Supporting Information

Pd(II), Ni(II), and Cu(II) complexes of *α*,*α*'-Ditolylmethanone Dipyrroethene

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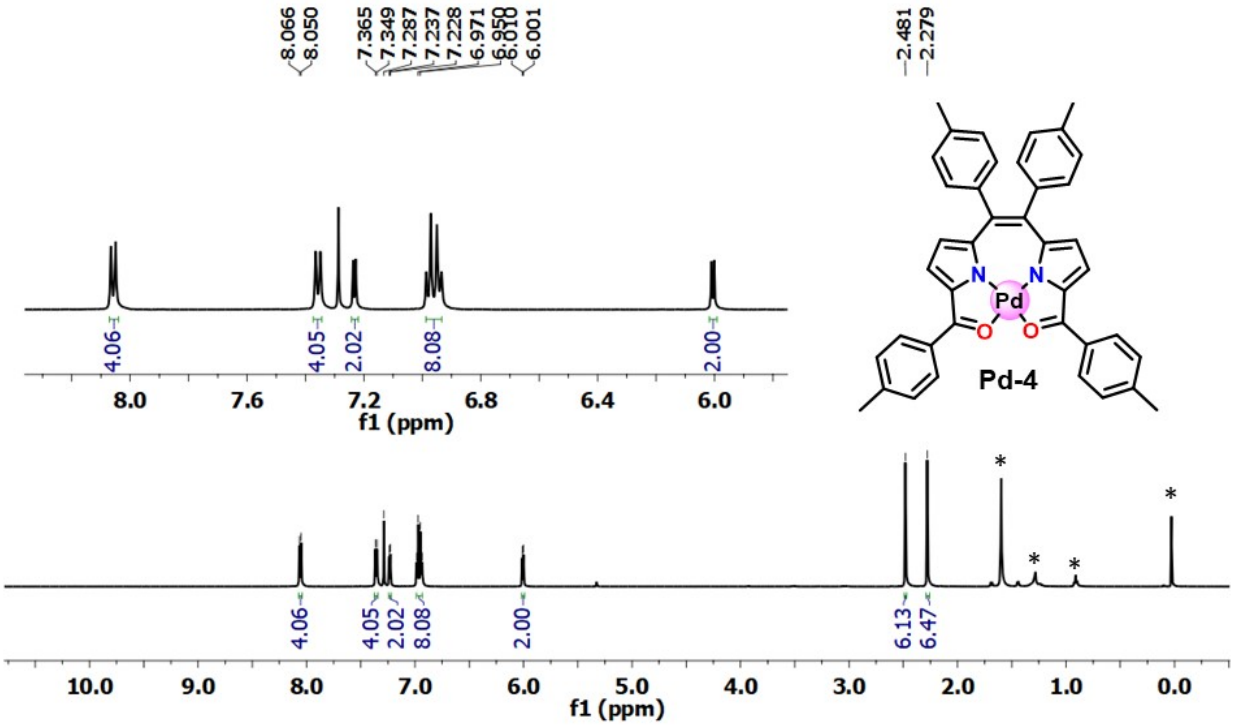

Figure S1. ^{1}H-NMR spectrum of **Pd-4** in $CDCl_3$ at room temperature. Note: Peaks marked with asterisk (*) are due to residual solvents.

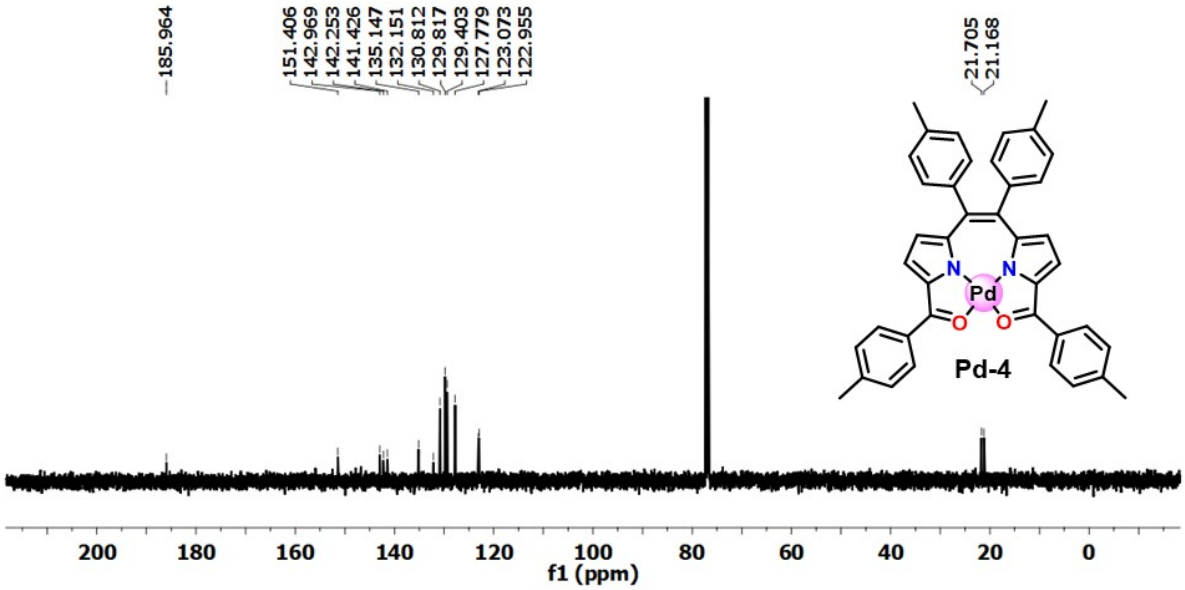

Figure S2. ^{13}C-NMR spectrum of **Pd-4** in $CDCl_3$ at room temperature.

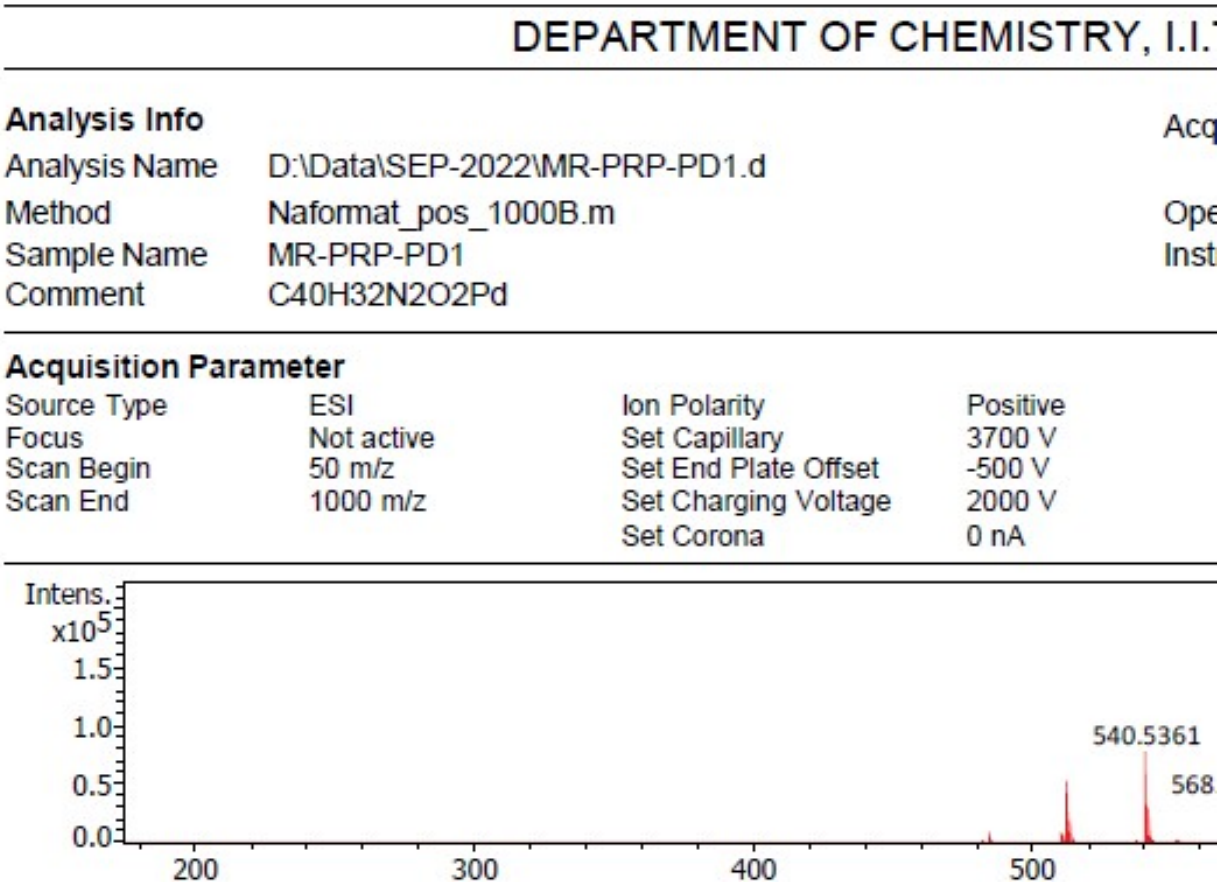

Figure S3. High resolution mass spectrum of **Pd-4**.

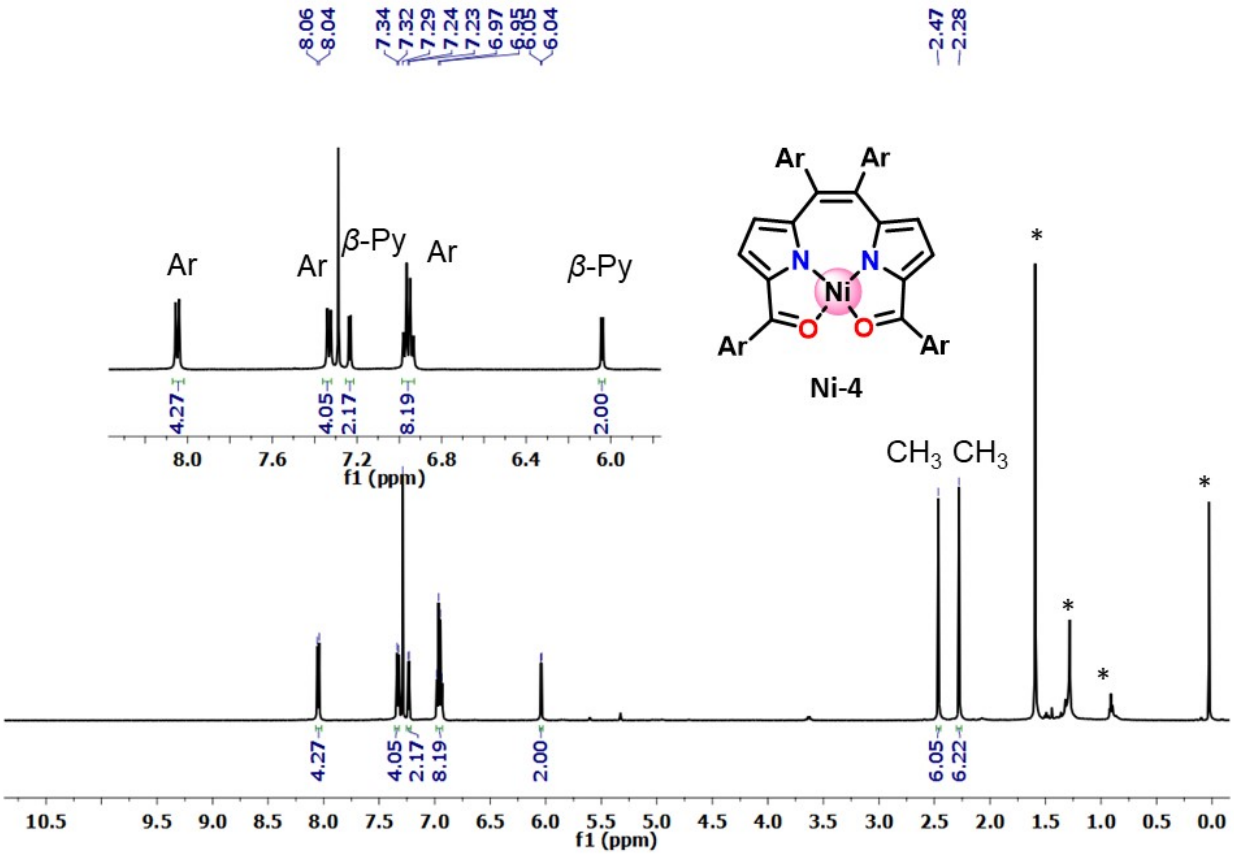

Figure S4. ^{1}H-NMR spectrum of **Ni-4** in $CDCl_3$ at room temperature. Note: Peaks marked with asterisk (*) are due to residual solvents.

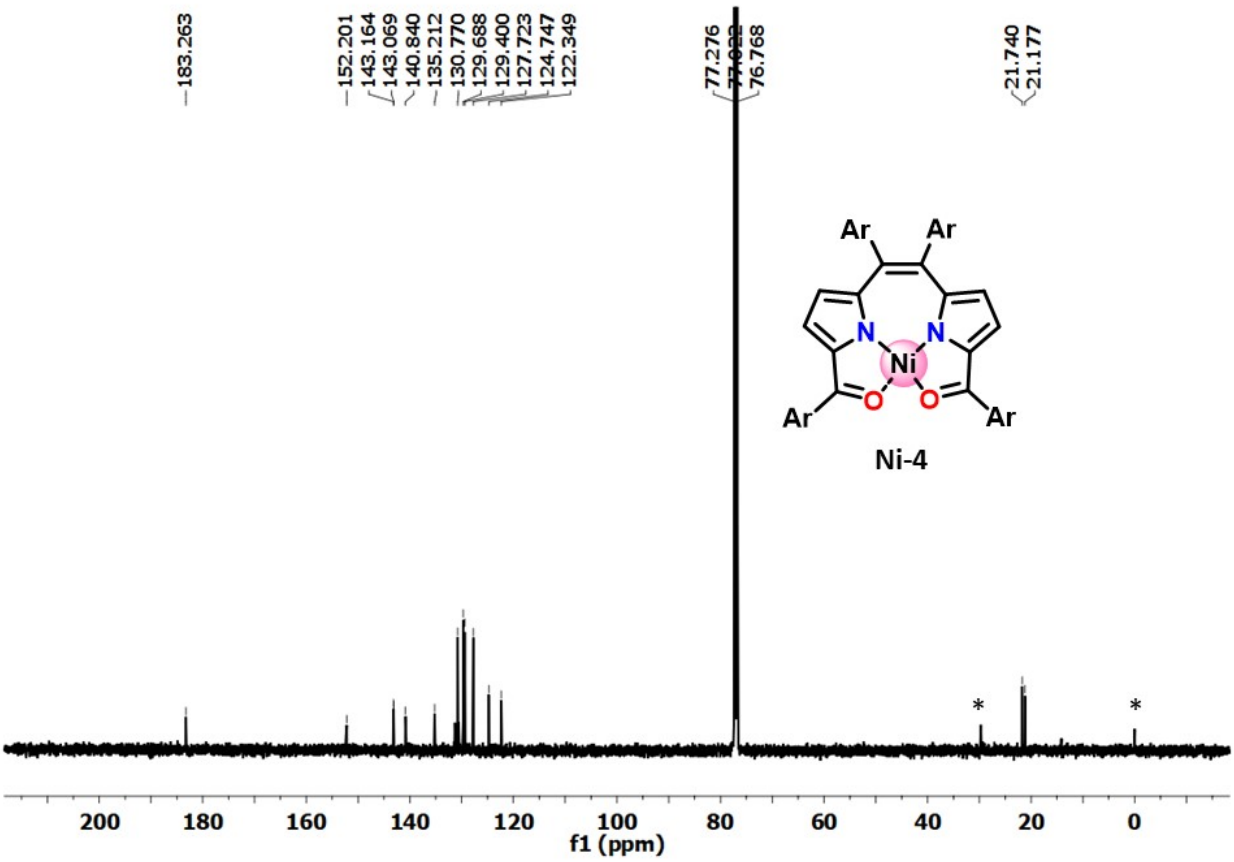

Figure S5. ^{13}C-NMR spectrum of **Ni-4** in $CDCl_3$ on at room temperature.

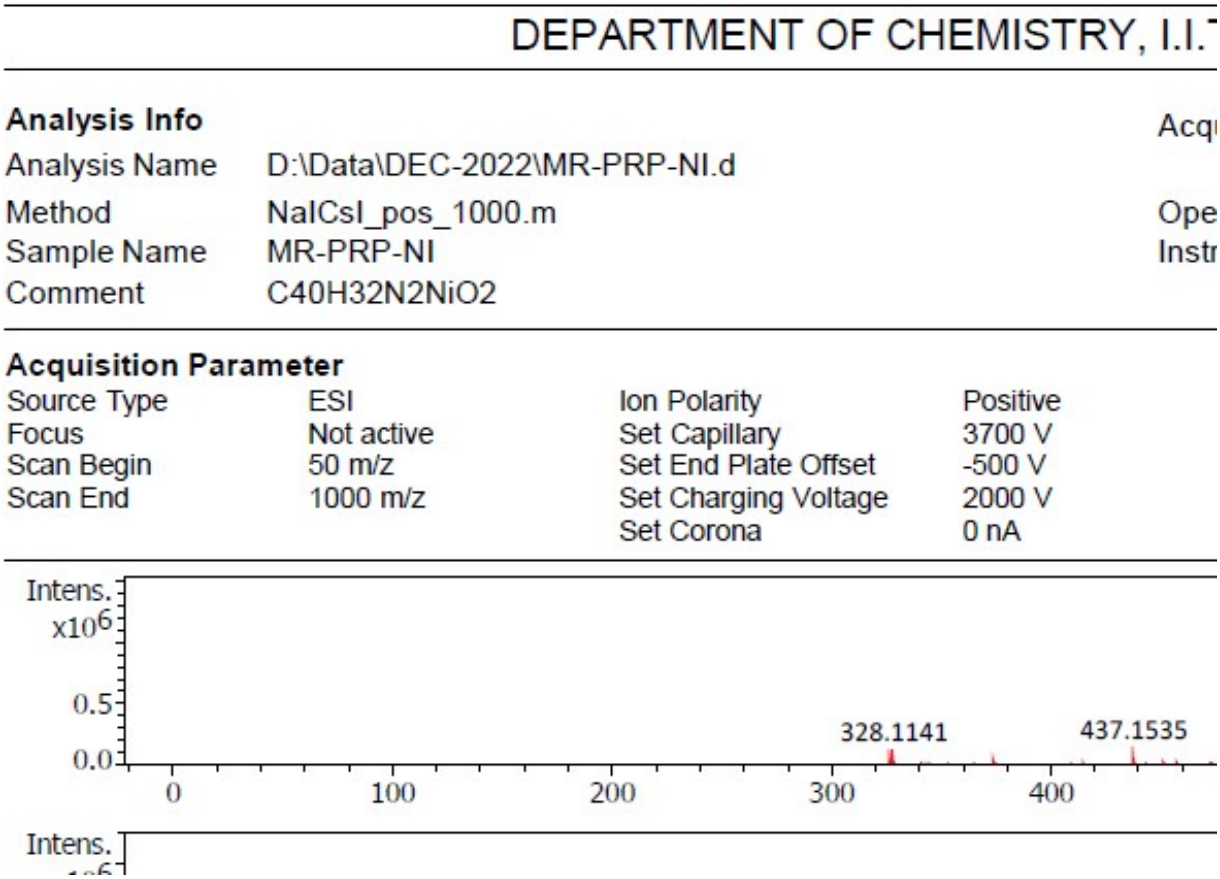

Figure S6. High resolution mass spectrum of **Ni-4**.

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Analysis Info

Analysis Name	D:\Data\NOV-2022\MR-PRP-CU.d
Method	Naformat_pos_1000a.m
Sample Name	MR-PRP-CU
Comment	C40H32N2O2Cu

Acquisition Parameter

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Scan End	1000 m/z	Set Charging Voltage	2000 V
		Set Corona	0 nA

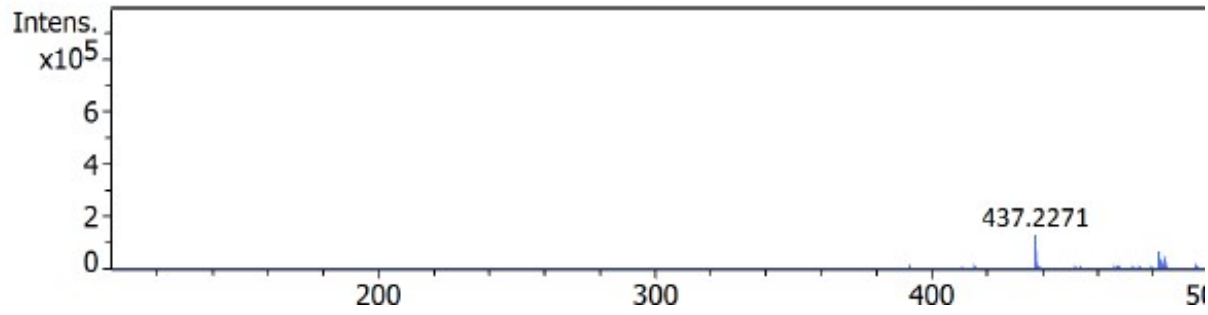


Figure S7. High resolution mass spectrum of **Cu-4**.

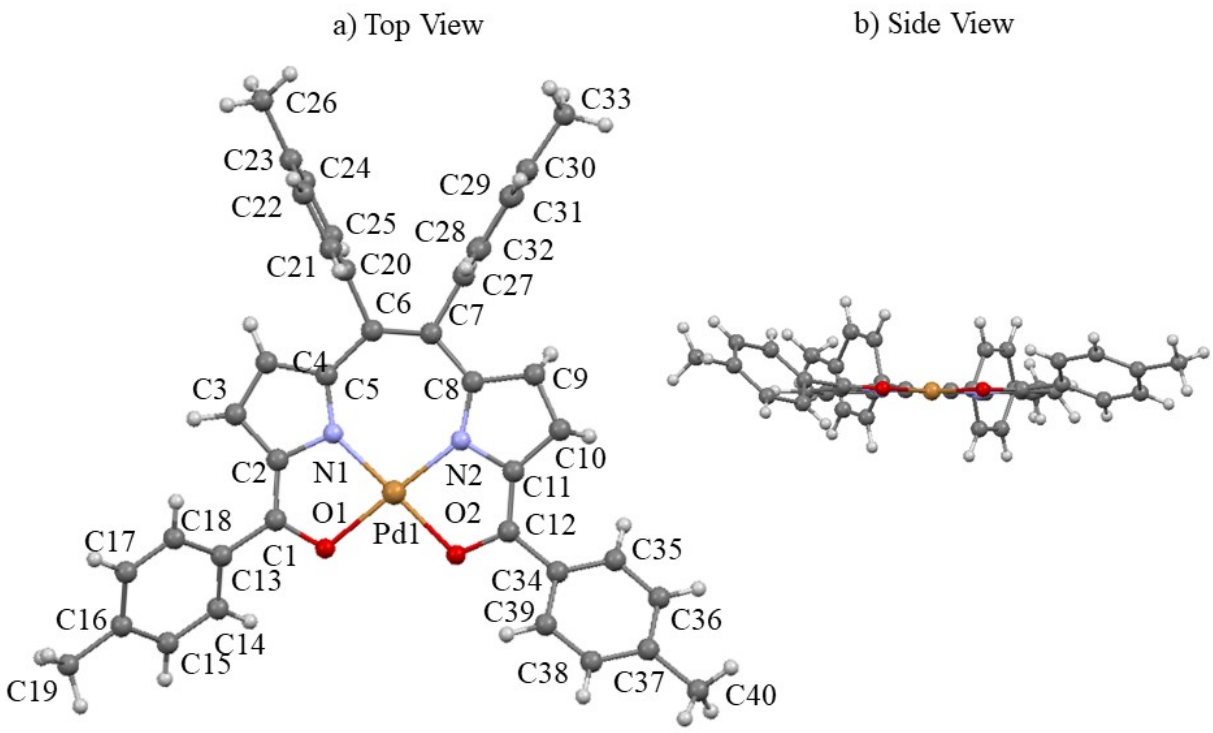


Figure S8. X-ray crystallographic structure (a) Top view and (b) Side view of **Pd-4**.

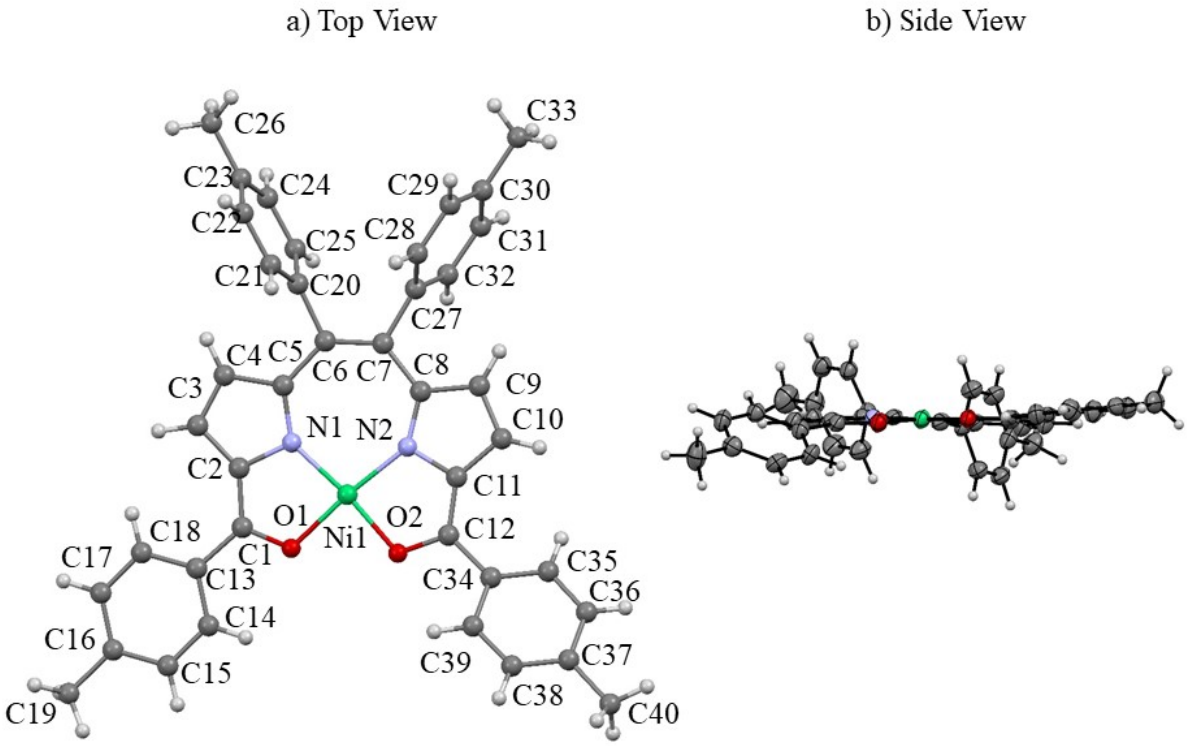


Figure S9. X-ray crystallographic structure (a) Top view and (b) Side view of **Ni-4**.

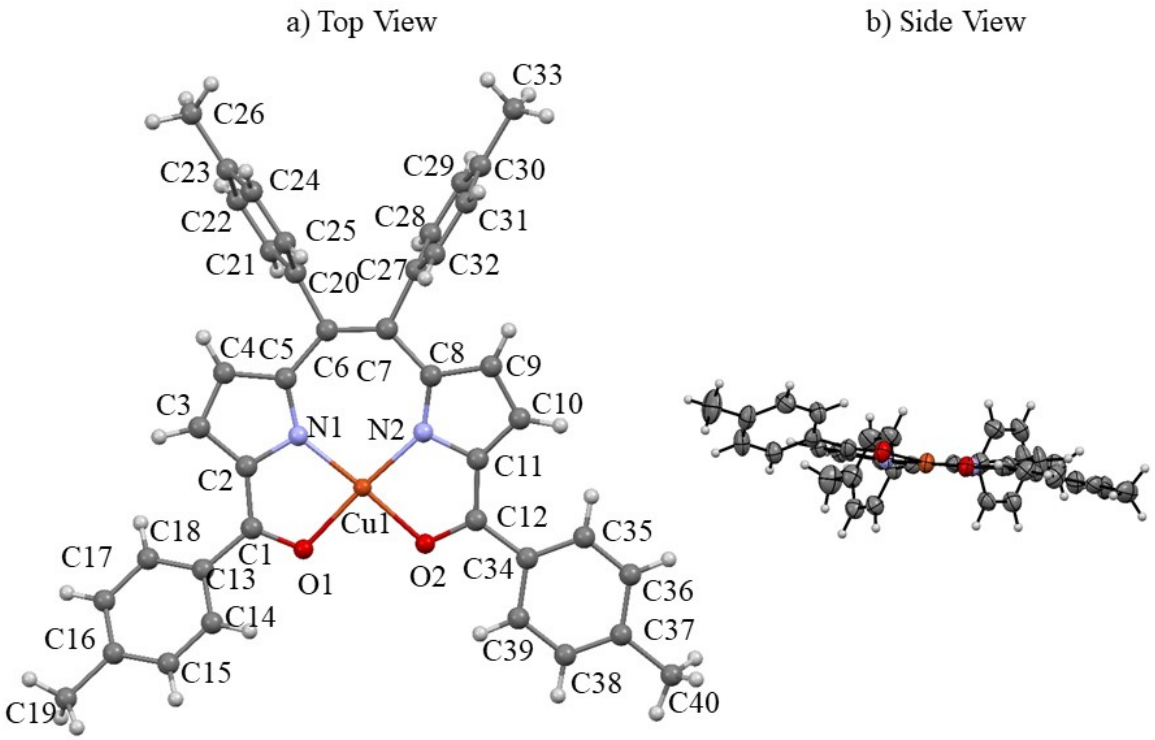


Figure S10. X-ray crystallographic structure (a) Top view and (b) Side view of **Cu-4**.

Table S1. Crystal data and structure refinement for **Pd-4**, **Ni-4** and **Cu-4**.

Compound	**Pd-4**	**Ni-4**	**Cu-4**
Empirical Formula	$C_{40}H_{32}N_2O_2Pd$	$C_{40}H_{32}N_2O_2Ni$	$C_{40}H_{32}N_2O_2Cu$
Crystal System	triclinic	triclinic	triclinic
Space Group	P-1	P-1	P-1
R_1 ($I > 2.00\sigma(I)$)	0.0438	0.0583	0.0637
wR_2 (All reflections)	0.1321	0.1659	0.1850
GOF	1.111	1.029	1.064
a [Å]	11.4482(4)	9.8300(5)	9.694(5)
b [Å]	11.8734(5)	11.2853(6)	11.558(6)
c [Å]	12.9557(5)	14.8021(6)	14.779(8)
α [°]	81.174(4)	96.813(4)	98.82(2)
β [°]	65.549(4)	106.561(4)	103.760(18)
γ [°]	88.541(3)	96.781(4)	97.860(18)
V [Å^3]	1582.72(12)	1542.80(13)	1563.3(14)
Z	2	2	2
T [K]	150	100	150
δ_{calc} [g/cm^3]	1.425	1.359	1.352
F_{000}	696	660.0	662
$2\theta_{max}$ [°]	49.99	50	50
no. reflns measd. (unique)	27860	56131	35132
no. params.	416	410	410
CCDC no.	2196178	2233882	2233881

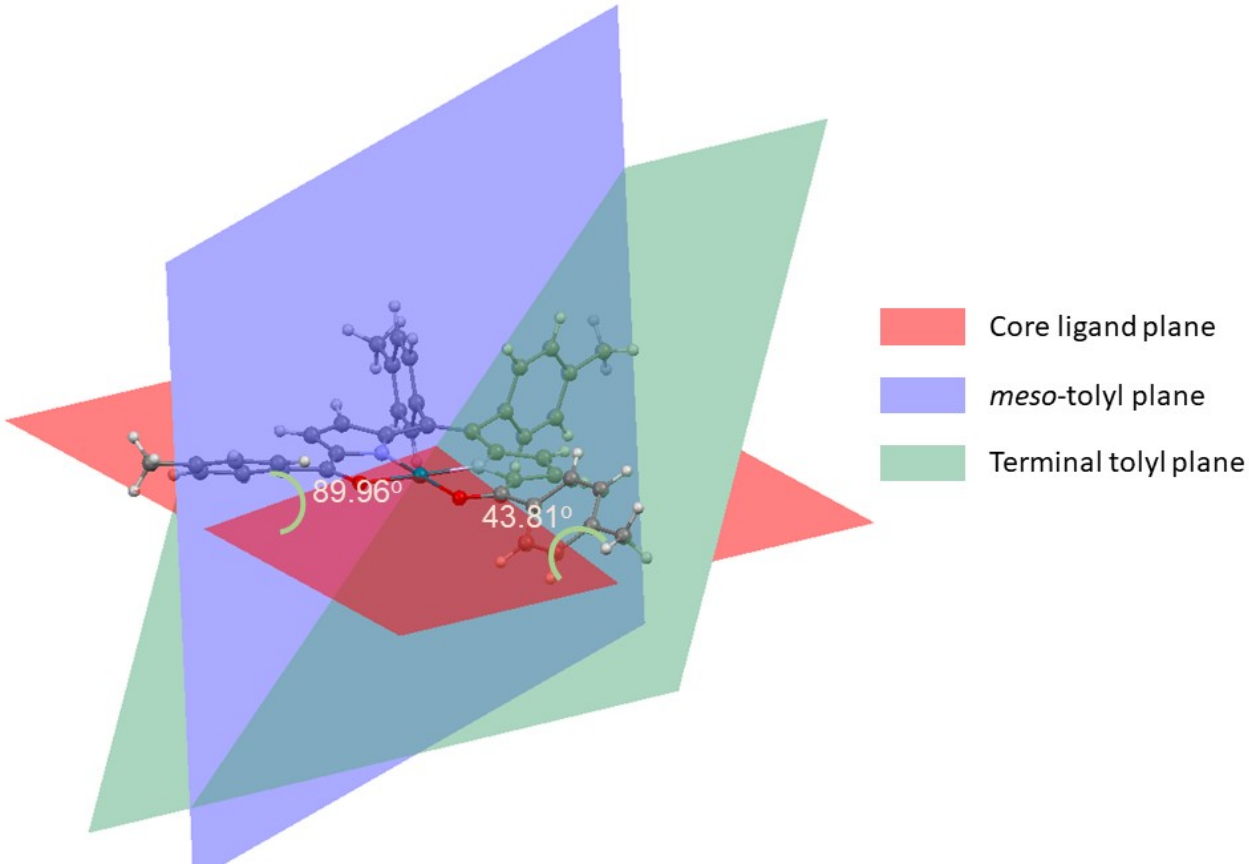


Figure S11. Angle made by the terminal and *meso*-tolyl groups with the ligand plane of **Pd-4**.

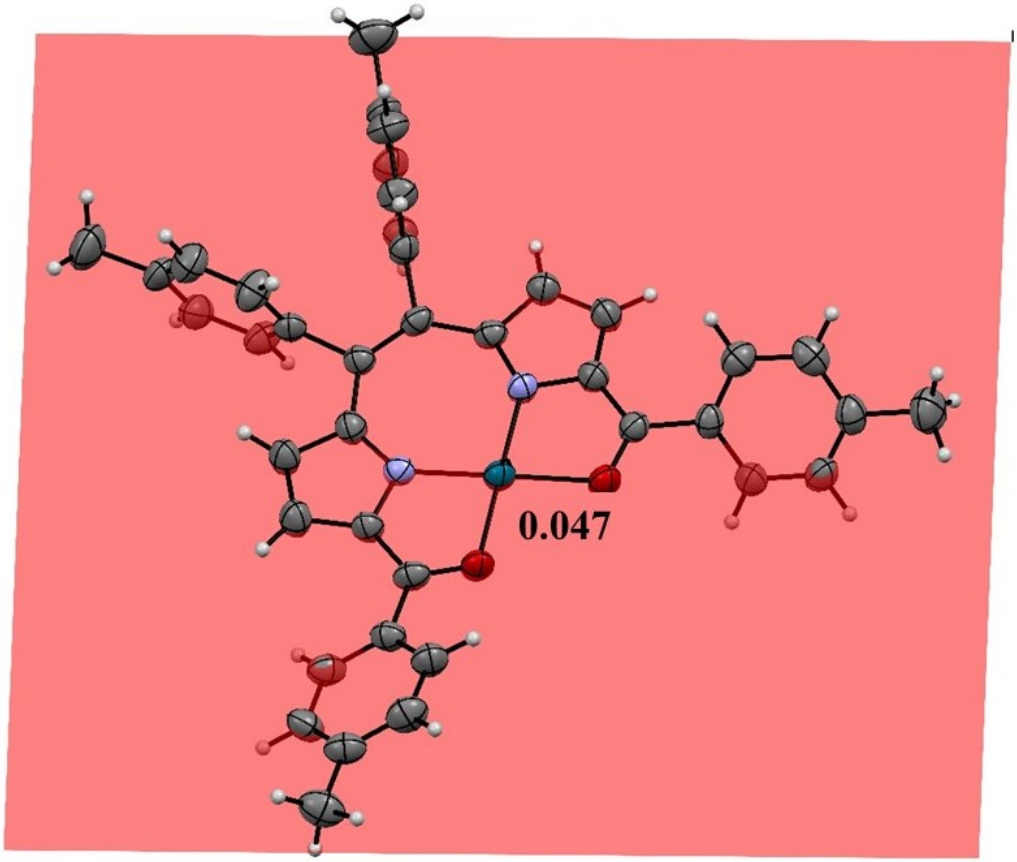


Figure S12. Deviation of Pd atom in **Pd-4** from mean plane constructed by 16 atoms (red plane).

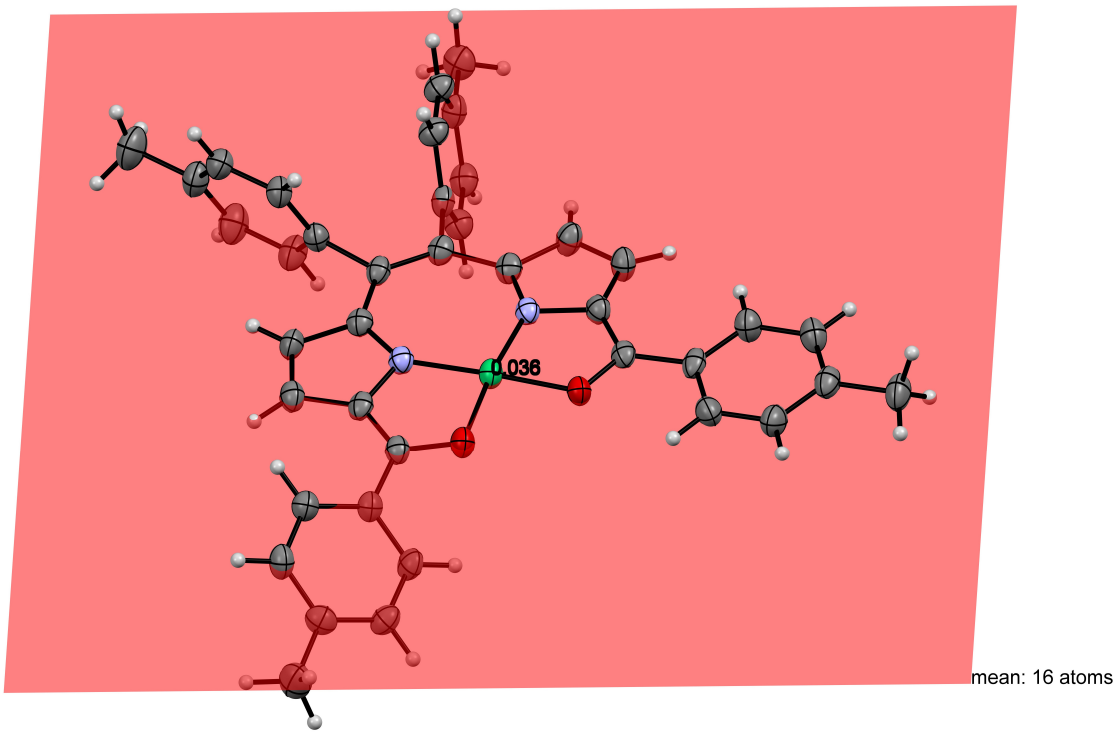


Figure S13. Deviation of Ni atom in **Ni-4** from mean plane constructed by 16 atoms (red plane).

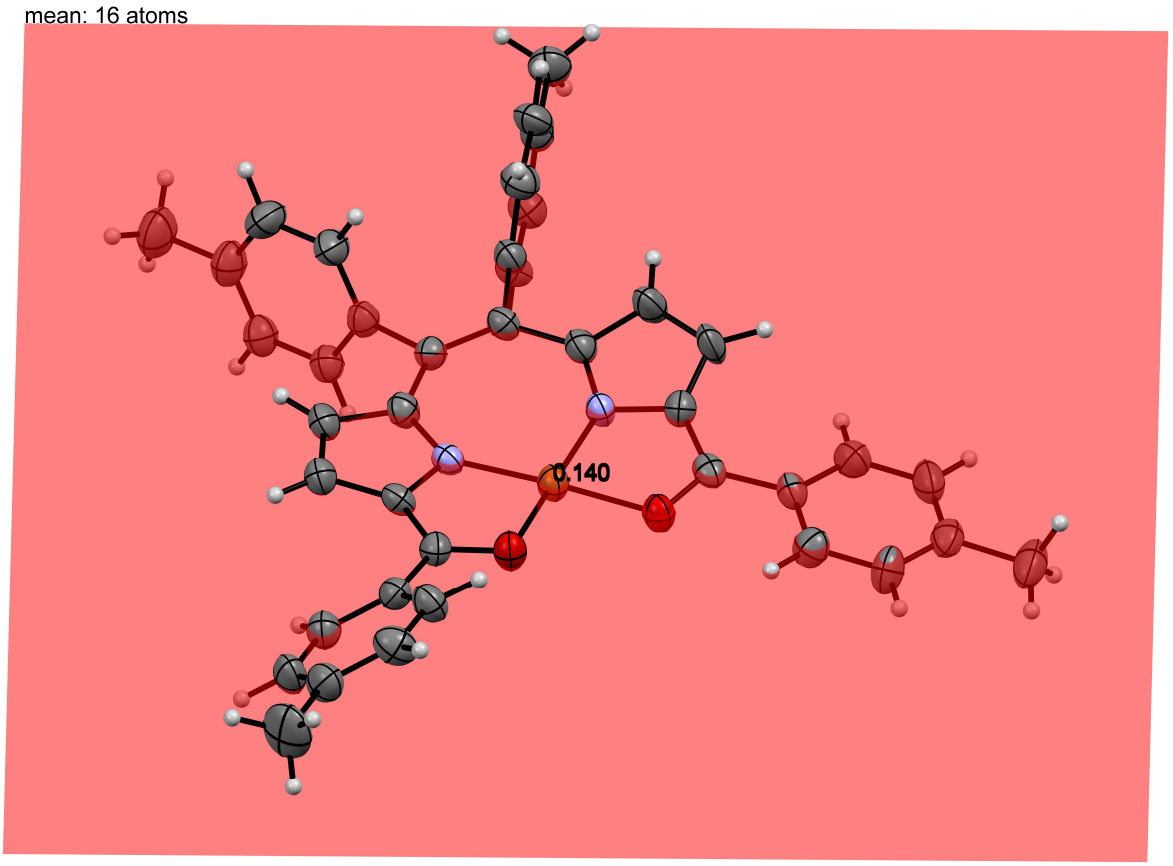


Figure S14. Deviation of Cu atom in **Cu-4** from mean plane constructed by 16 atoms (red plane).

Table S2. Bond Lengths for **Pd-4**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd01	O2	2.031(3)	C34	C39	1.404(7)
Pd01	O1	2.045(3)	C25	C24	1.383(7)
Pd01	N1	1.950(4)	C27	C32	1.384(7)
Pd01	N2	1.955(4)	C27	C28	1.363(7)
O2	C12	1.288(6)	C8	C9	1.434(7)
O1	C1	1.276(6)	C13	C14	1.394(7)
N1	C5	1.348(6)	C13	C18	1.388(7)
N1	C2	1.386(6)	C37	C36	1.390(7)
N2	C11	1.378(6)	C37	C38	1.388(8)
N2	C8	1.336(6)	C37	C40	1.502(7)
C20	C6	1.510(6)	C23	C24	1.386(8)
C20	C25	1.395(7)	C23	C22	1.384(8)
C20	C21	1.386(7)	C23	C26	1.519(7)
C5	C4	1.431(6)	C32	C31	1.406(7)
C5	C6	1.455(6)	C21	C22	1.383(7)
C3	C4	1.362(7)	C39	C38	1.395(7)
C3	C2	1.407(7)	C10	C9	1.372(7)
C1	C2	1.410(7)	C14	C15	1.381(7)
C1	C13	1.482(6)	C31	C30	1.373(8)
C11	C12	1.407(7)	C17	C16	1.387(8)
C11	C10	1.414(7)	C17	C18	1.418(7)
C6	C7	1.382(6)	C30	C29	1.384(8)

C35	C34	1.386(7)	C30	C33	1.529(7)
C35	C36	1.386(7)	C16	C15	1.362(8)
C7	C27	1.515(6)	C16	C19	1.523(8)
C7	C8	1.459(7)	C28	C29	1.383(8)
C34	C12	1.473(6)			

Table S3. Bond angles for **Pd-4**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	Pd01	O1	96.45(13)	C3	C2	C1	135.8(5)
N1	Pd01	O2	177.55(14)	C32	C27	C7	118.4(5)
N1	Pd01	O1	82.50(14)	C28	C27	C7	122.6(4)
N1	Pd01	N2	98.65(16)	C28	C27	C32	119.0(5)
N2	Pd01	O2	82.37(15)	N2	C8	C7	129.5(4)
N2	Pd01	O1	178.48(13)	N2	C8	C9	107.6(4)
C12	O2	Pd01	111.9(3)	C9	C8	C7	122.9(5)
C1	O1	Pd01	110.9(3)	C14	C13	C1	119.7(4)
C5	N1	Pd01	139.5(3)	C18	C13	C1	120.7(5)
C5	N1	C2	108.8(4)	C18	C13	C14	119.6(4)
C2	N1	Pd01	111.7(3)	O2	C12	C11	117.6(4)
C11	N2	Pd01	111.4(3)	O2	C12	C34	117.4(4)
C8	N2	Pd01	138.5(3)	C11	C12	C34	124.9(5)
C8	N2	C11	109.9(4)	C36	C37	C40	120.8(5)
C25	C20	C6	122.6(5)	C38	C37	C36	117.7(5)
C21	C20	C6	119.6(4)	C38	C37	C40	121.6(5)
C21	C20	C25	117.7(5)	C24	C23	C26	122.4(5)
N1	C5	C4	107.3(4)	C22	C23	C24	117.5(5)
N1	C5	C6	128.3(4)	C22	C23	C26	120.1(5)
C4	C5	C6	124.3(4)	C27	C32	C31	119.5(5)
C4	C3	C2	106.6(4)	C25	C24	C23	121.6(5)
O1	C1	C2	119.1(4)	C35	C36	C37	121.4(5)
O1	C1	C13	117.0(4)	C22	C21	C20	121.1(5)
C2	C1	C13	123.9(4)	C38	C39	C34	119.9(5)

C3	C4	C5	108.7(4)	C37	C38	C39	121.7(5)
N2	C11	C12	116.7(4)	C9	C10	C11	107.0(5)
N2	C11	C10	107.8(4)	C15	C14	C13	119.8(5)
C12	C11	C10	135.5(5)	C10	C9	C8	107.7(5)
C5	C6	C20	110.8(4)	C30	C31	C32	120.9(5)
C7	C6	C20	116.6(4)	C16	C17	C18	120.3(5)
C7	C6	C5	132.5(4)	C31	C30	C29	118.7(5)
C34	C35	C36	121.0(5)	C31	C30	C33	120.3(6)
C6	C7	C27	115.9(4)	C29	C30	C33	121.0(6)
C6	C7	C8	132.6(4)	C21	C22	C23	121.4(5)
C8	C7	C27	111.5(4)	C17	C16	C19	119.3(5)
C35	C34	C12	122.9(5)	C15	C16	C17	119.1(5)
C35	C34	C39	118.4(4)	C15	C16	C19	121.6(6)
C39	C34	C12	118.7(5)	C13	C18	C17	119.2(5)
C24	C25	C20	120.7(5)	C16	C15	C14	122.0(5)
N1	C2	C3	108.6(4)	C27	C28	C29	121.7(5)
N1	C2	C1	115.6(4)	C28	C29	C30	120.1(6)

Table S4. Bond Lengths for **Ni-4**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ni1	O1	1.854(2)	C16	C17	1.383(5)
Ni1	O2	1.861(2)	C16	C19	1.505(5)
Ni1	N1	1.822(3)	C17	C18	1.383(5)
Ni1	N2	1.833(3)	C20	C6	1.505(5)
O1	C1	1.280(4)	C20	C21	1.393(4)
O2	C12	1.296(4)	C20	C25	1.395(5)
N1	C2	1.400(4)	C21	C22	1.391(5)
N1	C5	1.372(4)	C22	C23	1.380(5)
N2	C8	1.354(4)	C23	C24	1.394(5)
N2	C11	1.395(4)	C23	C26	1.501(5)
C1	C13	1.477(4)	C25	C24	1.382(5)
C2	C1	1.409(5)	C27	C28	1.379(5)
C2	C3	1.408(5)	C27	C32	1.394(4)
C4	C3	1.357(5)	C28	C29	1.394(5)
C5	C4	1.430(5)	C29	C30	1.394(5)
C5	C6	1.457(5)	C30	C33	1.506(5)
C7	C6	1.378(5)	C31	C30	1.377(5)
C7	C27	1.514(4)	C32	C31	1.391(4)
C8	C7	1.451(5)	C34	C12	1.471(5)
C8	C9	1.427(5)	C34	C35	1.399(5)
C9	C10	1.367(5)	C35	C36	1.386(5)
C10	C11	1.419(5)	C36	C37	1.395(5)
C12	C11	1.393(5)	C37	C40	1.501(5)

C13	C14	1.391(5)	C38	C37	1.385(5)
C13	C18	1.397(5)	C39	C34	1.398(4)
C14	C15	1.384(5)	C39	C38	1.382(5)
C16	C15	1.393(5)			

Table S5. Bond angles for **Ni-4**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ni1	O2	88.61(10)	C11	C12	C34	126.4(3)
N1	Ni1	O1	85.74(11)	C14	C13	C1	119.0(3)
N1	Ni1	O2	173.56(10)	C14	C13	C18	117.1(3)
N1	Ni1	N2	99.25(12)	C18	C13	C1	123.9(3)
N2	Ni1	O1	174.68(11)	C15	C14	C13	121.5(4)
N2	Ni1	O2	86.51(11)	C14	C15	C16	121.2(4)
C1	O1	Ni1	114.1(2)	C15	C16	C19	121.3(4)
C12	O2	Ni1	112.5(2)	C17	C16	C15	117.4(3)
C2	N1	Ni1	112.1(2)	C17	C16	C19	121.3(4)
C5	N1	Ni1	140.2(2)	C18	C17	C16	121.6(4)
C5	N1	C2	107.4(3)	C17	C18	C13	121.2(4)
C8	N2	Ni1	141.5(2)	C21	C20	C6	120.4(3)
C8	N2	C11	107.4(3)	C21	C20	C25	117.2(3)
C11	N2	Ni1	111.0(2)	C25	C20	C6	122.3(3)
O1	C1	C2	115.7(3)	C22	C21	C20	121.7(3)
O1	C1	C13	116.4(3)	C23	C22	C21	120.9(3)
C2	C1	C13	127.9(3)	C22	C23	C24	117.5(3)
N1	C2	C1	112.3(3)	C22	C23	C26	121.6(3)
N1	C2	C3	108.9(3)	C24	C23	C26	120.9(3)
C3	C2	C1	138.7(3)	C25	C24	C23	122.0(3)
C4	C3	C2	107.2(3)	C24	C25	C20	120.6(3)
C3	C4	C5	108.8(3)	C28	C27	C7	121.9(3)
N1	C5	C4	107.7(3)	C28	C27	C32	118.6(3)
N1	C5	C6	128.2(3)	C32	C27	C7	119.3(3)

C4	C5	C6	124.0(3)	C27	C28	C29	120.8(3)
C5	C6	C20	111.0(3)	C30	C29	C28	121.0(3)
C7	C6	C5	131.1(3)	C29	C30	C33	120.5(4)
C7	C6	C20	117.9(3)	C31	C30	C29	117.5(3)
C6	C7	C8	130.9(3)	C31	C30	C33	122.0(3)
C6	C7	C27	118.0(3)	C30	C31	C32	122.2(3)
C8	C7	C27	111.0(3)	C31	C32	C27	119.8(3)
N2	C8	C7	127.9(3)	C35	C34	C12	123.0(3)
N2	C8	C9	108.4(3)	C39	C34	C12	118.5(3)
C9	C8	C7	123.5(3)	C39	C34	C35	118.5(3)
C10	C9	C8	108.9(3)	C36	C35	C34	120.5(3)
C9	C10	C11	105.8(3)	C35	C36	C37	120.8(3)
N2	C11	C10	109.5(3)	C36	C37	C40	121.2(3)
C12	C11	N2	113.5(3)	C38	C37	C36	118.3(3)
C12	C11	C10	136.9(3)	C38	C37	C40	120.5(3)
O2	C12	C11	116.5(3)	C39	C38	C37	121.6(3)
O2	C12	C34	117.0(3)	C38	C39	C34	120.2(3)

Table S6. Bond lengths for **Cu-4**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	O1	1.941(4)	C14	C15	1.521(8)
Cu1	O2	1.955(4)	C14	C16	1.388(8)
Cu1	N1	1.894(4)	C16	C17	1.395(8)
Cu1	N2	1.887(5)	C18	C19	1.421(8)
O1	C22	1.285(6)	C19	C20	1.376(8)
O2	C33	1.285(6)	C20	C21	1.394(8)
N1	C1	1.364(7)	C21	C22	1.431(8)
N1	C32	1.378(7)	C22	C23	1.479(8)
N2	C18	1.359(7)	C23	C24	1.393(8)
N2	C21	1.383(7)	C23	C28	1.396(8)
C1	C2	1.456(8)	C24	C25	1.381(8)
C1	C30	1.424(8)	C25	C26	1.399(9)
C2	C3	1.509(7)	C26	C27	1.366(9)
C2	C10	1.377(7)	C26	C29	1.509(8)
C3	C4	1.388(8)	C27	C28	1.387(8)
C3	C9	1.388(8)	C30	C31	1.369(8)
C4	C5	1.391(8)	C31	C32	1.420(7)
C5	C6	1.390(9)	C32	C33	1.420(8)
C6	C7	1.522(8)	C33	C34	1.466(8)
C6	C8	1.389(9)	C34	C35	1.392(8)
C8	C9	1.396(7)	C34	C40	1.399(8)
C10	C11	1.523(8)	C35	C36	1.372(8)
C10	C18	1.473(7)	C36	C37	1.383(8)

C11	C12	1.389(8)	C37	C38	1.508(9)
C11	C17	1.382(8)	C37	C39	1.388(9)
C12	C13	1.403(8)	C39	C40	1.389(8)
C13	C14	1.389(9)			

Table S7. Bond angles for **Cu-4**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	Cu1	O1	92.00(16)	C17	C16	C14	122.4(6)
N1	Cu1	O1	176.77(18)	C16	C17	C11	120.2(6)
N1	Cu1	O2	85.08(17)	C10	C18	N2	128.1(5)
N2	Cu1	O1	84.71(17)	C19	C18	N2	108.7(5)
N2	Cu1	O2	172.09(17)	C19	C18	C10	123.1(5)
N2	Cu1	N1	98.36(19)	C20	C19	C18	107.4(5)
C22	O1	Cu1	112.2(4)	C21	C20	C19	107.0(5)
C33	O2	Cu1	111.5(4)	C20	C21	N2	109.5(5)
C1	N1	Cu1	141.3(4)	C22	C21	N2	113.7(5)
C32	N1	Cu1	110.7(4)	C22	C21	C20	136.7(5)
C32	N1	C1	107.6(5)	C21	C22	O1	117.0(5)
C18	N2	Cu1	139.3(4)	C23	C22	O1	116.9(5)
C21	N2	Cu1	111.6(4)	C23	C22	C21	126.1(5)
C21	N2	C18	107.4(5)	C24	C23	C22	123.5(5)
C2	C1	N1	127.2(5)	C28	C23	C22	118.8(5)
C30	C1	N1	107.9(5)	C28	C23	C24	117.6(5)
C30	C1	C2	124.9(5)	C25	C24	C23	121.2(6)
C3	C2	C1	110.6(5)	C26	C25	C24	120.9(6)
C10	C2	C1	131.9(5)	C27	C26	C25	117.7(6)
C10	C2	C3	117.4(5)	C29	C26	C25	120.5(6)
C4	C3	C2	121.7(5)	C29	C26	C27	121.7(6)
C9	C3	C2	119.5(5)	C28	C27	C26	122.1(6)
C9	C3	C4	118.6(5)	C27	C28	C23	120.4(6)
C5	C4	C3	121.0(6)	C31	C30	C1	109.1(5)

C6	C5	C4	121.0(6)	C32	C31	C30	105.4(5)
C7	C6	C5	120.6(6)	C31	C32	N1	109.9(5)
C8	C6	C5	117.6(6)	C33	C32	N1	115.5(5)
C8	C6	C7	121.8(6)	C33	C32	C31	134.4(5)
C9	C8	C6	121.8(6)	C32	C33	O2	117.3(5)
C8	C9	C3	120.1(6)	C34	C33	O2	117.6(5)
C11	C10	C2	118.1(5)	C34	C33	C32	125.0(5)
C18	C10	C2	131.4(5)	C35	C34	C33	119.3(5)
C18	C10	C11	110.4(5)	C40	C34	C33	122.5(5)
C12	C11	C10	120.3(5)	C40	C34	C35	118.1(5)
C17	C11	C10	121.0(5)	C36	C35	C34	121.7(5)
C17	C11	C12	118.4(6)	C37	C36	C35	120.8(6)
C13	C12	C11	120.9(6)	C38	C37	C36	120.7(6)
C14	C13	C12	121.1(6)	C39	C37	C36	118.1(6)
C15	C14	C13	121.6(6)	C39	C37	C38	121.2(6)
C16	C14	C13	117.0(6)	C40	C39	C37	121.8(6)
C16	C14	C15	121.4(6)	C39	C40	C34	119.5(6)

Table S8. Electrochemical data of **Pd-4**, **Ni-4**, **Cu-4** and **4** in CH_2Cl_2

Compounds	Oxidation (V)		Reduction (V)
Pd-4	**0.75**	**1.02**	**-1.63**
Ni-4	**0.92**	**-**	**-1.52**
Cu-4	**0.88**	**-**	**--**
4	**0.96**	**1.30**	**-1.75**

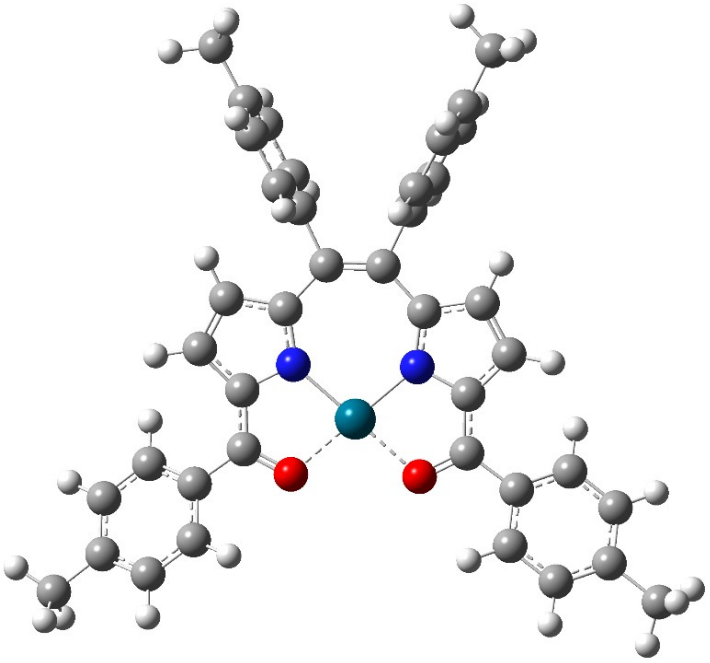


Figure S15. DFT Optimized structure of **Pd-4**.

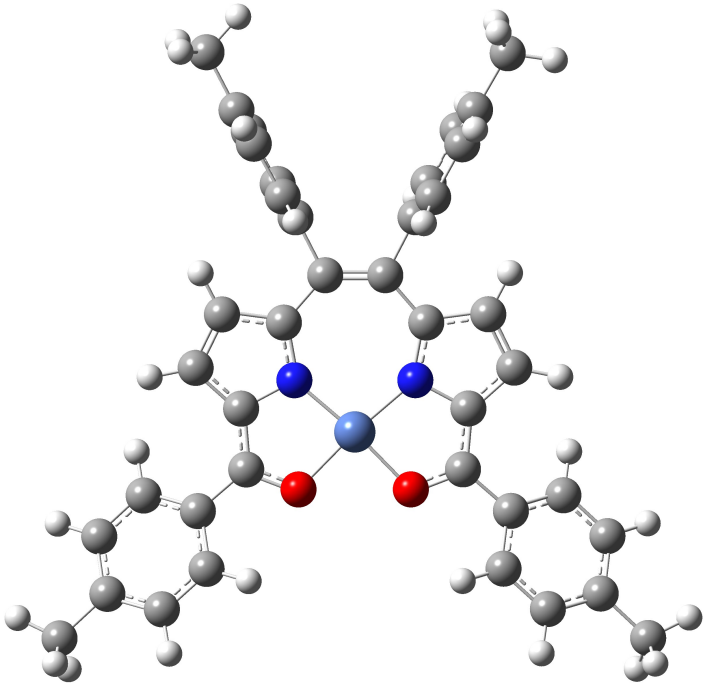


Figure S16. DFT Optimized structure of **Ni-4**.

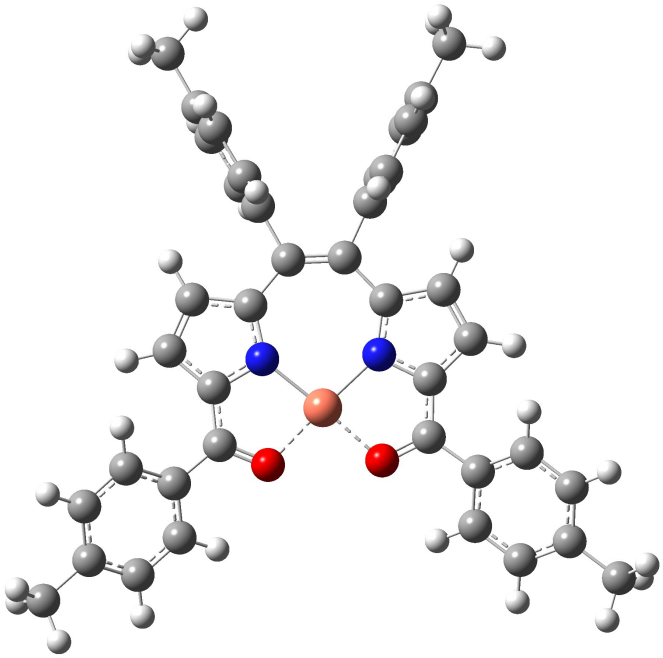


Figure S17. DFT Optimized structure of **Cu-4**.

Table S9. S0 optimized geometry of the compound **Pd-4** at B3LYP/6-31g (d,p)/LANL2DZ level of theory

Sum of imaginary frequencies= 0

Total Energy (hartree) = -1930.318440

Atom	X	Y	Z	Atom	X	Y	Z
O	2.857829	-1.55726	-0.01948	H	0.045776	-4.81097	-0.18647
O	2.856272	1.560046	-0.02467	C	0.85893	-2.73648	-0.011
N	0.223303	1.502194	0.011395	C	2.276919	-2.7026	0.009683
N	0.224651	-1.50176	0.010887	C	3.139928	-3.90193	0.038232
C	-1.12003	1.683808	-0.04865	C	2.75297	-5.09515	0.668873
C	-2.1886	0.686328	-0.0389	H	1.799608	-5.14969	1.182319
C	-3.55179	1.342035	-0.0262	C	3.609833	-6.1929	0.686194
C	-4.21422	1.655855	-1.21989	H	3.299247	-7.10342	1.192292
H	-3.75575	1.393029	-2.16904	C	4.870754	-6.13962	0.076857
C	-5.45204	2.297329	-1.20366	C	5.25842	-4.93744	-0.53504
H	-5.94829	2.523052	-2.14485	H	6.237728	-4.86806	-1.00213
C	-6.06791	2.654744	0.003511	C	4.414735	-3.83301	-0.54924
C	-7.39684	3.373509	0.01524	H	4.725567	-2.90388	-1.01451
H	-7.91076	3.248865	0.972941	C	5.781361	-7.34328	0.065876
H	-8.05907	3.003937	-0.7743	H	5.663221	-7.91681	-0.86223
H	-7.2693	4.451076	-0.14906	H	5.561883	-8.01951	0.897065
C	-5.39907	2.345828	1.19436	H	6.833531	-7.05007	0.132655
H	-5.85331	2.609552	2.146639	C	-1.35259	3.10387	-0.12642
C	-4.15934	1.705676	1.181225	H	-2.32123	3.570474	-0.19433
H	-3.6583	1.48207	2.118912	C	-0.13216	3.747577	-0.11453
C	-2.18791	-0.68858	-0.04037	H	0.040692	4.810703	-0.19465
C	-3.55066	-1.3452	-0.03088	C	0.85628	2.737575	-0.01408
C	-4.20068	-1.67662	-1.22608	C	2.274422	2.705046	0.004124
H	-3.73179	-1.42958	-2.17443	C	3.137201	3.904644	0.030347
C	-5.43519	-2.32562	-1.21298	C	4.409593	3.836392	-0.56263
H	-5.91859	-2.57187	-2.15563	H	4.717454	2.908728	-1.03275
C	-6.06121	-2.66854	-0.00743	C	5.250926	4.942577	-0.55575
C	-7.4142	-3.34049	0.00531	H	6.225274	4.876234	-1.03355
H	-7.54053	-3.97084	0.890917	C	4.865438	6.144418	0.058328
H	-7.55901	-3.9673	-0.88005	C	5.798734	7.330266	0.091653
H	-8.22485	-2.60076	0.015069	H	6.51595	7.243354	0.917628
C	-5.401	-2.34794	1.185826	H	5.252327	8.267445	0.230859
H	-5.85759	-2.61154	2.137083	H	6.379442	7.407916	-0.83271

C	-4.16553	-1.70071	1.175798	C	3.604423	6.199387	0.666958
H	-3.66919	-1.47184	2.114701	H	3.290559	7.113871	1.163864
C	-1.1184	-1.68496	-0.04945	C	2.749748	5.099713	0.656963
C	-1.34941	-3.10548	-0.12383	H	1.794685	5.156958	1.166909
H	-2.31751	-3.57342	-0.19058	Pd	1.503967	0.000729	-0.00313
C	-0.12832	-3.7478	-0.10958				

Table S10. S0 optimized geometry of the compound **Ni-4** at B3LYP/6-31g (d,p) level of theory

Sum of imaginary frequencies= 0

Total Energy (hartree) = -3311.206304

Atom	X	Y	Z
Ni	1.423336	0.00076	0.072213
O	2.752649	-1.290301	0.11464
O	2.749808	1.294829	0.113391
N	0.236	-1.392755	-0.011544
N	0.232947	1.39159	-0.01199
C	-1.104482	1.636426	-0.002777
C	0.895581	-2.615521	-0.015583
C	4.532571	3.422039	0.551254
H	4.760631	2.46904	1.015556
C	2.301979	-2.492619	0.017433
C	-3.544973	-1.385589	0.00969
C	-1.297776	3.062065	0.002838
H	-2.255385	3.556988	0.018359
C	3.263837	3.604893	-0.026132
C	-2.202289	0.688235	0.004583
C	-1.100922	-1.640476	-0.001599
C	2.977593	4.831516	-0.644926
H	2.025912	4.976047	-1.143395
C	3.271584	-3.599543	-0.020285
C	-1.291156	-3.066493	0.010522
H	-2.247648	-3.563497	0.029562
C	-4.176395	-1.722665	1.213156
H	-3.702781	-1.460897	2.154913
C	-3.547675	1.376933	0.013629
C	-2.200767	-0.694652	0.003665
C	2.296582	2.495941	0.013294
C	-0.059544	3.664946	-0.001085
H	0.148368	4.724131	0.03478
C	0.889931	2.615754	-0.020441
C	-5.39862	-2.393635	1.216583
H	-5.867492	-2.643283	2.165481
C	-4.193498	1.712214	-1.182475
H	-3.732061	1.447685	-2.129483
C	-4.167323	-1.757782	-1.188144

H	-3.686317	-1.523696	-2.133525
C	5.469107	4.447335	0.534568
H	6.440126	4.291899	0.998153
C	5.197172	-5.671616	-0.063904
C	4.540624	-3.41255	0.555138
H	4.767119	-2.457994	1.017
C	-0.051604	-3.666684	0.008436
H	0.158683	-4.725238	0.04895
C	-6.030868	-2.754485	0.020212
C	5.479465	-4.435728	0.539478
H	6.450743	-4.277051	1.001423
C	3.926644	5.850328	-0.663595
H	3.689775	6.790563	-1.154541
C	3.938667	-5.844883	-0.653604
H	3.70332	-6.786721	-1.142198
C	5.184783	5.681239	-0.071859
C	-5.420235	2.375187	-1.172037
H	-5.90406	2.616677	-2.115522
C	-5.38993	-2.428277	-1.181365
H	-5.852041	-2.704952	-2.126062
C	-4.161547	1.740362	1.218703
H	-3.67443	1.498325	2.158915
C	2.987318	-4.828178	-0.635966
H	2.03533	-4.975945	-1.1329
C	-7.371136	-3.450983	0.025852
H	-7.492658	-4.079241	0.91354
H	-7.497397	-4.084599	-0.857263
H	-8.195257	-2.726398	0.026115
C	6.234043	-6.767533	-0.097297
H	7.03533	-6.531144	-0.808069
H	5.797674	-7.723806	-0.397725
H	6.704112	-6.901507	0.882567
C	-5.388153	2.40325	1.225762
H	-5.846587	2.666856	2.176
C	-6.039948	2.734334	0.031214
C	6.219194	6.779441	-0.1065
H	6.690735	6.913925	0.872564
H	5.780205	7.734911	-0.405696
H	7.01969	6.545198	-0.818887
C	-7.353437	3.480301	0.040405
H	-7.195259	4.566266	0.043099
H	-7.945608	3.237908	0.928094
H	-7.954846	3.243118	-0.842334

Table S11. S0 optimized geometry of the compound **Cu-4** at B3LYP/6-31g (d,p) level of theory

Sum of imaginary frequencies= 0

Total Energy (hartree) = -3443.326896

Atom	X	Y	Z
Cu	1.504232	0.001291	-0.116041
O	2.856044	-1.397079	-0.149958
O	2.851773	1.403871	-0.150876
N	0.25777	1.433575	-0.011044
N	0.262173	-1.434856	-0.012084
C	-1.078798	1.662081	-0.045532
C	-2.164818	0.687627	-0.032214
C	-3.51493	1.369324	-0.016828
C	-4.174689	1.694034	-1.208227
H	-3.723389	1.422907	-2.158232
C	-5.402117	2.355644	-1.189779
H	-5.896466	2.588974	-2.129873
C	-6.009317	2.723421	0.017187
C	-7.324036	3.467107	0.034794
H	-7.909041	3.225615	0.927515
H	-7.931742	3.226804	-0.842766
H	-7.167979	4.553398	0.033924
C	-5.343713	2.403126	1.207056
H	-5.792119	2.673629	2.160166
C	-4.11575	1.742975	1.191704
H	-3.617499	1.510083	2.128411
C	-2.16269	-0.69653	-0.03279
C	-3.511132	-1.3815	-0.018979
C	-4.1531	-1.735827	-1.211942
H	-3.687019	-1.488735	-2.16145
C	-5.375904	-2.405664	-1.195643
H	-5.852907	-2.668508	-2.136916
C	-5.9985	-2.74835	0.011063
C	-7.339541	-3.443208	0.027165
H	-7.455796	-4.069602	0.916824
H	-7.472551	-4.078457	-0.853874
H	-8.162888	-2.717727	0.031202
C	-5.346946	-2.405486	1.202227
H	-5.801229	-2.668098	2.154732
C	-4.123512	-1.736687	1.18904

H	-3.634327	-1.489809	2.126899
C	-1.073694	-1.667661	-0.044849
C	-1.277488	-3.089456	-0.089005
H	-2.235409	-3.583142	-0.130061
C	-0.037927	-3.697676	-0.084261
H	0.164448	-4.756813	-0.147941
C	0.915567	-2.652096	-0.02721
C	2.335909	-2.564188	-0.043838
C	3.24455	-3.725203	0.025997
C	2.901092	-4.916097	0.685323
H	1.946709	-4.995088	1.193081
C	3.80034	-5.977493	0.738471
H	3.522174	-6.885927	1.266339
C	5.063097	-5.889835	0.137509
C	5.407648	-4.689726	-0.503221
H	6.38751	-4.593359	-0.964034
C	4.520868	-3.621406	-0.552705
H	4.797275	-2.692263	-1.038671
C	6.021319	-7.055183	0.166032
H	5.944617	-7.649367	-0.753245
H	5.813299	-7.724608	1.005386
H	7.059238	-6.718273	0.246868
C	-1.287001	3.083031	-0.09516
H	-2.246444	3.573417	-0.139752
C	-0.049377	3.695215	-0.09109
H	0.149802	4.754737	-0.158471
C	0.907304	2.652824	-0.029613
C	2.327924	2.569434	-0.046182
C	3.23268	3.733522	0.022454
C	4.509751	3.633192	-0.555206
H	4.789607	2.704323	-1.039722
C	5.392922	4.704525	-0.506516
H	6.373436	4.610795	-0.966489
C	5.043893	5.904363	0.132322
C	5.998305	7.072855	0.160058
H	7.037056	6.739508	0.245035
H	5.785676	7.744174	0.996736
H	5.922492	7.663922	-0.761283
C	3.780401	5.988658	0.732194
H	3.498814	6.896907	1.258564
C	2.884757	4.924171	0.679872
H	1.929718	5.000623	1.186789

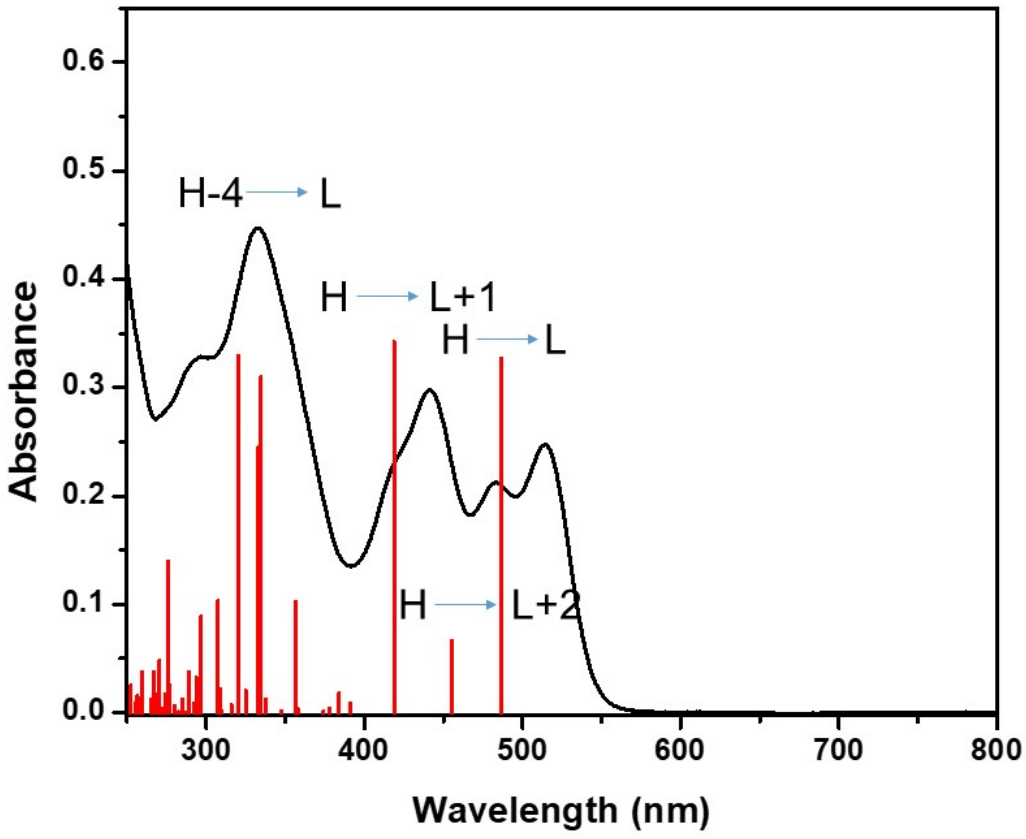


Figure S18. TD-DFT predicted electronic transitions (red sticks) and the normalized experimental UV-Vis absorption spectra (black line) of **Pd-4**.

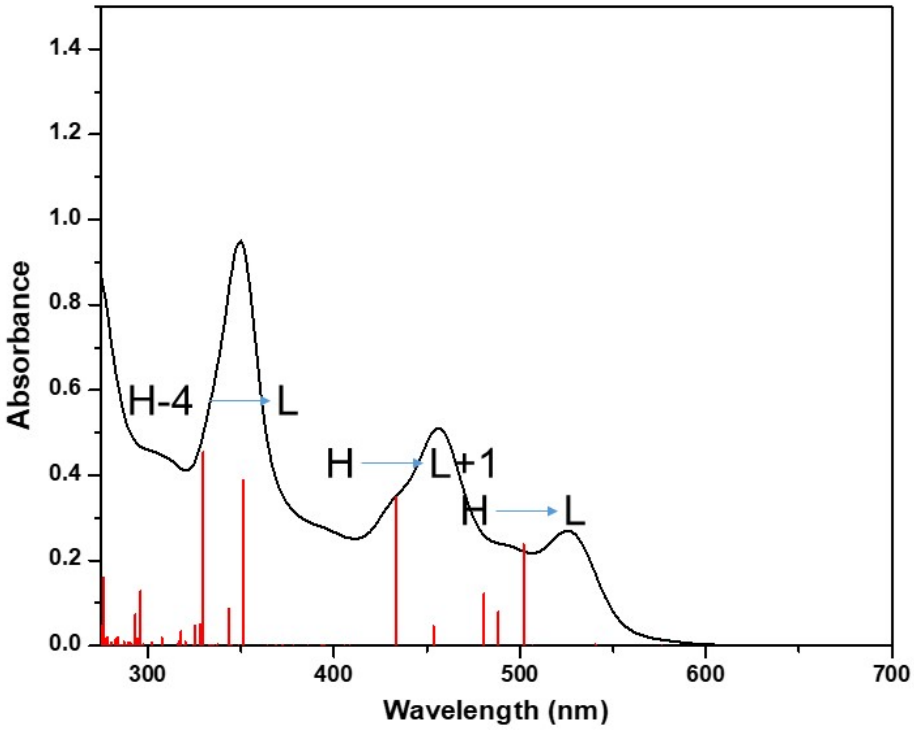


Figure S19. TD-DFT predicted electronic transitions (red sticks) and the experimental UV-Vis absorption spectra (black line) of **Ni-4**.

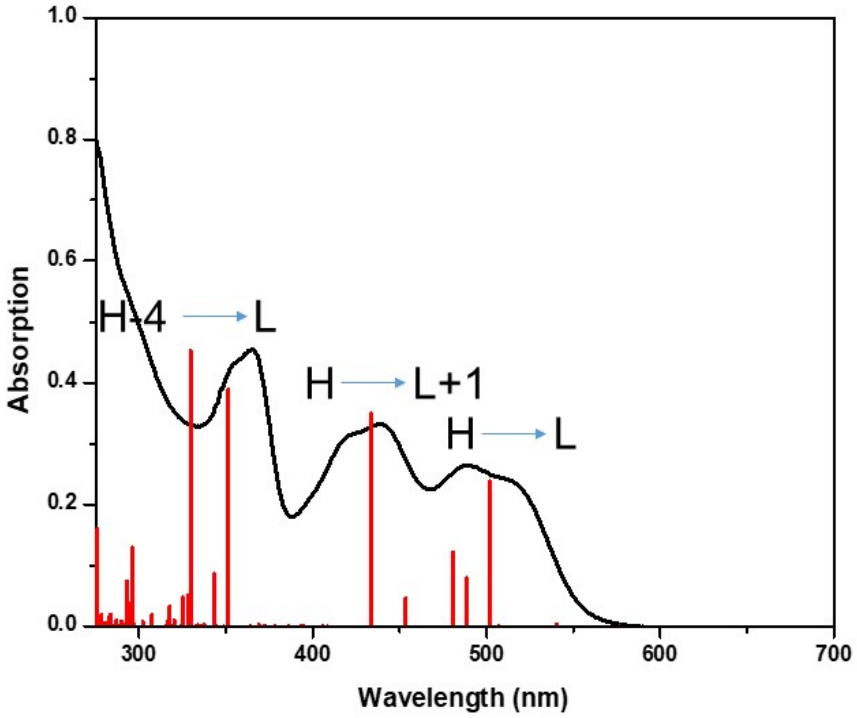


Figure S20. TD-DFT predicted electronic transitions (red sticks) and the normalized experimental UV-Vis absorption spectra (black line) of **Cu-4**.

Table S12. Major and minor transitions calculated using TD-DFT studies of **Pd-4**.

Wavelength (nm)	Osc. Strength	Major contributions	Minor contributions
486.4987	0.3273	HOMO->LUMO (89%)	HOMO->L+2 (9%)
455.4893	0.0666	HOMO->L+2 (90%)	HOMO->LUMO (8%)
418.9504	0.3424	HOMO->L+1 (93%)	H-4->LUMO (5%)
391.2284	0.0089	H-7->L+2 (27%), H-3->LUMO (30%), H-3->L+2 (32%)	H-7->LUMO (2%)
383.852	0.018	H-7->L+2 (31%), H-3->L+2 (48%)	H-17->L+2 (2%), H-14->L+2 (3%), H-10->L+2 (5%), H-7->LUMO (5%), H-3->LUMO (2%)
377.9775	0.0038	H-1->LUMO (96%)	
374.1789	0.0012	H-4->L+2 (26%), H-2->LUMO (17%), H-2->L+2 (43%)	H-16->L+2 (4%), H-15->L+2 (3%), H-4->LUMO (3%), H-1->LUMO (3%)
358.3151	0.0032	H-7->LUMO (25%), H-7->L+2 (10%), H-3->LUMO (53%)	H-10->LUMO (2%), H-3->L+2 (7%)
356.5223	0.1028	H-2->LUMO (72%), H-2->L+2 (10%)	H-15->L+2 (2%), H-4->L+2 (8%), H-3->L+1 (5%)
347.4504	0.0015	H-7->LUMO (61%), H-7->L+2 (21%), H-3->LUMO (11%)	
337.7396	0.0125	H-1->L+1 (95%)	H-2->L+1 (2%)
334.5048	0.3095	H-4->LUMO (72%)	H-4->L+2 (2%), H-3->L+1 (9%), H-2->L+2 (7%), HOMO->L+1 (3%)
332.2904	0.1828	H-3->L+1 (75%)	H-4->LUMO (4%), H-4->L+2 (2%), H-2->LUMO (6%), H-2->L+1 (6%)
332.237	0.2445	H-2->L+1 (79%)	H-4->L+1 (7%), H-3->L+1 (6%), H-1->L+1 (3%)
324.9487	0.0207	H-5->LUMO (18%), H-4->LUMO (10%), H-4->L+2 (34%), H-2->L+2 (18%)	H-8->L+2 (4%), H-5->L+2 (7%), H-1->L+2 (5%)
320.5217	0.3297	H-5->LUMO (77%)	H-4->L+2 (6%), H-2->L+2 (4%), H-1->L+2 (4%)
316.2701	0.0025	H-1->L+2 (86%)	H-6->LUMO (4%), H-4->L+2 (3%), H-2->L+2 (5%)
316.0202	0.0076	H-6->LUMO (89%)	H-7->LUMO (2%), H-1->L+2 (3%)
309.3495	0.0021	H-7->L+1 (91%)	H-6->L+1 (3%)
309.018	0.0217	H-4->L+1 (64%), HOMO->L+3 (20%)	H-13->L+2 (5%), H-2->L+1 (6%)
307.3176	0.1032	H-18->L+2 (17%), H-13->L+2 (50%)	H-14->L+2 (3%), H-13->LUMO (2%), H-10->LUMO (5%), H-6->L+2 (3%), H-4->L+1 (7%)
296.62	0.0888	H-10->LUMO (24%), H-9->LUMO (11%), H-5->L+1 (40%), HOMO->L+3 (13%)	H-4->L+1 (5%)

295.9191	0.0045	H-12->LUMO (20%), H-8->LUMO (67%)	H-11->L+1 (5%)
295.1794	0.0003	H-11->LUMO (36%), H-9->LUMO (42%)	H-12->L+1 (6%), H-10->LUMO (5%), HOMO->L+6 (2%)
293.704	0.0327	H-11->LUMO (24%), H-9->LUMO (42%), H-5->L+1 (13%)	H-12->L+1 (3%), H-10->LUMO (2%), H-4->L+1 (4%), HOMO->L+3 (6%)
292.2295	0.0089	H-12->LUMO (56%), H-8->LUMO (24%)	H-11->L+1 (7%)
289.2637	0.0376	H-11->LUMO (13%), H-10->LUMO (44%), H-5->L+1 (30%)	
287.1733	0.0003	H-6->L+1 (93%)	H-7->L+1 (3%)
284.8967	0.0123	H-5->L+1 (13%), HOMO->L+3 (54%)	H-18->L+2 (5%), H-11->LUMO (3%), H-10->LUMO (7%), H-4->L+1 (8%)
282.2891	0.0006	HOMO->L+4 (91%)	HOMO->L+5 (7%)
280.1586	0.0064	H-5->L+2 (87%)	H-8->L+2 (2%), H-4->L+2 (4%), H-2->L+2 (4%)
277.0906	0.025	HOMO->L+5 (72%), HOMO->L+7 (14%)	H-10->L+1 (3%), H-8->L+2 (2%), HOMO->L+4 (7%)
275.962	0.1398	H-8->L+1 (85%)	H-13->LUMO (4%)
275.6858	0.0038	H-13->LUMO (65%)	H-14->LUMO (7%), H-13->L+2 (2%), H-10->LUMO (2%), H-8->L+1 (4%), H-6->L+2 (4%), HOMO->L+6 (3%)
274.277	0.0175	H-8->L+2 (79%)	H-16->L+2 (2%), H-4->L+2 (8%), HOMO->L+5 (3%)
272.391	0.0003	HOMO->L+6 (75%)	H-13->LUMO (3%), H-12->L+1 (5%), H-11->LUMO (8%)
272.0861	0.0037	H-12->LUMO (11%), HOMO->L+5 (11%), HOMO->L+7 (62%)	H-11->L+1 (7%), H-10->L+1 (3%)
270.903	0.0003	H-6->L+2 (87%)	H-13->LUMO (3%), H-13->L+2 (3%), H-7->L+2 (2%)
270.4775	0.0477	H-9->L+1 (82%)	H-10->L+1 (8%), HOMO->L+7 (5%)
269.133	0.0168	H-10->L+1 (73%), H-9->L+1 (14%)	HOMO->L+7 (4%), HOMO->L+8 (4%)
266.7187	0.0378	H-10->L+2 (63%), H-9->L+2 (17%)	H-14->L+2 (3%), H-13->LUMO (4%), H-7->L+2 (4%)
265.0594	0.0062	H-11->L+1 (74%), HOMO->L+7 (10%)	H-12->LUMO (6%), HOMO->L+5 (3%)
264.9518	0.012	H-12->L+1 (73%), HOMO->L+6 (11%)	H-11->LUMO (7%)
259.5332	0.0373	H-14->LUMO (16%), H-14->L+2 (11%), H-10->L+2 (20%), H-9->L+2 (32%)	H-17->LUMO (2%), H-17->L+2 (5%), H-13->LUMO (4%), H-3->L+2 (6%)
257.6991	0.0134	H-16->LUMO (18%), H-15->LUMO (18%), H-13->L+1 (52%)	H-14->L+1 (3%)
256.5792	0.016	H-14->LUMO (49%), H-9->L+2 (31%)	H-17->LUMO (5%), H-13->LUMO (3%), H-10->L+2 (4%)

255.1745	0.0083	H-12->L+2 (62%), H-11->L+2 (29%)	H-1->L+3 (4%)
255.1168	0.0004	H-1->L+3 (88%)	H-11->L+2 (7%)
255.0905	0.002	H-12->L+2 (33%), H-11->L+2 (58%)	H-1->L+3 (4%)
252.5548	0.0252	HOMO->L+8 (76%)	H-15->LUMO (2%), H-10->L+1 (3%), H-4->L+3 (6%), H-2->L+3 (6%)

Table S13. Major and minor transitions calculated using TD-DFT studies of **Ni-4**.

Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
731.9451739	0.0001	HOMO(A)->LUMO(A) (47%), HOMO(B)->LUMO(B) (45%)	
576.4293692	0	HOMO(A)->L+1(A) (44%), HOMO(B)->L+1(B) (44%)	H-3(A)->LUMO(A) (4%), H-2(B)->LUMO(B) (4%)
540.5894616	0.0035	H-16(B)->L+2(B) (37%), H-4(B)->L+2(B) (31%), HOMO(B)->L+2(B) (11%)	H-13(B)->L+2(B) (9%), H-4(B)->LUMO(B) (2%)
506.7611911	0	H-17(B)->L+2(B) (49%), H-3(B)->L+2(B) (24%)	H-1(A)->LUMO(A) (7%), H-17(B)->LUMO(B) (2%), H-7(B)->L+2(B) (4%), H-5(B)->L+2(B) (4%), H-2(B)->L+2(B) (3%)
501.8587048	0.2387	HOMO(A)->LUMO(A) (28%), HOMO(B)->LUMO(B) (32%), HOMO(B)->L+2(B) (29%)	H-16(B)->L+2(B) (4%), H-4(B)->L+2(B) (4%)
488.3767007	0.0787	H-14(B)->L+2(B) (14%), H-12(B)->L+2(B) (27%), HOMO(B)->L+2(B) (33%)	HOMO(A)->LUMO(A) (7%), H-16(B)->L+2(B) (2%), H-13(B)->L+2(B) (2%), HOMO(B)->LUMO(B) (7%)
480.5588876	0.1211	HOMO(A)->LUMO(A) (10%), H-14(B)->L+2(B) (32%), H-12(B)->L+2(B) (15%), HOMO(B)->LUMO(B) (10%), HOMO(B)->L+2(B) (24%)	H-19(B)->L+2(B) (4%)
453.6394315	0.0015	H-1(A)->LUMO(A) (87%)	H-17(B)->L+2(B) (4%), H-3(B)->L+2(B) (2%)
453.5564567	0.0451	H-23(B)->L+2(B) (25%), H-19(B)->L+2(B) (36%), H-12(B)->L+2(B) (11%)	H-1(A)->LUMO(A) (3%), HOMO(A)->LUMO(A) (2%), H-32(B)->L+2(B) (3%), H-16(B)->L+2(B) (3%), H-14(B)->L+2(B) (5%), HOMO(B)->LUMO(B) (2%), HOMO(B)->L+2(B) (2%)
433.480851	0.3488	HOMO(A)->L+1(A) (47%), HOMO(B)->L+1(B) (45%)	H-3(A)->LUMO(A) (2%), H-2(B)->LUMO(B) (2%)
408.5550236	0	H-5(A)->LUMO(A) (16%), H-4(B)->LUMO(B) (22%)	H-7(A)->LUMO(A) (2%), H-6(A)->L+1(A) (3%), H-4(A)->L+1(A) (2%), H-3(A)->L+1(A) (7%), H-1(A)->L+1(A) (4%), HOMO(A)->L+2(A) (9%), H-3(B)->L+1(B) (4%), H-2(B)->L+1(B) (8%), HOMO(B)->L+3(B) (9%)
405.826955	0.0001	H-3(A)->LUMO(A) (34%), H-2(B)->LUMO(B) (35%)	H-8(A)->LUMO(A) (2%), H-6(A)->LUMO(A) (4%), H-5(A)->L+1(A) (2%), HOMO(A)->L+1(A) (3%), H-7(B)->LUMO(B) (2%), H-5(B)->LUMO(B) (2%), H-4(B)->L+1(B) (3%), H-3(B)->LUMO(B) (2%), HOMO(B)->L+1(B) (3%)

394.8666932	0	H-1(A)->L+1(A) (63%)	H-10(A)->LUMO(A) (3%), H-3(A)->L+1(A) (3%), HOMO(A)->L+2(A) (5%), H-9(B)->LUMO(B) (3%), H-7(B)->L+1(B) (2%), H-2(B)->L+1(B) (3%), HOMO(B)->L+3(B) (5%)
393.4382414	0.0011	H-4(A)->LUMO(A) (23%), H-3(B)->LUMO(B) (33%)	H-6(A)->LUMO(A) (6%), H-5(A)->L+1(A) (7%), H-3(A)->LUMO(A) (6%), HOMO(A)->L+1(A) (2%), H-4(B)->L+1(B) (9%), H-2(B)->LUMO(B) (3%), HOMO(B)->L+1(B) (2%)
385.7868972	0	H-1(A)->L+1(A) (27%), H-4(B)->LUMO(B) (12%)	H-8(A)->L+1(A) (3%), H-5(A)->LUMO(A) (9%), H-4(A)->L+1(A) (4%), H-3(A)->L+1(A) (4%), HOMO(A)->L+2(A) (7%), H-9(B)->LUMO(B) (2%), H-7(B)->L+1(B) (3%), H-3(B)->L+1(B) (4%), H-2(B)->L+1(B) (3%), HOMO(B)->L+3(B) (7%)
378.4621276	0	H-8(A)->LUMO(A) (21%), H-7(B)->LUMO(B) (21%)	H-12(A)->L+4(A) (2%), H-11(A)->L+3(A) (2%), H-10(A)->L+1(A) (8%), H-9(A)->L+1(A) (2%), H-8(A)->L+2(A) (2%), H-5(A)->L+1(A) (2%), H-11(B)->L+5(B) (2%), H-10(B)->L+4(B) (2%), H-9(B)->L+1(B) (8%), H-8(B)->L+1(B) (3%), H-7(B)->L+3(B) (2%), H-4(B)->L+1(B) (2%)
372.4926934	0.0007	H-2(A)->LUMO(A) (94%)	H-1(B)->LUMO(B) (3%)
368.9786114	0.002	H-1(B)->LUMO(B) (94%)	H-2(A)->LUMO(A) (3%)
364.2629874	0.0001	H-8(A)->L+1(A) (10%), H-7(B)->L+1(B) (10%), H-3(B)->L+1(B) (13%)	H-13(A)->LUMO(A) (2%), H-10(A)->LUMO(A) (9%), H-9(A)->LUMO(A) (2%), H-6(A)->L+1(A) (2%), H-4(A)->L+1(A) (7%), H-3(A)->L+1(A) (6%), HOMO(A)->L+2(A) (2%), H-13(B)->LUMO(B) (2%), H-9(B)->LUMO(B) (9%), H-8(B)->LUMO(B) (2%), H-2(B)->L+1(B) (4%), HOMO(B)->L+3(B) (2%)
351.4191577	0.3881	H-3(A)->LUMO(A) (33%), H-2(B)->LUMO(B) (34%), H-2(B)->L+2(B) (19%)	H-4(A)->LUMO(A) (2%)
348.8581683	0.0001	H-3(A)->L+1(A) (11%), H-2(A)->L+6(A) (10%), H-2(B)->L+1(B) (11%), H-1(B)->L+7(B) (10%)	H-9(A)->L+8(A) (2%), H-7(A)->L+9(A) (4%), H-6(A)->L+5(A) (2%), H-2(A)->L+5(A) (3%), HOMO(A)->L+2(A) (7%), H-8(B)->L+9(B) (2%), H-6(B)->L+10(B) (4%), H-5(B)->L+6(B) (3%), H-1(B)->L+6(B) (3%), HOMO(B)->L+3(B) (7%)
344.7644542	0.0002	H-3(A)->L+1(A) (11%), HOMO(A)->L+2(A) (11%), H-	H-7(A)->L+9(A) (3%), H-4(A)->L+1(A) (2%), H-2(A)->L+5(A) (3%),

		2(B)->L+1(B) (11%), HOMO(B)->L+3(B) (11%)	H-2(A)->L+6(A) (7%), HOMO(A)->LUMO(A) (2%), H-6(B)->L+10(B) (3%), H-5(B)->L+1(B) (2%), H-5(B)->L+6(B) (2%), H-1(B)->L+6(B) (2%), H-1(B)->L+7(B) (7%), HOMO(B)->LUMO(B) (2%)
343.3228838	0.0857	H-2(B)->L+2(B) (63%)	H-4(A)->LUMO(A) (5%), H-3(A)->LUMO(A) (7%), H-7(B)->L+2(B) (5%), H-5(B)->L+2(B) (2%), H-3(B)->LUMO(B) (2%), H-2(B)->LUMO(B) (9%)
337.5464676	0.0032	H-4(A)->L+1(A) (13%), H-4(B)->LUMO(B) (29%), H-3(B)->L+1(B) (19%)	H-10(A)->LUMO(A) (2%), H-6(A)->L+1(A) (5%), H-5(A)->L+2(A) (2%), H-2(A)->L+1(A) (3%), H-9(B)->LUMO(B) (3%), H-4(B)->L+3(B) (3%), H-2(B)->L+1(B) (4%), H-1(B)->L+1(B) (3%)
335.4187669	0.0004	H-2(A)->L+9(A) (13%), H-1(B)->L+10(B) (13%)	H-9(A)->L+3(A) (2%), H-9(A)->L+5(A) (3%), H-9(A)->L+6(A) (2%), H-7(A)->L+5(A) (3%), H-7(A)->L+6(A) (7%), H-6(A)->LUMO(A) (3%), H-6(A)->L+8(A) (3%), H-5(A)->L+6(A) (2%), H-4(A)->L+8(A) (2%), H-2(A)->L+1(A) (2%), H-8(B)->L+4(B) (2%), H-8(B)->L+6(B) (3%), H-8(B)->L+7(B) (2%), H-6(B)->L+6(B) (3%), H-6(B)->L+7(B) (9%), H-5(B)->LUMO(B) (3%), H-5(B)->L+9(B) (5%)
334.5950425	0.0004	H-2(A)->L+1(A) (56%), H-1(B)->L+1(B) (27%)	H-2(B)->L+1(B) (3%)
333.9011985	0.0017	H-5(A)->LUMO(A) (31%), H-4(B)->LUMO(B) (14%), H-1(B)->L+1(B) (22%)	H-10(A)->LUMO(A) (2%), H-3(A)->L+1(A) (6%), H-2(A)->L+1(A) (8%), H-3(B)->L+1(B) (5%), H-2(B)->L+1(B) (7%)
332.593468	0	H-5(A)->LUMO(A) (14%), H-2(A)->L+1(A) (25%), H-1(B)->L+1(B) (42%)	H-7(A)->LUMO(A) (3%), H-4(B)->LUMO(B) (6%), H-3(B)->L+1(B) (2%), H-2(B)->L+1(B) (3%)
329.8153677	0.4529	H-4(A)->LUMO(A) (19%), H-3(B)->LUMO(B) (49%)	H-6(A)->LUMO(A) (8%), H-5(A)->L+1(A) (4%), H-3(A)->LUMO(A) (5%), HOMO(A)->L+1(A) (2%), H-2(B)->LUMO(B) (3%)
328.1220373	0.0495	H-5(A)->L+1(A) (11%), H-4(A)->LUMO(A) (21%), H-4(B)->L+1(B) (39%)	H-10(A)->L+1(A) (3%), H-6(A)->LUMO(A) (2%), H-9(B)->L+1(B) (3%), H-3(B)->LUMO(B) (2%), H-3(B)->L+3(B) (2%), H-2(B)->LUMO(B) (2%), H-2(B)->L+3(B) (2%)
325.3153679	0.0476	H-5(A)->LUMO(A) (13%), H-3(A)->L+1(A) (39%), H-2(B)-	H-6(A)->L+1(A) (3%), H-4(A)->L+1(A) (2%), H-4(B)->LUMO(B)

		>L+1(B) (32%)	(5%)
324.6169372	0.0008	H-12(A)->L+1(A) (15%), H-11(A)->LUMO(A) (29%), H-11(B)->L+1(B) (14%), H-10(B)->LUMO(B) (24%)	H-11(A)->L+2(A) (2%), H-10(B)->L+3(B) (2%)
324.5404628	0.0006	H-12(A)->LUMO(A) (30%), H-11(A)->L+1(A) (15%), H-11(B)->LUMO(B) (26%), H-10(B)->L+1(B) (14%)	H-12(A)->L+2(A) (2%), H-11(B)->L+3(B) (2%)
320.1823025	0.008	H-6(A)->LUMO(A) (60%), H-4(A)->LUMO(A) (17%)	H-3(A)->LUMO(A) (2%), H-5(B)->LUMO(B) (6%), H-4(B)->L+1(B) (2%)
319.3658055	0.0005	H-7(A)->LUMO(A) (79%)	H-5(A)->LUMO(A) (6%), H-2(A)->L+1(A) (2%), H-6(B)->LUMO(B) (7%)
317.6719696	0.0324	H-6(B)->LUMO(B) (10%), H-5(B)->LUMO(B) (73%)	H-6(A)->LUMO(A) (6%), H-4(A)->LUMO(A) (3%), H-3(B)->LUMO(B) (2%)
316.8601115	0.0089	H-6(B)->LUMO(B) (77%)	H-7(A)->LUMO(A) (8%), H-5(B)->LUMO(B) (8%)
315.9557427	0.0024	H-1(B)->L+2(B) (95%)	H-5(B)->LUMO(B) (2%), H-2(B)->L+2(B) (2%)
307.5386159	0.004	H-4(A)->L+1(A) (26%), HOMO(A)->L+2(A) (16%), H-3(B)->L+1(B) (27%), HOMO(B)->L+3(B) (15%)	H-6(A)->L+1(A) (7%)
307.4471025	0.018	H-5(A)->L+1(A) (50%), H-4(B)->L+1(B) (33%)	H-10(A)->L+1(A) (2%), H-7(A)->L+1(A) (4%), H-6(A)->LUMO(A) (2%)
302.1646349	0.0065	H-17(B)->L+2(B) (15%), H-7(B)->L+2(B) (10%), H-3(B)->L+2(B) (59%)	H-7(B)->LUMO(B) (6%)
297.3384647	0.0023	H-9(A)->LUMO(A) (47%), H-6(A)->L+1(A) (12%), H-8(B)->LUMO(B) (11%)	H-10(A)->LUMO(A) (7%), H-4(A)->L+1(A) (4%), H-2(A)->L+6(A) (2%), H-5(B)->L+1(B) (6%), H-1(B)->L+7(B) (2%)
296.081655	0.1291	H-10(A)->LUMO(A) (13%), H-9(A)->LUMO(A) (10%), H-9(B)->LUMO(B) (18%), H-8(B)->LUMO(B) (10%)	H-11(A)->LUMO(A) (6%), H-8(A)->L+1(A) (2%), H-6(A)->L+1(A) (2%), HOMO(A)->L+2(A) (2%), H-16(B)->L+2(B) (2%), H-12(B)->LUMO(B) (3%), H-10(B)->LUMO(B) (6%), H-5(B)->L+1(B) (2%), H-4(B)->L+2(B) (5%), HOMO(B)->L+3(B) (2%)
295.5804916	0.011	H-7(B)->LUMO(B) (13%)	H-12(A)->LUMO(A) (2%), H-12(A)->L+4(A) (5%), H-11(A)->L+3(A) (4%), H-10(A)->LUMO(A) (2%), H-9(A)->LUMO(A) (2%), H-8(A)->LUMO(A) (7%), HOMO(A)->L+3(A) (5%), HOMO(A)->L+7(A) (2%), H-17(B)->L+2(B) (3%), H-

			11(B)->L+5(B) (5%), H-10(B)->L+4(B) (4%), H-8(B)->LUMO(B) (5%), H-5(B)->L+1(B) (5%), H-4(B)->L+2(B) (2%), H-3(B)->L+2(B) (6%), HOMO(B)->L+4(B) (3%), HOMO(B)->L+6(B) (2%), HOMO(B)->L+8(B) (2%)
295.5452624	0.0383	H-8(B)->LUMO(B) (18%), H-5(B)->L+1(B) (15%)	H-12(A)->L+4(A) (2%), H-10(A)->LUMO(A) (5%), H-9(A)->LUMO(A) (6%), H-8(A)->LUMO(A) (2%), H-6(A)->L+1(A) (3%), HOMO(A)->L+2(A) (4%), H-16(B)->L+2(B) (2%), H-9(B)->LUMO(B) (5%), H-7(B)->LUMO(B) (4%), H-4(B)->L+2(B) (6%), H-3(B)->L+2(B) (2%), HOMO(B)->L+3(B) (4%)
294.7022724	0.0166	H-12(A)->LUMO(A) (17%), H-8(A)->LUMO(A) (26%), H-11(B)->LUMO(B) (21%), H-7(B)->LUMO(B) (13%)	H-11(A)->L+1(A) (3%), HOMO(A)->L+5(A) (2%), H-10(B)->L+1(B) (4%), HOMO(B)->L+4(B) (3%)
293.9616213	0.0079	H-16(B)->L+2(B) (16%), H-4(B)->L+2(B) (35%)	H-11(A)->LUMO(A) (5%), H-9(A)->LUMO(A) (4%), H-13(B)->L+2(B) (4%), H-10(B)->LUMO(B) (6%), H-9(B)->L+2(B) (4%), H-8(B)->LUMO(B) (5%), H-5(B)->L+1(B) (7%)
293.238554	0.0737	H-11(A)->LUMO(A) (17%), H-9(A)->LUMO(A) (13%), H-6(A)->L+1(A) (10%), H-10(B)->LUMO(B) (14%)	H-12(A)->L+1(A) (2%), H-3(A)->L+1(A) (2%), HOMO(A)->L+2(A) (7%), HOMO(A)->L+4(A) (4%), H-11(B)->L+1(B) (3%), H-9(B)->LUMO(B) (2%), H-8(B)->LUMO(B) (8%), H-3(B)->L+1(B) (4%), HOMO(B)->L+3(B) (5%), HOMO(B)->L+5(B) (2%)
292.8160999	0.0002	H-10(A)->LUMO(A) (18%), H-9(B)->LUMO(B) (15%)	H-12(A)->L+3(A) (5%), H-12(A)->L+5(A) (2%), H-11(A)->L+4(A) (7%), H-6(A)->L+1(A) (3%), H-5(A)->LUMO(A) (2%), H-13(B)->LUMO(B) (2%), H-12(B)->LUMO(B) (2%), H-11(B)->L+4(B) (6%), H-11(B)->L+6(B) (2%), H-10(B)->LUMO(B) (5%), H-10(B)->L+5(B) (7%), HOMO(B)->L+5(B) (3%)
292.4431385	0.0003	H-7(A)->L+1(A) (24%), H-8(B)->LUMO(B) (11%), H-6(B)->L+1(B) (24%)	H-9(A)->LUMO(A) (2%), H-6(A)->L+1(A) (8%), H-5(A)->L+1(A) (3%), H-4(A)->L+1(A) (4%), H-5(B)->L+1(B) (7%)
292.1468296	0.0001	H-7(A)->L+1(A) (18%), H-6(A)->L+1(A) (12%), H-8(B)-	H-9(A)->LUMO(A) (5%), H-4(A)->L+1(A) (6%), H-5(B)->L+1(B) (9%)

		>LUMO(B) (16%), H-6(B)->L+1(B) (17%)	
290.7355915	0.0039	H-12(A)->LUMO(A) (15%), H-8(A)->LUMO(A) (24%), H-11(B)->LUMO(B) (15%), H-7(B)->LUMO(B) (23%)	H-11(A)->L+1(A) (2%), HOMO(A)->L+3(A) (6%), H-10(B)->L+1(B) (2%), HOMO(B)->L+4(B) (4%)
290.0554287	0.0071	H-7(A)->L+1(A) (18%), H-6(A)->L+1(A) (11%), H-6(B)->L+1(B) (21%), H-5(B)->L+1(B) (22%)	H-10(A)->LUMO(A) (3%), H-5(A)->L+1(A) (2%), H-4(A)->L+1(A) (7%), H-9(B)->LUMO(B) (4%), H-3(B)->L+1(B) (2%)
289.560916	0.0068	H-7(A)->L+1(A) (25%), H-6(B)->L+1(B) (28%), H-5(B)->L+1(B) (14%)	H-10(A)->LUMO(A) (4%), H-6(A)->L+1(A) (6%), H-5(A)->L+1(A) (2%), H-4(A)->L+1(A) (6%), H-9(B)->LUMO(B) (5%)
288.2682934	0.0001	HOMO(A)->L+5(A) (15%), HOMO(A)->L+6(A) (17%), HOMO(B)->L+6(B) (24%), HOMO(B)->L+7(B) (33%)	H-7(A)->L+1(A) (2%), HOMO(B)->L+4(B) (2%)
287.5862707	0.0019	HOMO(A)->L+4(A) (11%), HOMO(B)->L+3(B) (12%), HOMO(B)->L+5(B) (11%)	H-11(A)->LUMO(A) (9%), H-10(A)->LUMO(A) (3%), H-4(A)->L+1(A) (4%), HOMO(A)->L+2(A) (7%), H-12(B)->LUMO(B) (9%), H-10(B)->LUMO(B) (3%), H-9(B)->LUMO(B) (6%), H-4(B)->L+2(B) (2%), H-3(B)->L+1(B) (4%)
287.0735442	0.0087	HOMO(A)->L+4(A) (25%), HOMO(B)->L+5(B) (25%)	H-10(A)->LUMO(A) (9%), H-4(A)->L+1(A) (2%), HOMO(A)->L+2(A) (6%), HOMO(A)->L+6(A) (2%), H-10(B)->LUMO(B) (6%), HOMO(B)->L+3(B) (2%)
286.967233	0.0002	HOMO(A)->L+3(A) (31%), HOMO(B)->L+4(B) (38%)	H-8(A)->LUMO(A) (2%), H-8(A)->L+4(A) (2%), HOMO(A)->L+5(A) (4%), H-7(B)->L+5(B) (2%), HOMO(B)->L+6(B) (3%)
286.3574682	0.001	HOMO(A)->L+5(A) (20%), HOMO(A)->L+6(A) (35%), HOMO(B)->L+7(B) (25%)	HOMO(B)->L+6(B) (9%)
285.414809	0.0002	HOMO(A)->L+5(A) (15%), HOMO(A)->L+6(A) (21%), HOMO(B)->L+6(B) (25%), HOMO(B)->L+7(B) (22%)	
283.7166888	0.0185	H-12(B)->LUMO(B) (49%)	H-14(A)->LUMO(A) (5%), H-12(A)->L+3(A) (2%), H-11(A)->L+4(A) (2%), H-10(A)->LUMO(A) (2%), H-15(B)->L+1(B) (6%), H-14(B)->LUMO(B) (2%), H-11(B)->L+4(B) (2%), H-10(B)->L+5(B) (2%), H-9(B)->LUMO(B) (4%), H-7(B)->L+1(B) (2%), HOMO(B)->L+5(B) (6%)
282.5142255	0.0148	HOMO(A)->L+3(A) (19%), HOMO(A)->L+5(A) (18%), HOMO(A)->L+6(A) (16%), HOMO(B)->L+4(B) (15%), HOMO(B)->L+6(B) (14%), HOMO(B)->L+7(B) (11%)	

280.3423168	0.0054	H-7(B)->L+1(B) (26%)	H-13(A)->LUMO(A) (4%), H-12(A)->L+3(A) (5%), H-11(A)->L+4(A) (6%), H-8(A)->L+1(A) (9%), H-13(B)->LUMO(B) (2%), H-12(B)->LUMO(B) (2%), H-11(B)->L+4(B) (5%), H-10(B)->L+5(B) (6%), H-9(B)->LUMO(B) (6%), H-8(B)->LUMO(B) (2%)
279.9372161	0.0001	H-2(A)->L+5(A) (14%), H-1(B)->L+6(B) (14%)	H-7(A)->L+8(A) (4%), H-2(A)->L+3(A) (7%), H-2(A)->L+6(A) (7%), H-2(A)->L+7(A) (2%), H-12(B)->LUMO(B) (2%), H-7(B)->L+1(B) (2%), H-6(B)->L+9(B) (4%), H-5(B)->L+2(B) (8%), H-5(B)->L+7(B) (2%), H-1(B)->L+4(B) (7%), H-1(B)->L+7(B) (6%)
279.8045474	0.0005	H-5(B)->L+2(B) (75%)	H-2(A)->L+5(A) (2%), H-7(B)->L+2(B) (5%), H-3(B)->L+2(B) (2%), H-2(B)->L+2(B) (5%), H-1(B)->L+6(B) (2%)
278.8166614	0.0007	H-10(A)->L+1(A) (13%), H-9(B)->L+1(B) (20%)	H-12(A)->L+4(A) (6%), H-11(A)->L+3(A) (4%), H-9(A)->L+1(A) (4%), H-8(A)->LUMO(A) (5%), H-1(A)->L+2(A) (2%), H-15(B)->LUMO(B) (3%), H-12(B)->L+1(B) (3%), H-11(B)->L+5(B) (6%), H-10(B)->L+4(B) (4%), H-8(B)->L+1(B) (7%), H-7(B)->LUMO(B) (6%), H-5(B)->L+2(B) (2%)
278.1785798	0.018	HOMO(A)->L+3(A) (24%), HOMO(A)->L+5(A) (15%), HOMO(B)->L+4(B) (23%), HOMO(B)->L+6(B) (14%)	H-12(A)->LUMO(A) (7%), HOMO(A)->L+6(A) (3%), H-11(B)->LUMO(B) (8%), HOMO(B)->L+7(B) (3%)
278.0351019	0.0043	HOMO(A)->L+4(A) (41%), HOMO(B)->L+5(B) (36%)	H-11(A)->LUMO(A) (6%), H-10(B)->LUMO(B) (6%), H-6(B)->L+2(B) (4%)
276.9606242	0.0167	H-6(B)->L+2(B) (88%)	HOMO(B)->L+5(B) (2%)
276.1033137	0.1601	H-8(A)->L+1(A) (24%), H-7(B)->L+1(B) (35%)	H-13(A)->LUMO(A) (5%), H-13(B)->LUMO(B) (8%), H-9(B)->LUMO(B) (3%), H-9(B)->L+2(B) (2%), H-6(B)->L+2(B) (3%), HOMO(B)->L+3(B) (2%), HOMO(B)->L+11(B) (2%)
276.0418413	0.0036	H-1(A)->L+2(A) (11%), H-15(B)->LUMO(B) (24%), H-12(B)->L+1(B) (16%)	H-15(A)->LUMO(A) (7%), H-14(A)->L+1(A) (4%), H-12(A)->L+4(A) (2%), H-11(A)->L+3(A) (2%), H-10(A)->L+1(A) (2%), HOMO(A)->L+7(A) (3%), H-14(B)->L+1(B) (2%), H-11(B)->L+5(B) (2%), H-10(B)->L+4(B) (2%), H-5(B)->L+2(B) (2%), HOMO(B)->L+8(B) (3%)

274.422738	0.0499	H-13(A)->LUMO(A) (12%), H-8(A)->L+1(A) (35%), H-13(B)->LUMO(B) (11%)	H-10(A)->LUMO(A) (4%), HOMO(A)->L+2(A) (2%), HOMO(A)->L+8(A) (3%), HOMO(A)->L+10(A) (2%), HOMO(B)->L+3(B) (2%), HOMO(B)->L+9(B) (2%)
273.8106336	0.0008	H-9(A)->L+1(A) (27%), H-9(B)->L+1(B) (10%), H-8(B)->L+1(B) (21%)	H-10(A)->L+1(A) (9%), H-7(A)->L+6(A) (2%), H-2(A)->L+9(A) (3%), HOMO(A)->L+7(A) (2%), H-6(B)->L+7(B) (2%), H-1(B)->L+10(B) (3%), HOMO(B)->L+8(B) (2%)
272.7384963	0.0005	HOMO(A)->L+7(A) (19%), HOMO(B)->L+8(B) (20%)	H-10(A)->L+1(A) (2%), H-9(A)->L+1(A) (7%), H-3(A)->L+2(A) (7%), H-1(A)->L+2(A) (3%), H-15(B)->LUMO(B) (3%), H-8(B)->L+1(B) (6%), H-2(B)->L+3(B) (7%)
272.6785129	0.0004		H-13(A)->LUMO(A) (3%), H-9(A)->L+8(A) (4%), H-8(A)->L+1(A) (3%), H-6(A)->L+3(A) (2%), H-6(A)->L+5(A) (4%), H-6(A)->L+6(A) (2%), H-4(A)->L+1(A) (2%), H-4(A)->L+5(A) (3%), H-3(A)->L+5(A) (2%), H-2(A)->L+5(A) (3%), H-2(A)->L+6(A) (7%), H-13(B)->LUMO(B) (3%), H-8(B)->L+9(B) (4%), H-5(B)->L+1(B) (3%), H-5(B)->L+4(B) (3%), H-5(B)->L+6(B) (7%), H-5(B)->L+7(B) (3%), H-2(B)->L+6(B) (2%), H-1(B)->L+6(B) (3%), H-1(B)->L+7(B) (7%)
271.4249283	0.0681	H-9(A)->L+1(A) (38%), H-8(B)->L+1(B) (40%)	H-10(A)->L+1(A) (6%), H-1(A)->L+2(A) (2%), HOMO(A)->L+7(A) (2%), H-7(B)->L+2(B) (4%), HOMO(B)->L+8(B) (2%)
270.849775	0.0295	H-9(B)->L+2(B) (64%), H-8(B)->L+2(B) (17%)	H-7(B)->L+1(B) (5%), H-4(B)->L+2(B) (5%)
270.0768794	0.0303	H-10(A)->L+1(A) (32%), H-9(B)->L+1(B) (21%), H-7(B)->L+2(B) (15%)	H-9(A)->L+1(A) (7%), HOMO(A)->L+7(A) (2%), H-17(B)->L+2(B) (3%), H-8(B)->L+1(B) (9%), HOMO(B)->L+8(B) (2%)
269.7067501	0.0035	H-9(B)->L+1(B) (15%), H-7(B)->L+2(B) (47%)	H-10(A)->L+1(A) (5%), H-1(A)->L+2(A) (8%), H-17(B)->L+2(B) (7%), H-5(B)->L+2(B) (3%), H-2(B)->L+2(B) (2%)
268.8995251	0	H-12(A)->LUMO(A) (16%), H-11(A)->L+1(A) (30%), H-11(B)->LUMO(B) (17%), H-10(B)->L+1(B) (27%)	H-11(B)->L+2(B) (2%)
268.6722712	0	H-12(A)->L+1(A) (30%), H-11(A)->LUMO(A) (16%), H-	H-10(B)->L+2(B) (2%)

		11(B)->L+1(B) (26%), H-10(B)->LUMO(B) (17%)	
267.0231586	0.0006	H-2(A)->L+8(A) (16%), H-1(B)->L+9(B) (16%)	H-9(A)->L+6(A) (2%), H-7(A)->L+1(A) (3%), H-7(A)->L+3(A) (3%), H-7(A)->L+5(A) (8%), H-7(A)->L+6(A) (3%), H-6(A)->L+9(A) (2%), H-2(A)->L+10(A) (3%), H-1(A)->L+2(A) (5%), H-8(B)->L+7(B) (2%), H-6(B)->L+1(B) (2%), H-6(B)->L+4(B) (4%), H-6(B)->L+6(B) (8%), H-6(B)->L+7(B) (4%), H-5(B)->L+10(B) (2%), H-1(B)->L+11(B) (3%)
266.1575961	0.0097	H-1(A)->L+2(A) (42%), H-15(B)->LUMO(B) (12%), H-12(B)->L+1(B) (11%)	H-11(A)->L+1(A) (3%), H-10(A)->L+1(A) (2%), HOMO(A)->L+7(A) (2%), H-10(B)->L+1(B) (3%), H-9(B)->L+1(B) (4%), H-2(B)->L+3(B) (2%)
264.9914359	0.0084	H-12(A)->L+1(A) (33%), H-11(B)->L+1(B) (36%)	H-14(A)->LUMO(A) (6%), H-11(A)->LUMO(A) (4%), H-11(A)->L+1(A) (3%), HOMO(A)->L+4(A) (2%), H-10(B)->LUMO(B) (5%), H-10(B)->L+1(B) (3%), HOMO(B)->L+5(B) (2%)
264.8895291	0.0055	H-11(A)->L+1(A) (32%), H-10(B)->L+1(B) (32%)	H-12(A)->LUMO(A) (3%), H-12(A)->L+1(A) (3%), H-3(A)->L+2(A) (3%), H-1(A)->L+2(A) (2%), H-11(B)->LUMO(B) (5%), H-11(B)->L+1(B) (3%), H-2(B)->L+3(B) (3%), HOMO(B)->L+8(B) (2%)
264.3868067	0.0022	H-3(A)->L+2(A) (17%), HOMO(A)->L+7(A) (11%), H-2(B)->L+3(B) (20%), HOMO(B)->L+8(B) (10%)	H-11(A)->L+1(A) (4%), H-6(A)->L+2(A) (2%), H-1(A)->L+2(A) (7%), H-15(B)->LUMO(B) (2%), H-10(B)->L+1(B) (3%)
262.9457775	0.0028	H-14(A)->LUMO(A) (56%), H-12(B)->LUMO(B) (11%)	H-15(A)->L+1(A) (6%), H-13(A)->LUMO(A) (3%), H-12(A)->L+1(A) (6%), H-14(B)->LUMO(B) (6%), H-11(B)->L+1(B) (2%)
259.957632	0.0005	H-9(B)->L+2(B) (12%), H-8(B)->L+2(B) (58%)	HOMO(A)->L+8(A) (6%), HOMO(A)->L+10(A) (2%), H-13(B)->LUMO(B) (2%), HOMO(B)->L+9(B) (7%), HOMO(B)->L+11(B) (2%)
259.1317832	0.0004	H-13(A)->L+1(A) (15%), H-4(A)->L+2(A) (13%), H-13(B)->L+1(B) (17%), H-3(B)->L+3(B) (21%)	H-6(A)->L+2(A) (4%), H-3(A)->L+2(A) (2%), HOMO(A)->L+7(A) (3%), H-3(B)->L+11(B) (2%), HOMO(B)->L+8(B) (4%)
257.2659785	0.0057	H-10(B)->L+2(B) (91%)	H-11(B)->L+1(B) (4%)
257.1165945	0.0051	H-11(B)->L+2(B) (91%)	H-10(B)->L+1(B) (4%)
255.7799043	0.0034	H-14(B)->LUMO(B) (54%), HOMO(B)->L+10(B) (10%)	H-14(A)->LUMO(A) (7%), HOMO(A)->L+7(A) (2%),

			HOMO(A)->L+9(A) (7%), H-15(B)->L+1(B) (3%), HOMO(B)->L+8(B) (2%)
255.758799	0.003	HOMO(A)->L+7(A) (37%), HOMO(B)->L+8(B) (36%)	H-10(A)->L+1(A) (2%), H-15(B)->L+2(B) (2%), H-14(B)->LUMO(B) (2%), H-9(B)->L+1(B) (3%)
255.7218732	0.002	HOMO(A)->L+9(A) (21%), H-14(B)->LUMO(B) (20%), HOMO(B)->L+10(B) (30%)	H-14(A)->LUMO(A) (2%), H-3(A)->L+6(A) (2%), H-5(B)->L+7(B) (2%), H-2(B)->L+7(B) (2%)
254.2796058	0.0268	HOMO(A)->L+8(A) (37%), HOMO(A)->L+9(A) (10%), HOMO(B)->L+9(B) (38%)	H-13(B)->LUMO(B) (2%), HOMO(B)->L+10(B) (6%)
253.3702395	0.0072	HOMO(A)->L+9(A) (42%), HOMO(B)->L+10(B) (36%)	HOMO(A)->L+8(A) (7%), HOMO(B)->L+9(B) (9%)
251.4127406	0.0001	H-2(A)->L+2(A) (74%), H-1(B)->L+3(B) (16%)	
250.7821619	0.0002	H-5(A)->L+2(A) (15%), HOMO(A)->L+8(A) (14%), H-4(B)->L+3(B) (23%)	H-2(A)->L+2(A) (3%), HOMO(A)->L+10(A) (9%), H-13(B)->LUMO(B) (3%), HOMO(B)->L+9(B) (4%), HOMO(B)->L+11(B) (5%)

Table S14. Major and minor transitions calculated using TD-DFT studies of **Cu-4**.

Wavelength (nm)	Osc. Strength	Major contribs	Minor contribs
731.9451739	0.0001	HOMO(A)->LUMO(A) (47%), HOMO(B)->LUMO(B) (45%)	
576.4293692	0	HOMO(A)->L+1(A) (44%), HOMO(B)->L+1(B) (44%)	H-3(A)->LUMO(A) (4%), H-2(B)->LUMO(B) (4%)
540.5894616	0.0035	H-16(B)->L+2(B) (37%), H-4(B)->L+2(B) (31%), HOMO(B)->L+2(B) (11%)	H-13(B)->L+2(B) (9%), H-4(B)->LUMO(B) (2%)
506.7611911	0	H-17(B)->L+2(B) (49%), H-3(B)->L+2(B) (24%)	H-1(A)->LUMO(A) (7%), H-17(B)->LUMO(B) (2%), H-7(B)->L+2(B) (4%), H-5(B)->L+2(B) (4%), H-2(B)->L+2(B) (3%)
501.8587048	0.2387	HOMO(A)->LUMO(A) (28%), HOMO(B)->LUMO(B) (32%), HOMO(B)->L+2(B) (29%)	H-16(B)->L+2(B) (4%), H-4(B)->L+2(B) (4%)
488.3767007	0.0787	H-14(B)->L+2(B) (14%), H-12(B)->L+2(B) (27%), HOMO(B)->L+2(B) (33%)	HOMO(A)->LUMO(A) (7%), H-16(B)->L+2(B) (2%), H-13(B)->L+2(B) (2%), HOMO(B)->LUMO(B) (7%)
480.5588876	0.1211	HOMO(A)->LUMO(A) (10%), H-14(B)->L+2(B) (32%), H-12(B)->L+2(B) (15%), HOMO(B)->LUMO(B) (10%), HOMO(B)->L+2(B) (24%)	H-19(B)->L+2(B) (4%)
453.6394315	0.0015	H-1(A)->LUMO(A) (87%)	H-17(B)->L+2(B) (4%), H-3(B)->L+2(B) (2%)
453.5564567	0.0451	H-23(B)->L+2(B) (25%), H-19(B)->L+2(B) (36%), H-12(B)->L+2(B) (11%)	H-1(A)->LUMO(A) (3%), HOMO(A)->LUMO(A) (2%), H-32(B)->L+2(B) (3%), H-16(B)->L+2(B) (3%), H-14(B)->L+2(B) (5%), HOMO(B)->LUMO(B) (2%), HOMO(B)->L+2(B) (2%)
433.480851	0.3488	HOMO(A)->L+1(A) (47%), HOMO(B)->L+1(B) (45%)	H-3(A)->LUMO(A) (2%), H-2(B)->LUMO(B) (2%)
408.5550236	0	H-5(A)->LUMO(A) (16%), H-4(B)->LUMO(B) (22%)	H-7(A)->LUMO(A) (2%), H-6(A)->L+1(A) (3%), H-4(A)->L+1(A) (2%), H-3(A)->L+1(A) (7%), H-1(A)->L+1(A) (4%), HOMO(A)->L+2(A) (9%), H-3(B)->L+1(B) (4%), H-2(B)->L+1(B) (8%), HOMO(B)->L+3(B) (9%)
405.826955	0.0001	H-3(A)->LUMO(A) (34%), H-2(B)->LUMO(B) (35%)	H-8(A)->LUMO(A) (2%), H-6(A)->LUMO(A) (4%), H-5(A)->L+1(A) (2%), HOMO(A)->L+1(A) (3%), H-7(B)->LUMO(B) (2%), H-5(B)->LUMO(B) (2%), H-4(B)->L+1(B) (3%), H-3(B)->LUMO(B) (2%), HOMO(B)->L+1(B) (3%)
394.8666932	0	H-1(A)->L+1(A) (63%)	H-10(A)->LUMO(A) (3%), H-3(A)-

			>L+1(A) (3%), HOMO(A)->L+2(A) (5%), H-9(B)->LUMO(B) (3%), H-7(B)->L+1(B) (2%), H-2(B)->L+1(B) (3%), HOMO(B)->L+3(B) (5%)
393.4382414	0.0011	H-4(A)->LUMO(A) (23%), H-3(B)->LUMO(B) (33%)	H-6(A)->LUMO(A) (6%), H-5(A)->L+1(A) (7%), H-3(A)->LUMO(A) (6%), HOMO(A)->L+1(A) (2%), H-4(B)->L+1(B) (9%), H-2(B)->LUMO(B) (3%), HOMO(B)->L+1(B) (2%)
385.7868972	0	H-1(A)->L+1(A) (27%), H-4(B)->LUMO(B) (12%)	H-8(A)->L+1(A) (3%), H-5(A)->LUMO(A) (9%), H-4(A)->L+1(A) (4%), H-3(A)->L+1(A) (4%), HOMO(A)->L+2(A) (7%), H-9(B)->LUMO(B) (2%), H-7(B)->L+1(B) (3%), H-3(B)->L+1(B) (4%), H-2(B)->L+1(B) (3%), HOMO(B)->L+3(B) (7%)
378.4621276	0	H-8(A)->LUMO(A) (21%), H-7(B)->LUMO(B) (21%)	H-12(A)->L+4(A) (2%), H-11(A)->L+3(A) (2%), H-10(A)->L+1(A) (8%), H-9(A)->L+1(A) (2%), H-8(A)->L+2(A) (2%), H-5(A)->L+1(A) (2%), H-11(B)->L+5(B) (2%), H-10(B)->L+4(B) (2%), H-9(B)->L+1(B) (8%), H-8(B)->L+1(B) (3%), H-7(B)->L+3(B) (2%), H-4(B)->L+1(B) (2%)
372.4926934	0.0007	H-2(A)->LUMO(A) (94%)	H-1(B)->LUMO(B) (3%)
368.9786114	0.002	H-1(B)->LUMO(B) (94%)	H-2(A)->LUMO(A) (3%)
364.2629874	0.0001	H-8(A)->L+1(A) (10%), H-7(B)->L+1(B) (10%), H-3(B)->L+1(B) (13%)	H-13(A)->LUMO(A) (2%), H-10(A)->LUMO(A) (9%), H-9(A)->LUMO(A) (2%), H-6(A)->L+1(A) (2%), H-4(A)->L+1(A) (7%), H-3(A)->L+1(A) (6%), HOMO(A)->L+2(A) (2%), H-13(B)->LUMO(B) (2%), H-9(B)->LUMO(B) (9%), H-8(B)->LUMO(B) (2%), H-2(B)->L+1(B) (4%), HOMO(B)->L+3(B) (2%)
351.4191577	0.3881	H-3(A)->LUMO(A) (33%), H-2(B)->LUMO(B) (34%), H-2(B)->L+2(B) (19%)	H-4(A)->LUMO(A) (2%)
348.8581683	0.0001	H-3(A)->L+1(A) (11%), H-2(A)->L+6(A) (10%), H-2(B)->L+1(B) (11%), H-1(B)->L+7(B) (10%)	H-9(A)->L+8(A) (2%), H-7(A)->L+9(A) (4%), H-6(A)->L+5(A) (2%), H-2(A)->L+5(A) (3%), HOMO(A)->L+2(A) (7%), H-8(B)->L+9(B) (2%), H-6(B)->L+10(B) (4%), H-5(B)->L+6(B) (3%), H-1(B)->L+6(B) (3%), HOMO(B)->L+3(B) (7%)
344.7644542	0.0002	H-3(A)->L+1(A) (11%), HOMO(A)->L+2(A) (11%), H-2(B)->L+1(B) (11%), HOMO(B)->L+3(B) (11%)	H-7(A)->L+9(A) (3%), H-4(A)->L+1(A) (2%), H-2(A)->L+5(A) (3%), H-2(A)->L+6(A) (7%), HOMO(A)->LUMO(A) (2%), H-6(B)->L+10(B) (3%), H-5(B)->L+1(B) (2%), H-5(B)->L+6(B) (2%), H-1(B)->L+6(B) (2%), H-1(B)->L+7(B) (7%), HOMO(B)->LUMO(B) (2%)
343.3228838	0.0857	H-2(B)->L+2(B) (63%)	H-4(A)->LUMO(A) (5%), H-3(A)->LUMO(A) (7%), H-7(B)->L+2(B) (5%), H-

			5(B)->L+2(B) (2%), H-3(B)->LUMO(B) (2%), H-2(B)->LUMO(B) (9%)
337.5464676	0.0032	H-4(A)->L+1(A) (13%), H-4(B)->LUMO(B) (29%), H-3(B)->L+1(B) (19%)	H-10(A)->LUMO(A) (2%), H-6(A)->L+1(A) (5%), H-5(A)->L+2(A) (2%), H-2(A)->L+1(A) (3%), H-9(B)->LUMO(B) (3%), H-4(B)->L+3(B) (3%), H-2(B)->L+1(B) (4%), H-1(B)->L+1(B) (3%)
335.4187669	0.0004	H-2(A)->L+9(A) (13%), H-1(B)->L+10(B) (13%)	H-9(A)->L+3(A) (2%), H-9(A)->L+5(A) (3%), H-9(A)->L+6(A) (2%), H-7(A)->L+5(A) (3%), H-7(A)->L+6(A) (7%), H-6(A)->LUMO(A) (3%), H-6(A)->L+8(A) (3%), H-5(A)->L+6(A) (2%), H-4(A)->L+8(A) (2%), H-2(A)->L+1(A) (2%), H-8(B)->L+4(B) (2%), H-8(B)->L+6(B) (3%), H-8(B)->L+7(B) (2%), H-6(B)->L+6(B) (3%), H-6(B)->L+7(B) (9%), H-5(B)->LUMO(B) (3%), H-5(B)->L+9(B) (5%)
334.5950425	0.0004	H-2(A)->L+1(A) (56%), H-1(B)->L+1(B) (27%)	H-2(B)->L+1(B) (3%)
333.9011985	0.0017	H-5(A)->LUMO(A) (31%), H-4(B)->LUMO(B) (14%), H-1(B)->L+1(B) (22%)	H-10(A)->LUMO(A) (2%), H-3(A)->L+1(A) (6%), H-2(A)->L+1(A) (8%), H-3(B)->L+1(B) (5%), H-2(B)->L+1(B) (7%)
332.593468	0	H-5(A)->LUMO(A) (14%), H-2(A)->L+1(A) (25%), H-1(B)->L+1(B) (42%)	H-7(A)->LUMO(A) (3%), H-4(B)->LUMO(B) (6%), H-3(B)->L+1(B) (2%), H-2(B)->L+1(B) (3%)
329.8153677	0.4529	H-4(A)->LUMO(A) (19%), H-3(B)->LUMO(B) (49%)	H-6(A)->LUMO(A) (8%), H-5(A)->L+1(A) (4%), H-3(A)->LUMO(A) (5%), HOMO(A)->L+1(A) (2%), H-2(B)->LUMO(B) (3%)
328.1220373	0.0495	H-5(A)->L+1(A) (11%), H-4(A)->LUMO(A) (21%), H-4(B)->L+1(B) (39%)	H-10(A)->L+1(A) (3%), H-6(A)->LUMO(A) (2%), H-9(B)->L+1(B) (3%), H-3(B)->LUMO(B) (2%), H-3(B)->L+3(B) (2%), H-2(B)->LUMO(B) (2%), H-2(B)->L+3(B) (2%)
325.3153679	0.0476	H-5(A)->LUMO(A) (13%), H-3(A)->L+1(A) (39%), H-2(B)->L+1(B) (32%)	H-6(A)->L+1(A) (3%), H-4(A)->L+1(A) (2%), H-4(B)->LUMO(B) (5%)
324.6169372	0.0008	H-12(A)->L+1(A) (15%), H-11(A)->LUMO(A) (29%), H-11(B)->L+1(B) (14%), H-10(B)->LUMO(B) (24%)	H-11(A)->L+2(A) (2%), H-10(B)->L+3(B) (2%)
324.5404628	0.0006	H-12(A)->LUMO(A) (30%), H-11(A)->L+1(A) (15%), H-11(B)->LUMO(B) (26%), H-10(B)->L+1(B) (14%)	H-12(A)->L+2(A) (2%), H-11(B)->L+3(B) (2%)
320.1823025	0.008	H-6(A)->LUMO(A) (60%), H-4(A)->LUMO(A) (17%)	H-3(A)->LUMO(A) (2%), H-5(B)->LUMO(B) (6%), H-4(B)->L+1(B) (2%)
319.3658055	0.0005	H-7(A)->LUMO(A) (79%)	H-5(A)->LUMO(A) (6%), H-2(A)->L+1(A) (2%), H-6(B)->LUMO(B) (7%)

317.6719696	0.0324	H-6(B)->LUMO(B) (10%), H-5(B)->LUMO(B) (73%)	H-6(A)->LUMO(A) (6%), H-4(A)->LUMO(A) (3%), H-3(B)->LUMO(B) (2%)
316.8601115	0.0089	H-6(B)->LUMO(B) (77%)	H-7(A)->LUMO(A) (8%), H-5(B)->LUMO(B) (8%)
315.9557427	0.0024	H-1(B)->L+2(B) (95%)	H-5(B)->LUMO(B) (2%), H-2(B)->L+2(B) (2%)
307.5386159	0.004	H-4(A)->L+1(A) (26%), HOMO(A)->L+2(A) (16%), H-3(B)->L+1(B) (27%), HOMO(B)->L+3(B) (15%)	H-6(A)->L+1(A) (7%)
307.4471025	0.018	H-5(A)->L+1(A) (50%), H-4(B)->L+1(B) (33%)	H-10(A)->L+1(A) (2%), H-7(A)->L+1(A) (4%), H-6(A)->LUMO(A) (2%)
302.1646349	0.0065	H-17(B)->L+2(B) (15%), H-7(B)->L+2(B) (10%), H-3(B)->L+2(B) (59%)	H-7(B)->LUMO(B) (6%)
297.3384647	0.0023	H-9(A)->LUMO(A) (47%), H-6(A)->L+1(A) (12%), H-8(B)->LUMO(B) (11%)	H-10(A)->LUMO(A) (7%), H-4(A)->L+1(A) (4%), H-2(A)->L+6(A) (2%), H-5(B)->L+1(B) (6%), H-1(B)->L+7(B) (2%)
296.081655	0.1291	H-10(A)->LUMO(A) (13%), H-9(A)->LUMO(A) (10%), H-9(B)->LUMO(B) (18%), H-8(B)->LUMO(B) (10%)	H-11(A)->LUMO(A) (6%), H-8(A)->L+1(A) (2%), H-6(A)->L+1(A) (2%), HOMO(A)->L+2(A) (2%), H-16(B)->L+2(B) (2%), H-12(B)->LUMO(B) (3%), H-10(B)->LUMO(B) (6%), H-5(B)->L+1(B) (2%), H-4(B)->L+2(B) (5%), HOMO(B)->L+3(B) (2%)
295.5804916	0.011	H-7(B)->LUMO(B) (13%)	H-12(A)->LUMO(A) (2%), H-12(A)->L+4(A) (5%), H-11(A)->L+3(A) (4%), H-10(A)->LUMO(A) (2%), H-9(A)->LUMO(A) (2%), H-8(A)->LUMO(A) (7%), HOMO(A)->L+3(A) (5%), HOMO(A)->L+7(A) (2%), H-17(B)->L+2(B) (3%), H-11(B)->L+5(B) (5%), H-10(B)->L+4(B) (4%), H-8(B)->LUMO(B) (5%), H-5(B)->L+1(B) (5%), H-4(B)->L+2(B) (2%), H-3(B)->L+2(B) (6%), HOMO(B)->L+4(B) (3%), HOMO(B)->L+6(B) (2%), HOMO(B)->L+8(B) (2%)
295.5452624	0.0383	H-8(B)->LUMO(B) (18%), H-5(B)->L+1(B) (15%)	H-12(A)->L+4(A) (2%), H-10(A)->LUMO(A) (5%), H-9(A)->LUMO(A) (6%), H-8(A)->LUMO(A) (2%), H-6(A)->L+1(A) (3%), HOMO(A)->L+2(A) (4%), H-16(B)->L+2(B) (2%), H-9(B)->LUMO(B) (5%), H-7(B)->LUMO(B) (4%), H-4(B)->L+2(B) (6%), H-3(B)->L+2(B) (2%), HOMO(B)->L+3(B) (4%)
294.7022724	0.0166	H-12(A)->LUMO(A) (17%), H-8(A)->LUMO(A) (26%), H-11(B)->LUMO(B) (21%), H-7(B)-	H-11(A)->L+1(A) (3%), HOMO(A)->L+5(A) (2%), H-10(B)->L+1(B) (4%), HOMO(B)->L+4(B) (3%)

		>LUMO(B) (13%)	
293.9616213	0.0079	H-16(B)->L+2(B) (16%), H-4(B)->L+2(B) (35%)	H-11(A)->LUMO(A) (5%), H-9(A)->LUMO(A) (4%), H-13(B)->L+2(B) (4%), H-10(B)->LUMO(B) (6%), H-9(B)->L+2(B) (4%), H-8(B)->LUMO(B) (5%), H-5(B)->L+1(B) (7%)
293.238554	0.0737	H-11(A)->LUMO(A) (17%), H-9(A)->LUMO(A) (13%), H-6(A)->L+1(A) (10%), H-10(B)->LUMO(B) (14%)	H-12(A)->L+1(A) (2%), H-3(A)->L+1(A) (2%), HOMO(A)->L+2(A) (7%), HOMO(A)->L+4(A) (4%), H-11(B)->L+1(B) (3%), H-9(B)->LUMO(B) (2%), H-8(B)->LUMO(B) (8%), H-3(B)->L+1(B) (4%), HOMO(B)->L+3(B) (5%), HOMO(B)->L+5(B) (2%)
292.8160999	0.0002	H-10(A)->LUMO(A) (18%), H-9(B)->LUMO(B) (15%)	H-12(A)->L+3(A) (5%), H-12(A)->L+5(A) (2%), H-11(A)->L+4(A) (7%), H-6(A)->L+1(A) (3%), H-5(A)->LUMO(A) (2%), H-13(B)->LUMO(B) (2%), H-12(B)->LUMO(B) (2%), H-11(B)->L+4(B) (6%), H-11(B)->L+6(B) (2%), H-10(B)->LUMO(B) (5%), H-10(B)->L+5(B) (7%), HOMO(B)->L+5(B) (3%)
292.4431385	0.0003	H-7(A)->L+1(A) (24%), H-8(B)->LUMO(B) (11%), H-6(B)->L+1(B) (24%)	H-9(A)->LUMO(A) (2%), H-6(A)->L+1(A) (8%), H-5(A)->L+1(A) (3%), H-4(A)->L+1(A) (4%), H-5(B)->L+1(B) (7%)
292.1468296	0.0001	H-7(A)->L+1(A) (18%), H-6(A)->L+1(A) (12%), H-8(B)->LUMO(B) (16%), H-6(B)->L+1(B) (17%)	H-9(A)->LUMO(A) (5%), H-4(A)->L+1(A) (6%), H-5(B)->L+1(B) (9%)
290.7355915	0.0039	H-12(A)->LUMO(A) (15%), H-8(A)->LUMO(A) (24%), H-11(B)->LUMO(B) (15%), H-7(B)->LUMO(B) (23%)	H-11(A)->L+1(A) (2%), HOMO(A)->L+3(A) (6%), H-10(B)->L+1(B) (2%), HOMO(B)->L+4(B) (4%)
290.0554287	0.0071	H-7(A)->L+1(A) (18%), H-6(A)->L+1(A) (11%), H-6(B)->L+1(B) (21%), H-5(B)->L+1(B) (22%)	H-10(A)->LUMO(A) (3%), H-5(A)->L+1(A) (2%), H-4(A)->L+1(A) (7%), H-9(B)->LUMO(B) (4%), H-3(B)->L+1(B) (2%)
289.560916	0.0068	H-7(A)->L+1(A) (25%), H-6(B)->L+1(B) (28%), H-5(B)->L+1(B) (14%)	H-10(A)->LUMO(A) (4%), H-6(A)->L+1(A) (6%), H-5(A)->L+1(A) (2%), H-4(A)->L+1(A) (6%), H-9(B)->LUMO(B) (5%)
288.2682934	0.0001	HOMO(A)->L+5(A) (15%), HOMO(A)->L+6(A) (17%), HOMO(B)->L+6(B) (24%), HOMO(B)->L+7(B) (33%)	H-7(A)->L+1(A) (2%), HOMO(B)->L+4(B) (2%)
287.5862707	0.0019	HOMO(A)->L+4(A) (11%), HOMO(B)->L+3(B) (12%), HOMO(B)->L+5(B) (11%)	H-11(A)->LUMO(A) (9%), H-10(A)->LUMO(A) (3%), H-4(A)->L+1(A) (4%), HOMO(A)->L+2(A) (7%), H-12(B)->LUMO(B) (9%), H-10(B)->LUMO(B)

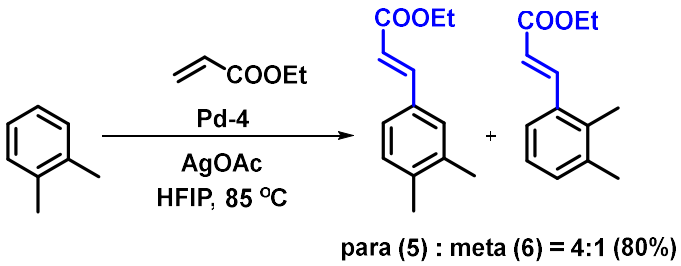
			(3%), H-9(B)->LUMO(B) (6%), H-4(B)->L+2(B) (2%), H-3(B)->L+1(B) (4%)
287.0735442	0.0087	HOMO(A)->L+4(A) (25%), HOMO(B)->L+5(B) (25%)	H-10(A)->LUMO(A) (9%), H-4(A)->L+1(A) (2%), HOMO(A)->L+2(A) (6%), HOMO(A)->L+6(A) (2%), H-10(B)->LUMO(B) (6%), HOMO(B)->L+3(B) (2%)
286.967233	0.0002	HOMO(A)->L+3(A) (31%), HOMO(B)->L+4(B) (38%)	H-8(A)->LUMO(A) (2%), H-8(A)->L+4(A) (2%), HOMO(A)->L+5(A) (4%), H-7(B)->L+5(B) (2%), HOMO(B)->L+6(B) (3%)
286.3574682	0.001	HOMO(A)->L+5(A) (20%), HOMO(A)->L+6(A) (35%), HOMO(B)->L+7(B) (25%)	HOMO(B)->L+6(B) (9%)
285.414809	0.0002	HOMO(A)->L+5(A) (15%), HOMO(A)->L+6(A) (21%), HOMO(B)->L+6(B) (25%), HOMO(B)->L+7(B) (22%)	
283.7166888	0.0185	H-12(B)->LUMO(B) (49%)	H-14(A)->LUMO(A) (5%), H-12(A)->L+3(A) (2%), H-11(A)->L+4(A) (2%), H-10(A)->LUMO(A) (2%), H-15(B)->L+1(B) (6%), H-14(B)->LUMO(B) (2%), H-11(B)->L+4(B) (2%), H-10(B)->L+5(B) (2%), H-9(B)->LUMO(B) (4%), H-7(B)->L+1(B) (2%), HOMO(B)->L+5(B) (6%)
282.5142255	0.0148	HOMO(A)->L+3(A) (19%), HOMO(A)->L+5(A) (18%), HOMO(A)->L+6(A) (16%), HOMO(B)->L+4(B) (15%), HOMO(B)->L+6(B) (14%), HOMO(B)->L+7(B) (11%)	
280.3423168	0.0054	H-7(B)->L+1(B) (26%)	H-13(A)->LUMO(A) (4%), H-12(A)->L+3(A) (5%), H-11(A)->L+4(A) (6%), H-8(A)->L+1(A) (9%), H-13(B)->LUMO(B) (2%), H-12(B)->LUMO(B) (2%), H-11(B)->L+4(B) (5%), H-10(B)->L+5(B) (6%), H-9(B)->LUMO(B) (6%), H-8(B)->LUMO(B) (2%)
279.9372161	0.0001	H-2(A)->L+5(A) (14%), H-1(B)->L+6(B) (14%)	H-7(A)->L+8(A) (4%), H-2(A)->L+3(A) (7%), H-2(A)->L+6(A) (7%), H-2(A)->L+7(A) (2%), H-12(B)->LUMO(B) (2%), H-7(B)->L+1(B) (2%), H-6(B)->L+9(B) (4%), H-5(B)->L+2(B) (8%), H-5(B)->L+7(B) (2%), H-1(B)->L+4(B) (7%), H-1(B)->L+7(B) (6%)
279.8045474	0.0005	H-5(B)->L+2(B) (75%)	H-2(A)->L+5(A) (2%), H-7(B)->L+2(B) (5%), H-3(B)->L+2(B) (2%), H-2(B)->L+2(B) (5%), H-1(B)->L+6(B) (2%)
278.8166614	0.0007	H-10(A)->L+1(A) (13%), H-9(B)->L+1(B) (20%)	H-12(A)->L+4(A) (6%), H-11(A)->L+3(A) (4%), H-9(A)->L+1(A) (4%), H-8(A)->LUMO(A) (5%), H-1(A)->L+2(A) (2%), H-15(B)->LUMO(B) (3%), H-12(B)->L+1(B) (3%), H-11(B)->L+5(B) (6%), H-10(B)->L+4(B) (4%), H-8(B)->L+1(B) (7%), H-7(B)->LUMO(B) (6%), H-5(B)->L+2(B) (2%)

278.1785798	0.018	HOMO(A)->L+3(A) (24%), HOMO(A)->L+5(A) (15%), HOMO(B)->L+4(B) (23%), HOMO(B)->L+6(B) (14%)	H-12(A)->LUMO(A) (7%), HOMO(A)->L+6(A) (3%), H-11(B)->LUMO(B) (8%), HOMO(B)->L+7(B) (3%)
278.0351019	0.0043	HOMO(A)->L+4(A) (41%), HOMO(B)->L+5(B) (36%)	H-11(A)->LUMO(A) (6%), H-10(B)->LUMO(B) (6%), H-6(B)->L+2(B) (4%)
276.9606242	0.0167	H-6(B)->L+2(B) (88%)	HOMO(B)->L+5(B) (2%)
276.1033137	0.1601	H-8(A)->L+1(A) (24%), H-7(B)->L+1(B) (35%)	H-13(A)->LUMO(A) (5%), H-13(B)->LUMO(B) (8%), H-9(B)->LUMO(B) (3%), H-9(B)->L+2(B) (2%), H-6(B)->L+2(B) (3%), HOMO(B)->L+3(B) (2%), HOMO(B)->L+11(B) (2%)
276.0418413	0.0036	H-1(A)->L+2(A) (11%), H-15(B)->LUMO(B) (24%), H-12(B)->L+1(B) (16%)	H-15(A)->LUMO(A) (7%), H-14(A)->L+1(A) (4%), H-12(A)->L+4(A) (2%), H-11(A)->L+3(A) (2%), H-10(A)->L+1(A) (2%), HOMO(A)->L+7(A) (3%), H-14(B)->L+1(B) (2%), H-11(B)->L+5(B) (2%), H-10(B)->L+4(B) (2%), H-5(B)->L+2(B) (2%), HOMO(B)->L+8(B) (3%)
274.422738	0.0499	H-13(A)->LUMO(A) (12%), H-8(A)->L+1(A) (35%), H-13(B)->LUMO(B) (11%)	H-10(A)->LUMO(A) (4%), HOMO(A)->L+2(A) (2%), HOMO(A)->L+8(A) (3%), HOMO(A)->L+10(A) (2%), HOMO(B)->L+3(B) (2%), HOMO(B)->L+9(B) (2%)
273.8106336	0.0008	H-9(A)->L+1(A) (27%), H-9(B)->L+1(B) (10%), H-8(B)->L+1(B) (21%)	H-10(A)->L+1(A) (9%), H-7(A)->L+6(A) (2%), H-2(A)->L+9(A) (3%), HOMO(A)->L+7(A) (2%), H-6(B)->L+7(B) (2%), H-1(B)->L+10(B) (3%), HOMO(B)->L+8(B) (2%)
272.7384963	0.0005	HOMO(A)->L+7(A) (19%), HOMO(B)->L+8(B) (20%)	H-10(A)->L+1(A) (2%), H-9(A)->L+1(A) (7%), H-3(A)->L+2(A) (7%), H-1(A)->L+2(A) (3%), H-15(B)->LUMO(B) (3%), H-8(B)->L+1(B) (6%), H-2(B)->L+3(B) (7%)
272.6785129	0.0004		H-13(A)->LUMO(A) (3%), H-9(A)->L+8(A) (4%), H-8(A)->L+1(A) (3%), H-6(A)->L+3(A) (2%), H-6(A)->L+5(A) (4%), H-6(A)->L+6(A) (2%), H-4(A)->L+1(A) (2%), H-4(A)->L+5(A) (3%), H-3(A)->L+5(A) (2%), H-2(A)->L+5(A) (3%), H-2(A)->L+6(A) (7%), H-13(B)->LUMO(B) (3%), H-8(B)->L+9(B) (4%), H-5(B)->L+1(B) (3%), H-5(B)->L+4(B) (3%), H-5(B)->L+6(B) (7%), H-5(B)->L+7(B) (3%), H-2(B)->L+6(B) (2%), H-1(B)->L+6(B) (3%), H-1(B)->L+7(B) (7%)
271.4249283	0.0681	H-9(A)->L+1(A) (38%), H-8(B)->L+1(B) (40%)	H-10(A)->L+1(A) (6%), H-1(A)->L+2(A) (2%), HOMO(A)->L+7(A) (2%), H-7(B)->L+2(B) (4%), HOMO(B)->L+8(B) (2%)

270.849775	0.0295	H-9(B)->L+2(B) (64%), H-8(B)->L+2(B) (17%)	H-7(B)->L+1(B) (5%), H-4(B)->L+2(B) (5%)
270.0768794	0.0303	H-10(A)->L+1(A) (32%), H-9(B)->L+1(B) (21%), H-7(B)->L+2(B) (15%)	H-9(A)->L+1(A) (7%), HOMO(A)->L+7(A) (2%), H-17(B)->L+2(B) (3%), H-8(B)->L+1(B) (9%), HOMO(B)->L+8(B) (2%)
269.7067501	0.0035	H-9(B)->L+1(B) (15%), H-7(B)->L+2(B) (47%)	H-10(A)->L+1(A) (5%), H-1(A)->L+2(A) (8%), H-17(B)->L+2(B) (7%), H-5(B)->L+2(B) (3%), H-2(B)->L+2(B) (2%)
268.8995251	0	H-12(A)->LUMO(A) (16%), H-11(A)->L+1(A) (30%), H-11(B)->LUMO(B) (17%), H-10(B)->L+1(B) (27%)	H-11(B)->L+2(B) (2%)
268.6722712	0	H-12(A)->L+1(A) (30%), H-11(A)->LUMO(A) (16%), H-11(B)->L+1(B) (26%), H-10(B)->LUMO(B) (17%)	H-10(B)->L+2(B) (2%)
267.0231586	0.0006	H-2(A)->L+8(A) (16%), H-1(B)->L+9(B) (16%)	H-9(A)->L+6(A) (2%), H-7(A)->L+1(A) (3%), H-7(A)->L+3(A) (3%), H-7(A)->L+5(A) (8%), H-7(A)->L+6(A) (3%), H-6(A)->L+9(A) (2%), H-2(A)->L+10(A) (3%), H-1(A)->L+2(A) (5%), H-8(B)->L+7(B) (2%), H-6(B)->L+1(B) (2%), H-6(B)->L+4(B) (4%), H-6(B)->L+6(B) (8%), H-6(B)->L+7(B) (4%), H-5(B)->L+10(B) (2%), H-1(B)->L+11(B) (3%)
266.1575961	0.0097	H-1(A)->L+2(A) (42%), H-15(B)->LUMO(B) (12%), H-12(B)->L+1(B) (11%)	H-11(A)->L+1(A) (3%), H-10(A)->L+1(A) (2%), HOMO(A)->L+7(A) (2%), H-10(B)->L+1(B) (3%), H-9(B)->L+1(B) (4%), H-2(B)->L+3(B) (2%)
264.9914359	0.0084	H-12(A)->L+1(A) (33%), H-11(B)->L+1(B) (36%)	H-14(A)->LUMO(A) (6%), H-11(A)->LUMO(A) (4%), H-11(A)->L+1(A) (3%), HOMO(A)->L+4(A) (2%), H-10(B)->LUMO(B) (5%), H-10(B)->L+1(B) (3%), HOMO(B)->L+5(B) (2%)
264.8895291	0.0055	H-11(A)->L+1(A) (32%), H-10(B)->L+1(B) (32%)	H-12(A)->LUMO(A) (3%), H-12(A)->L+1(A) (3%), H-3(A)->L+2(A) (3%), H-1(A)->L+2(A) (2%), H-11(B)->LUMO(B) (5%), H-11(B)->L+1(B) (3%), H-2(B)->L+3(B) (3%), HOMO(B)->L+8(B) (2%)
264.3868067	0.0022	H-3(A)->L+2(A) (17%), HOMO(A)->L+7(A) (11%), H-2(B)->L+3(B) (20%), HOMO(B)->L+8(B) (10%)	H-11(A)->L+1(A) (4%), H-6(A)->L+2(A) (2%), H-1(A)->L+2(A) (7%), H-15(B)->LUMO(B) (2%), H-10(B)->L+1(B) (3%)
262.9457775	0.0028	H-14(A)->LUMO(A) (56%), H-12(B)->LUMO(B) (11%)	H-15(A)->L+1(A) (6%), H-13(A)->LUMO(A) (3%), H-12(A)->L+1(A) (6%), H-14(B)->LUMO(B) (6%), H-11(B)->L+1(B) (2%)

259.957632	0.0005	H-9(B)->L+2(B) (12%), H-8(B)->L+2(B) (58%)	HOMO(A)->L+8(A) (6%), HOMO(A)->L+10(A) (2%), H-13(B)->LUMO(B) (2%), HOMO(B)->L+9(B) (7%), HOMO(B)->L+11(B) (2%)
259.1317832	0.0004	H-13(A)->L+1(A) (15%), H-4(A)->L+2(A) (13%), H-13(B)->L+1(B) (17%), H-3(B)->L+3(B) (21%)	H-6(A)->L+2(A) (4%), H-3(A)->L+2(A) (2%), HOMO(A)->L+7(A) (3%), H-3(B)->L+11(B) (2%), HOMO(B)->L+8(B) (4%)
257.2659785	0.0057	H-10(B)->L+2(B) (91%)	H-11(B)->L+1(B) (4%)
257.1165945	0.0051	H-11(B)->L+2(B) (91%)	H-10(B)->L+1(B) (4%)
255.7799043	0.0034	H-14(B)->LUMO(B) (54%), HOMO(B)->L+10(B) (10%)	H-14(A)->LUMO(A) (7%), HOMO(A)->L+7(A) (2%), HOMO(A)->L+9(A) (7%), H-15(B)->L+1(B) (3%), HOMO(B)->L+8(B) (2%)
255.758799	0.003	HOMO(A)->L+7(A) (37%), HOMO(B)->L+8(B) (36%)	H-10(A)->L+1(A) (2%), H-15(B)->L+2(B) (2%), H-14(B)->LUMO(B) (2%), H-9(B)->L+1(B) (3%)
255.7218732	0.002	HOMO(A)->L+9(A) (21%), H-14(B)->LUMO(B) (20%), HOMO(B)->L+10(B) (30%)	H-14(A)->LUMO(A) (2%), H-3(A)->L+6(A) (2%), H-5(B)->L+7(B) (2%), H-2(B)->L+7(B) (2%)
254.2796058	0.0268	HOMO(A)->L+8(A) (37%), HOMO(A)->L+9(A) (10%), HOMO(B)->L+9(B) (38%)	H-13(B)->LUMO(B) (2%), HOMO(B)->L+10(B) (6%)
253.3702395	0.0072	HOMO(A)->L+9(A) (42%), HOMO(B)->L+10(B) (36%)	HOMO(A)->L+8(A) (7%), HOMO(B)->L+9(B) (9%)
251.4127406	0.0001	H-2(A)->L+2(A) (74%), H-1(B)->L+3(B) (16%)	
250.7821619	0.0002	H-5(A)->L+2(A) (15%), HOMO(A)->L+8(A) (14%), H-4(B)->L+3(B) (23%)	H-2(A)->L+2(A) (3%), HOMO(A)->L+10(A) (9%), H-13(B)->LUMO(B) (3%), HOMO(B)->L+9(B) (4%), HOMO(B)->L+11(B) (5%)

Catalysis studies:



para (5) : meta (6) = 4:1 (80%)

The substrate for example *o*-xylene (30 µL, 0.25 mmol) was dissolved in hexafluoroisoproponol (HFIP, 2 mL). To the mixture ethyl acrylate (53 µL, 0.50 mmol), Silver acetate (83 mg, 0.50 mmol) and **Pd-4** catalyst (0-5 mol%) was added (Table S4) to optimize the ideal condition. The reaction mixture was stirred for 24 h at 85 °C. The reaction was monitored by TLC analysis where formation of a new non-polar UV-active spot was observed corresponding to the product. The reaction mixture was passed through celite resin followed by silica-gel column chromatography (Ethyl acetate/Pet ether = 5/95).

Table S15. Amount of catalyst added and yield of product obtained.

Amount of Pd-4 catalyst (mol%)	**Yield (%)**
0	<5
0.5	39
1	51
1.5	63
2	68
2.5	75
3	80
4	79
5	82

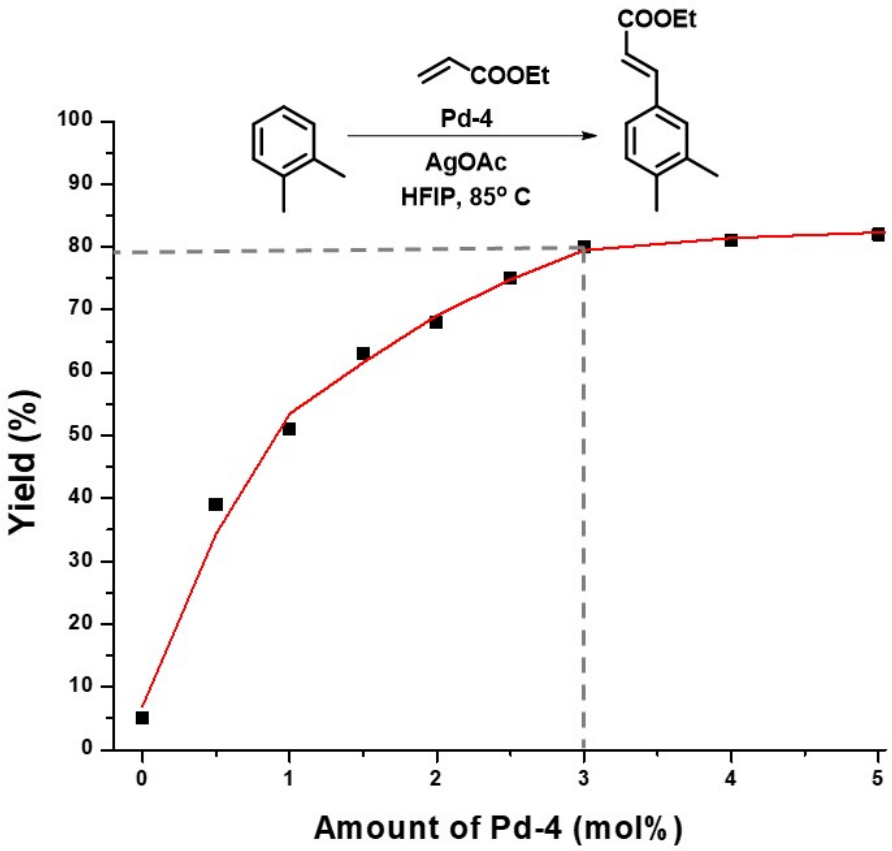


Figure S21. Schematic representation of yield of product formed upon change in amount of **Pd-4**.

Table S16. Optimization of solvent and oxidant.

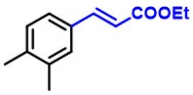
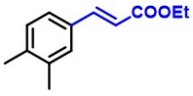
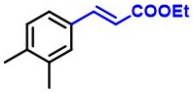
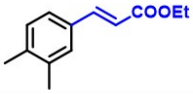
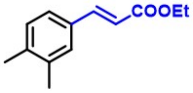
Substrate	Substrate	Oxidant	Solvent	Product	Temperature	Yield (%)
		AgOAc	HFIP		85 °C	80
		AgOAc	Dichloroethane		85 °C	20
		AgOAc	THF		70 °C	NA
		$Cu(OAc)_2$	HFIP		85 °C	< 5
		$FeCl_3$	HFIP		85 °C	< 5

Table S17. Control reactions.

Substrate	Substrate	Oxidant	Solvent	Catalyst	Temperature	Yield (%)
		AgOAc	HFIP	No	85 °C	< 5
		AgOAc	HFIP	**4** (3 mol%)	85 °C	< 5
		AgOAc	HFIP	$PdCl_2$ (3 mol%)	85 °C	38
		AgOAc	HFIP	**Cu-4** (3 mol%)	85 °C	< 5
		AgOAc	HFIP	**Ni-4** (3 mol%)	85 °C	< 5
		AgOAc	HFIP	**Pd-4** (3 mol%)	85 °C	80

General reaction scheme

The substrate, ***o*-xylene** (30 µL, 0.25 mmol) was dissolved in hexafluoroisoproponol (HFIP, 2 mL). To the mixture ethyl acrylate (53 µL, 0.50 mmol), Silver acetate (83 mg, 0.50 mmol) and **Pd-4** catalyst (3 mol%) was added and the reaction mixture was stirred for 24 h at 85 °C. The reaction was monitored by TLC analysis where formation of a new non-polar UV-active spot was observed corresponding to the product. The reaction mixture was passed through celite resin followed by silica-gel column chromatography (Ethyl acetate/Pet ether = 5/95).

6; Yield = 80% (40 mg) ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.67 (d, J = 16.0 Hz, 1H), 7.33 (s, 1H), 7.31 (s, 1H), 7.17 (d, J = 7.8 Hz, 1H), 6.41 (d, J = 16.0 Hz, 1H), 4.32 – 4.24 (m, 2H), 2.30 (s,

6H), 1.36 (t, J = 7.1 Hz, 5H). ^{13}C NMR (126 MHz, $CDCl_3$) δ = 167.31, 167.31, 144.82, 139.40, 137.11, 130.16, 129.29, 125.69, 116.96, 60.39, 19.81, 19.79, 14.36.

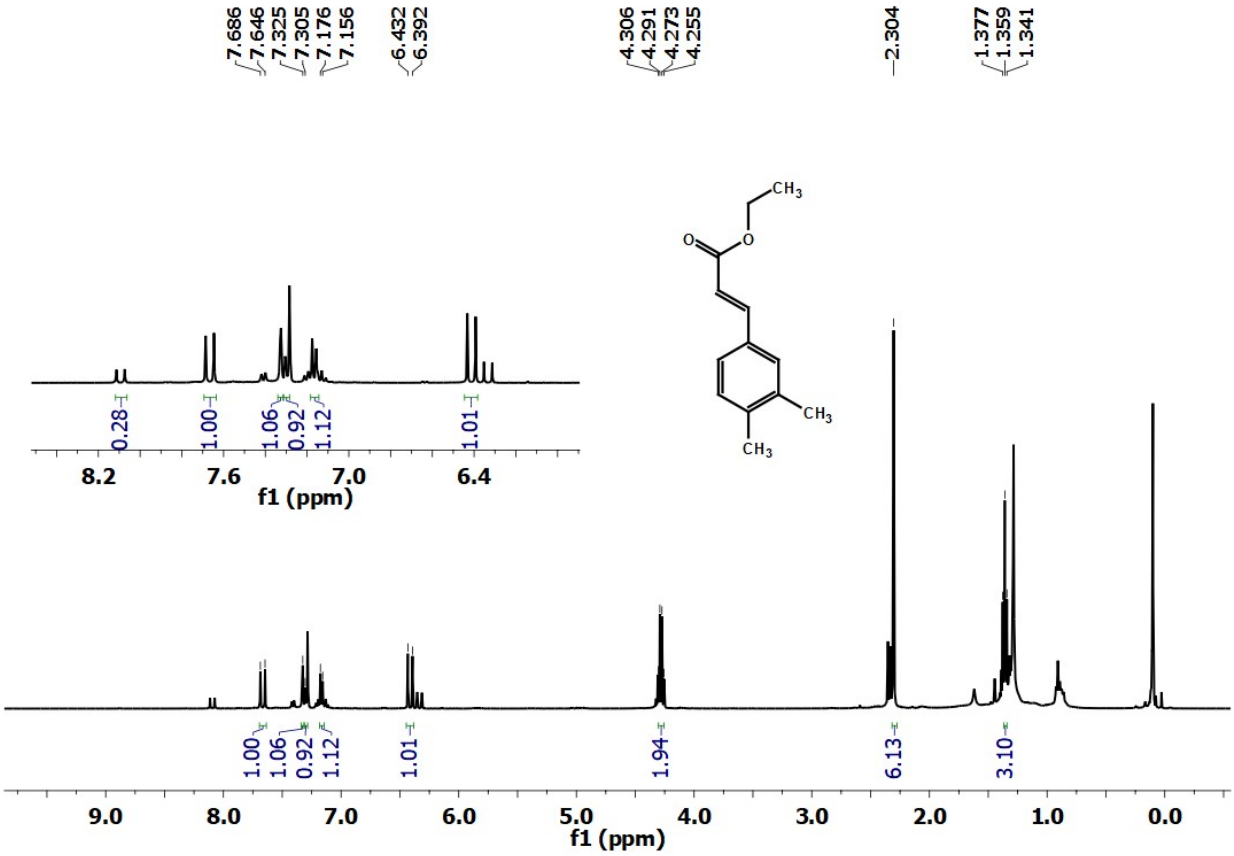


Figure S22. ^{1}H-NMR spectrum of **6** in $CDCl_3$ on 400 MHz instrument at room temperature. Note: Peaks marked with asterisk (*) are due to residual solvents.

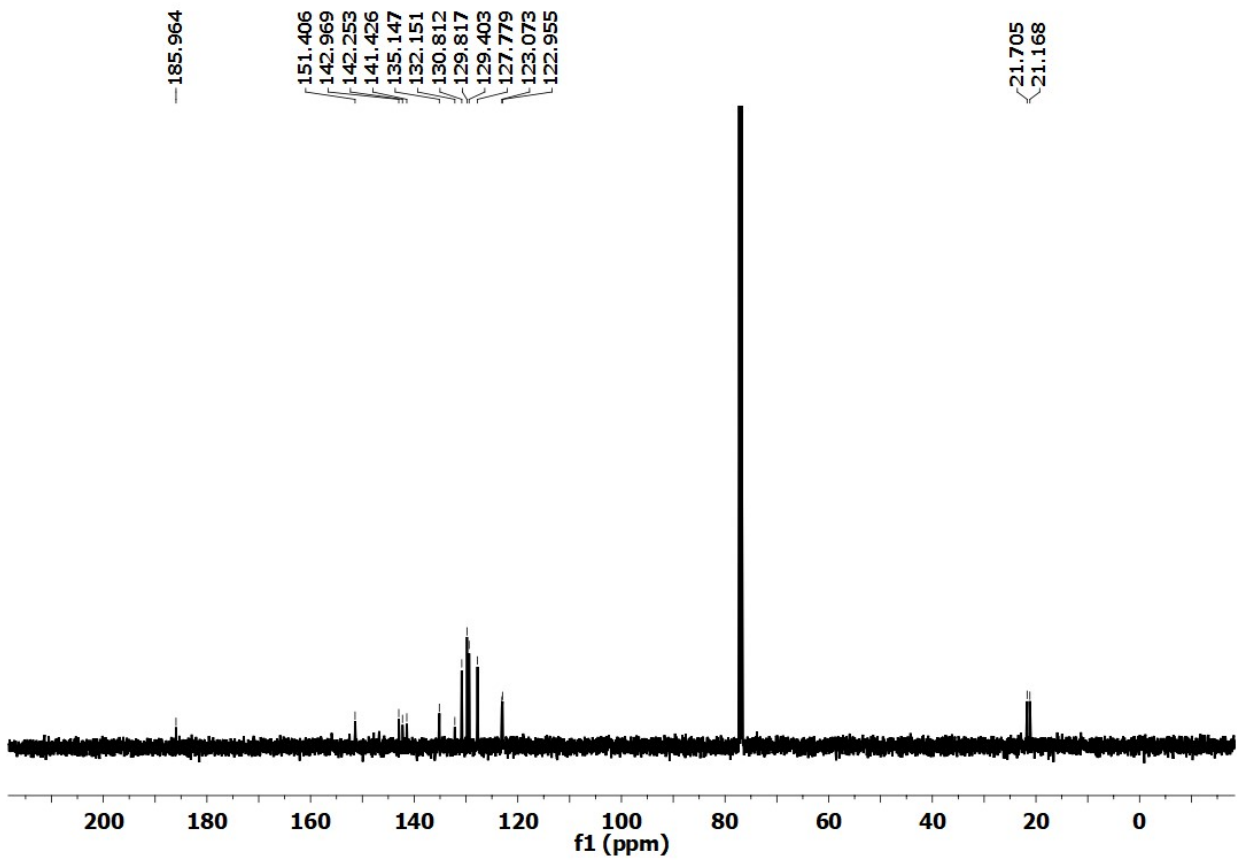


Figure S23. ^{13}C-NMR spectrum of **6** in $CDCl_3$ on 400 MHz instrument at room temperature. Note: Peaks marked with asterisk (*) are due to residual solvents.