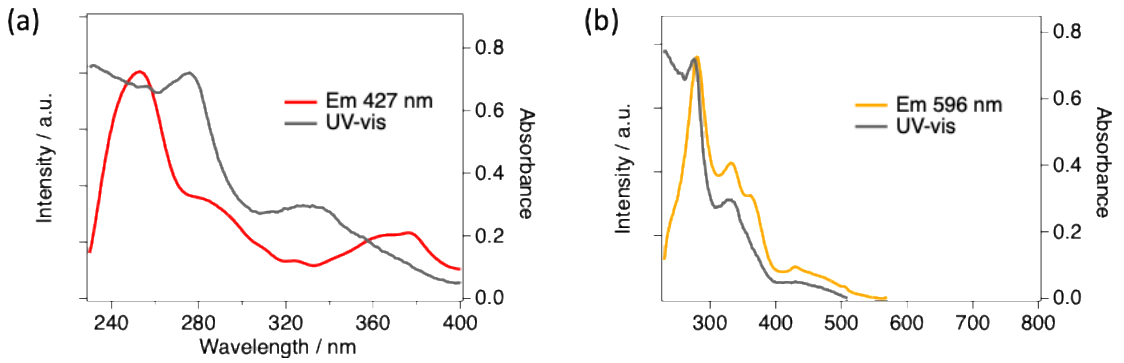

Figure S5: Excitation spectra and UV–vis spectra of a 1.0×10^{-5} M solution of ***R*-Pt** in dichloromethane: (a) at an emission wavelength of 427 nm, (b) at an emission wavelength of 596 nm.

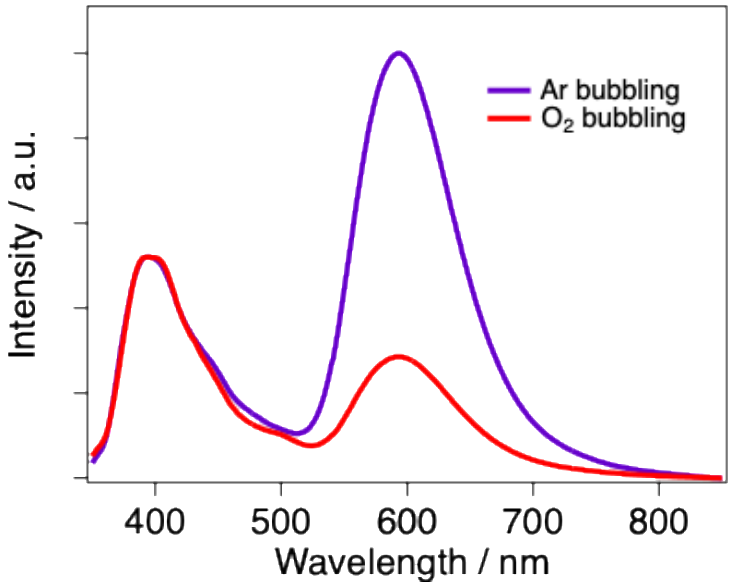

Figure S6: Emission spectra of a 1.0×10^{-5} M ***R*-Pt** solution in dichloromethane under Ar and O_2 bubbling conditions (λ_{ex} = 320 nm).

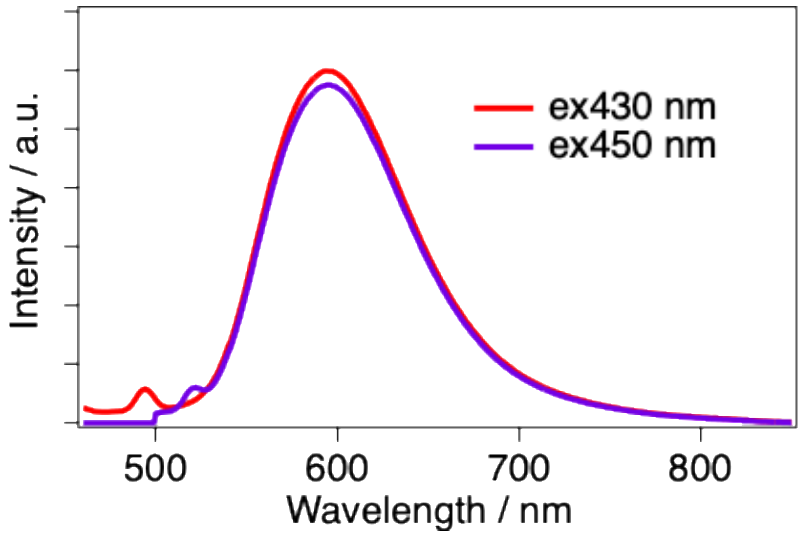

Figure S7: Emission spectra excited at the CT band of the absorption spectrum.

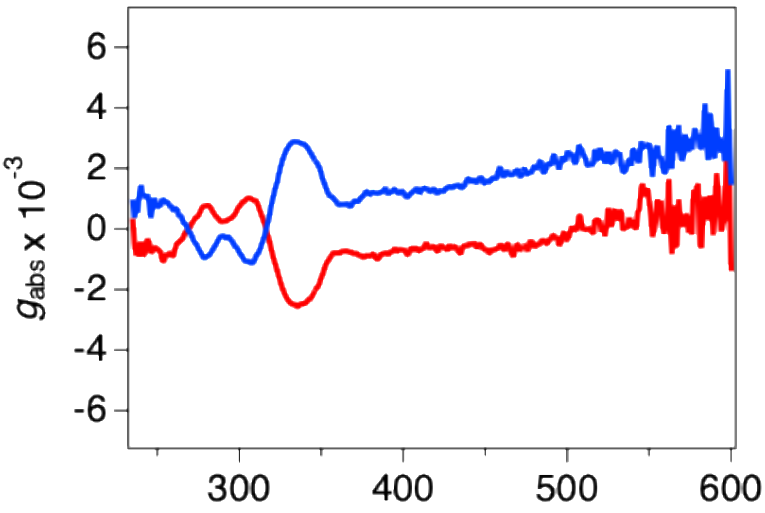

Figure S8: g_{abs} chart of ***R*/*S*-Pt** in 1.0×10^{-5} M dichloromethane solution.

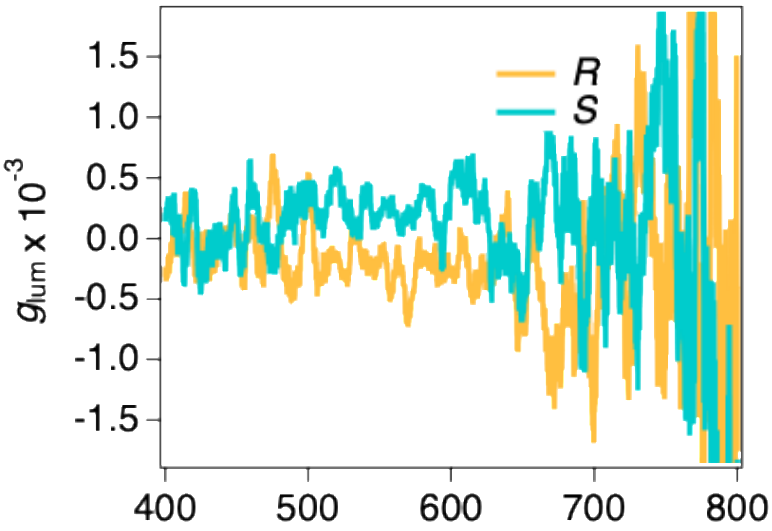

Figure S9: g_{lum} chart of ***R*/*S*-Pt** in PMMA matrices.

2. Theoretical calculations

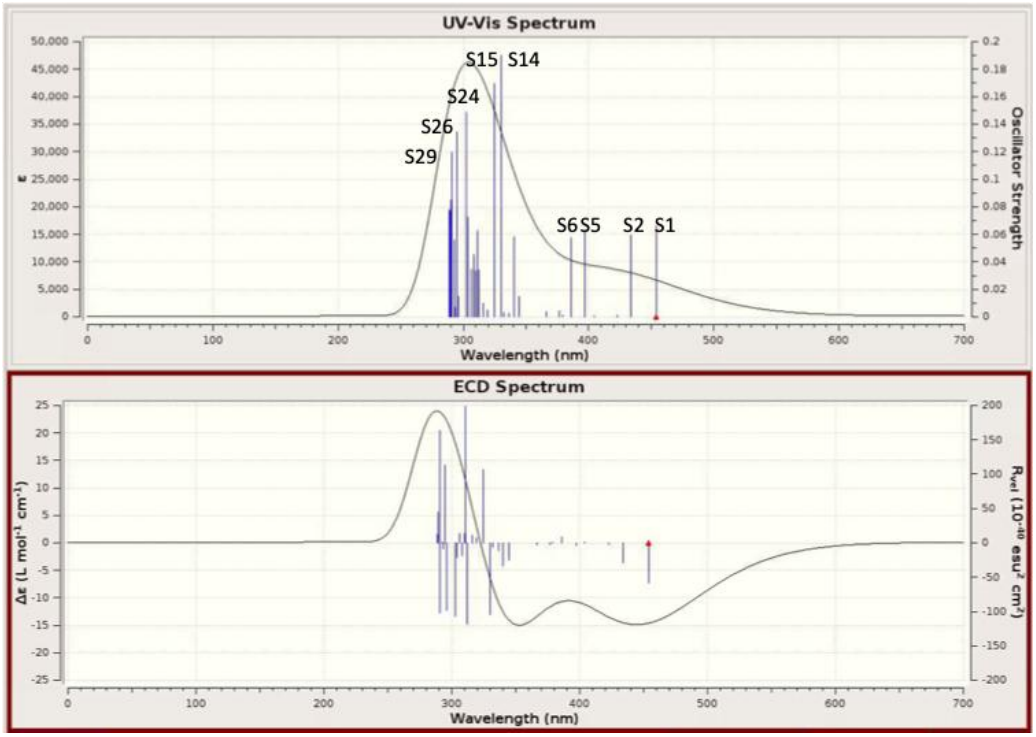

Figure S10: Simulated UV–vis and CD spectrum of ***R*-Pt** calculated by CAM-B3LYP/6-31+G(d,p).

Table S1: TD-DFT calculated excitation energies of ***R*-Pt** corresponding to the absorption wavelengths and main weight of transition.

Exited state	Excitation energy (OSC)	Dominant transitions (% weight)
1	2.7318 eV 453.86 nm (*f* = 0.0663)	232→234 (73%)
2	2.8576 eV 433.87 nm (*f* = 0.0594)	233→235 (85%)
5	3.1217 eV 397.17 nm (*f* = 0.0632)	227→234 (72%)
6	3.2125 eV 385.94 nm (*f* = 0.0578)	229→235 (100%)
14	3.7553 eV 330.16 nm (*f* = 0.1902)	226→236 (58%)
15	3.8173 eV 324.80 nm (*f* = 0.1698)	228→237 (82%)
24	4.1008 eV 302.34 nm (*f* = 0.1484)	221→234 (44%)
26	4.2097 eV 294.52 nm (*f* = 0.1345)	230→235 (21%) 231→241 (24%)
29	4.2622 eV 290.89 nm (*f* = 0.1196)	230→235 (22%) 232→240 (21%)

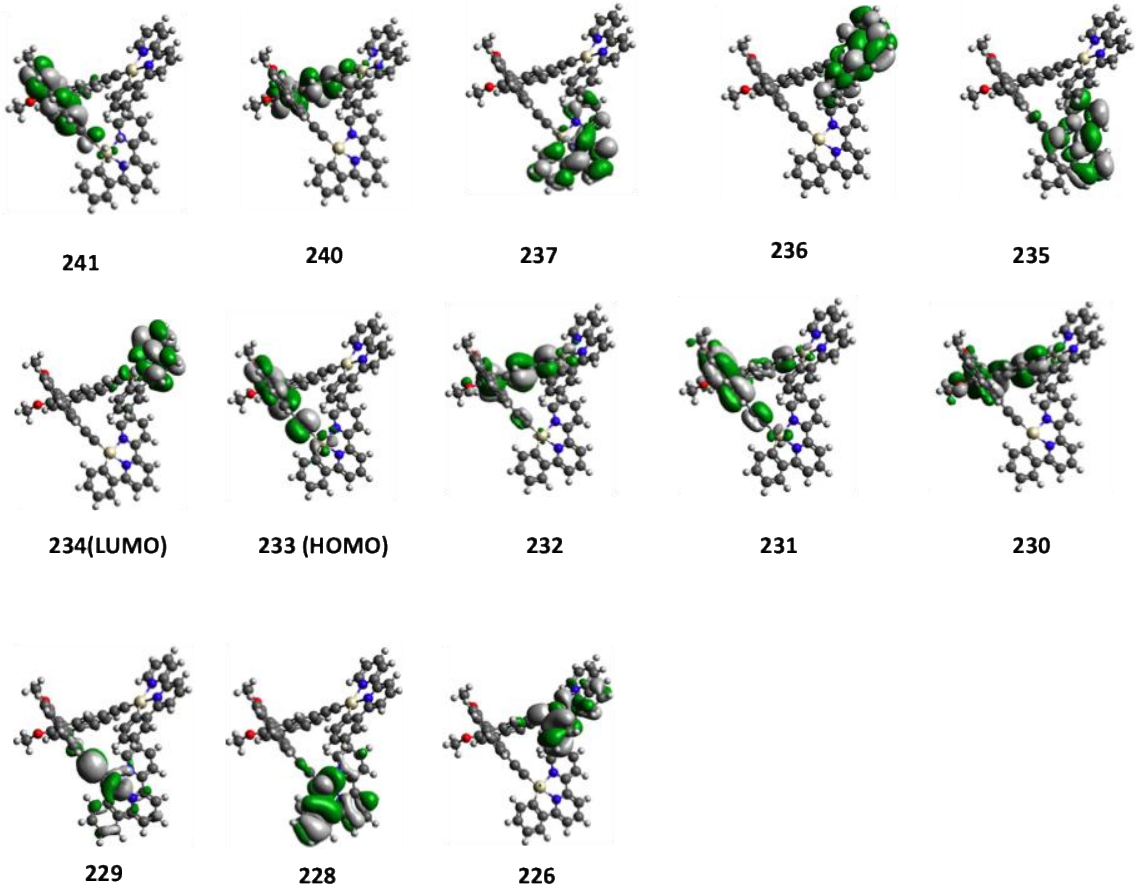

Figure S11: Dominant molecular orbitals of ***R*-Pt** related to the excitation listed in **Table S1.**

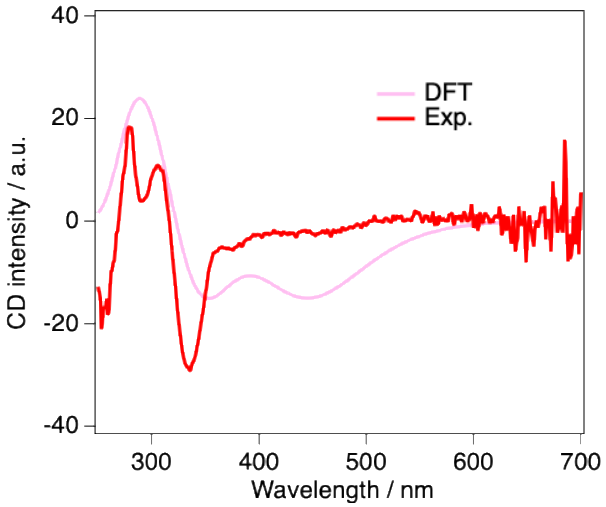

Figure S12: Experimental and simulated CD spectrum of ***R*-Pt** with TD-DFT calculation.

Table S2: Cartesian coordinates for ***R*-Pt** in ground state (S_0).

Atoms	X	Y	Z
C	1.07601	3.33509	-1.05702
C	0.23544	4.34734	-1.5934
C	0.04628	4.38624	-3.01675
C	0.71232	3.42887	-3.83099
C	1.50704	2.45612	-3.28267
H	1.22365	3.28458	0.01479
C	-0.43868	5.2973	-0.76205
C	-0.80536	5.36943	-3.56769
H	0.56848	3.47592	-4.90812
H	1.99954	1.72095	-3.91167
C	-1.462	6.27326	-2.76325
C	-1.28113	6.23562	-1.35809
H	-0.94786	5.40056	-4.64509
H	-2.11739	7.01046	-3.21097
C	-0.25259	5.32614	0.72211

C	-0.83961	4.34082	1.5791
C	0.49758	6.35522	1.28961
C	-1.58555	3.24319	1.07359
C	-0.65514	4.43755	3.00028
C	0.6727	6.44971	2.69235
H	-1.73232	3.15111	0.00435
C	-1.23091	3.44567	3.84202
C	0.10136	5.51032	3.5215
H	1.25576	7.25685	3.11896
C	-1.93239	2.38919	3.32285
H	-1.09232	3.53519	4.9171
H	0.23867	5.58414	4.59755
H	-2.35521	1.62886	3.97166
O	1.0505	7.25452	0.4181
O	-1.91455	7.10416	-0.51389
C	-2.79985	8.06674	-1.05454
H	-3.63848	7.60039	-1.58836
H	-3.19015	8.62521	-0.2017
H	-2.28736	8.76243	-1.7326
C	1.80995	8.33066	0.93381
H	2.69312	7.98424	1.48728
H	2.13982	8.90639	0.0668
H	1.21252	8.9803	1.58753
C	1.68911	2.38285	-1.8645
C	2.44845	1.31987	-1.28991
C	-2.10863	2.25994	1.90768
C	3.04196	0.38747	-0.75256
C	-2.76781	1.1176	1.36691
C	-3.27847	0.11557	0.87195
C	-8.29946	-2.42617	1.63152
C	-7.66826	-3.21484	0.67446
C	-6.37931	-2.88558	0.22781

C	-6.3573	-0.96554	1.70754
C	-7.64056	-1.30339	2.14418
H	-9.29714	-2.68242	1.9758
H	-8.18296	-4.0862	0.27692
H	-5.85838	-0.09156	2.11254
H	-8.13359	-0.68599	2.89126
C	-5.65934	-3.67654	-0.77992
C	-6.07618	-4.83321	-1.45337
C	-3.57683	-3.73368	-1.95032
C	-5.22168	-5.42795	-2.37959
H	-7.05281	-5.2592	-1.2556
C	-3.95991	-4.88645	-2.64001
H	-5.53887	-6.32328	-2.90568
H	-3.29973	-5.35343	-3.3608
C	-2.28102	-3.0196	-2.08381
C	-1.24782	-3.44008	-2.92376
C	-0.0592	-2.71135	-2.96746
H	-1.36625	-4.32976	-3.53178
C	-0.99514	-1.20008	-1.36705
C	0.07674	-1.57174	-2.17748
H	0.75291	-3.03589	-3.61083
H	-0.96022	-0.32279	-0.73039
H	0.98714	-0.98108	-2.16019
N	-2.13495	-1.90132	-1.3174
Pt	-3.88282	-1.50324	-0.06032
C	4.71558	-4.44658	2.61318
C	4.13196	-3.34139	1.97533
C	6.10862	-3.04833	0.66655
C	6.71986	-4.1438	1.27977
C	6.0044	-4.83819	2.26003
H	4.16661	-4.98925	3.37365
H	7.72151	-4.45423	1.00829

H	6.46007	-5.69278	2.75073
C	6.7052	-2.19041	-0.38889
C	7.99764	-2.37072	-0.88992
C	8.47809	-1.51227	-1.87611
H	8.62306	-3.17075	-0.51139
C	6.38036	-0.35762	-1.807
C	7.65843	-0.48633	-2.34482
H	9.48101	-1.6435	-2.27022
H	5.69103	0.41885	-2.12368
H	7.99609	0.20427	-3.10967
C	2.80347	-2.75538	2.18383
C	1.88115	-3.26235	3.11366
C	1.22897	-1.01384	1.57916
C	0.63844	-2.65561	3.26896
H	2.13016	-4.13164	3.71746
C	0.31549	-1.52928	2.50331
H	0.97143	-0.13174	1.00412
H	-0.07542	-3.05351	3.98387
H	-0.65395	-1.0509	2.61628
N	5.91533	-1.18391	-0.86002
Pt	3.95022	-1.11605	0.12901
N	-4.42776	-3.17866	-1.06186
C	-5.69381	-1.73816	0.74681
N	4.85914	-2.69096	1.02918
C	2.47817	-1.61161	1.38483