Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Theoretical Study of Radiative and Nonradiative Decay Rates for Cu(I) Complexes with Double Heteroleptic Ligands

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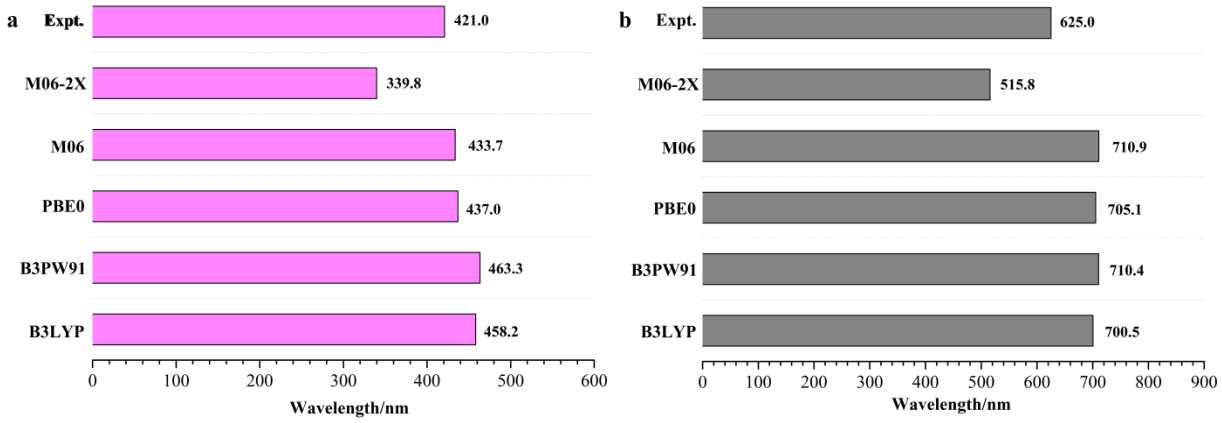


Fig. S1. Absorption(a) and emission(b) spectra obtained by TDDFT method with different functionals for **3**, together with experimentally (unit: nm).

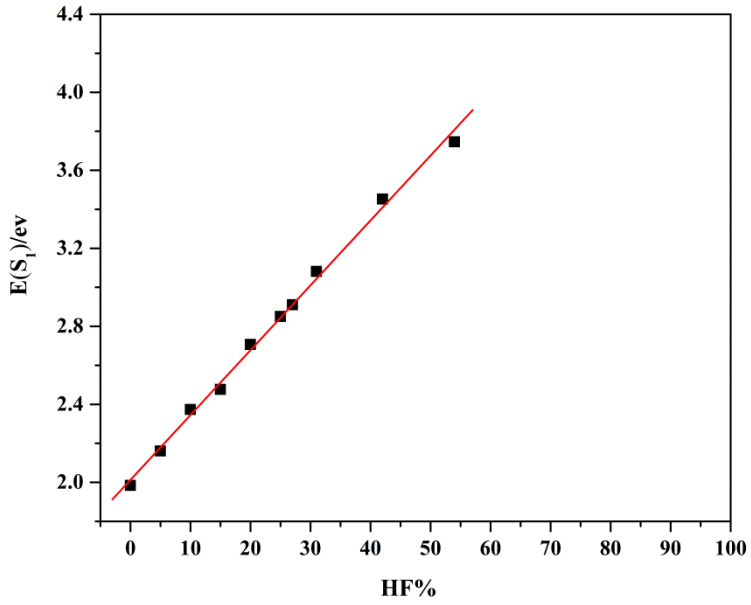


Fig. S2. Dependence of $E(S_1)$ of **3** on the HF% in TD-DFT functionals.

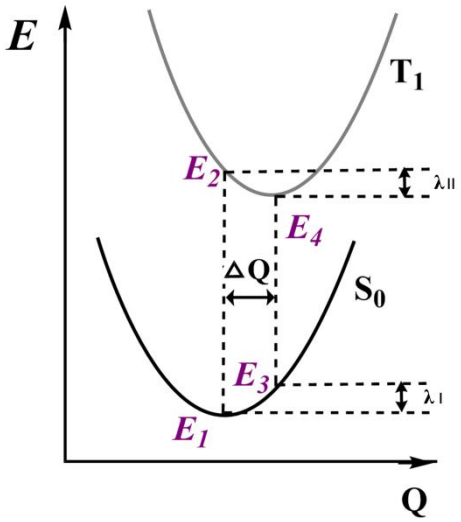


Fig. S3. *Dushin* program to deal with changes in the electronic state process of reorganization energy diagram.

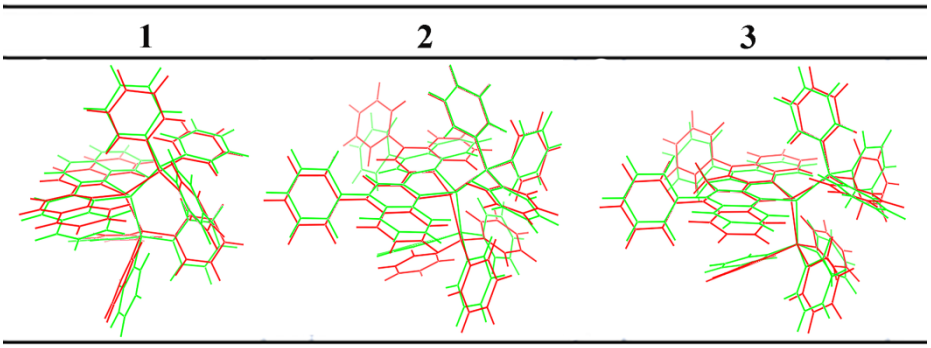


Fig. S4. Super imposed structures of S_0 (green) and T_1 (red) states of the studied complexes.

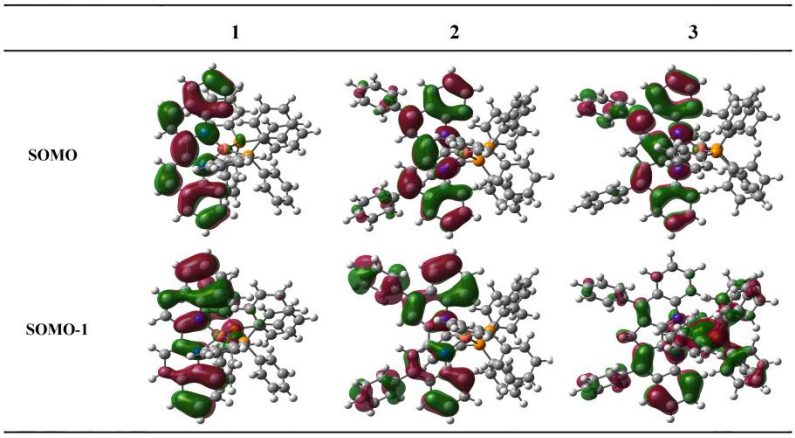
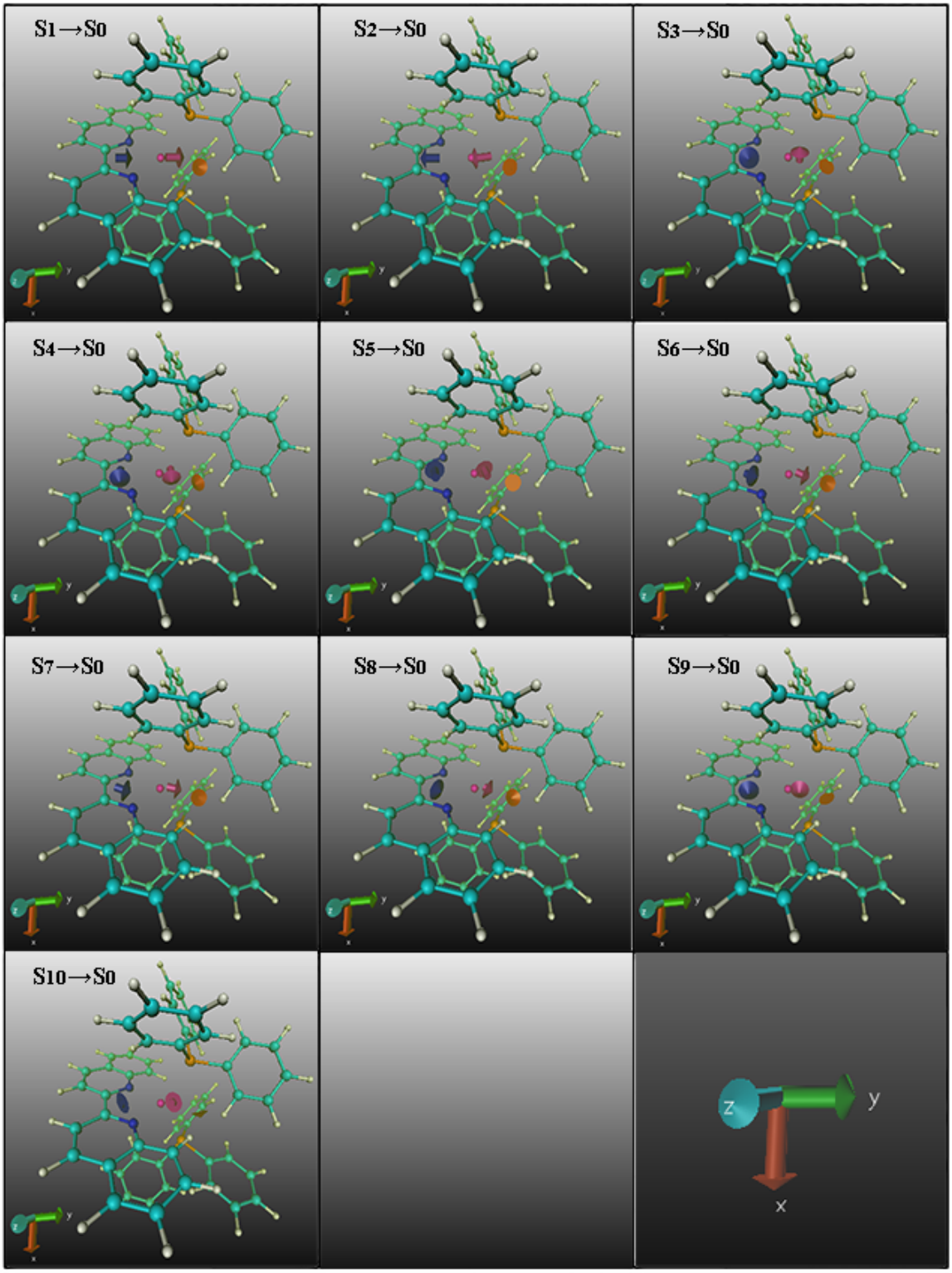


Fig. S5. Spin density plot for the lowest T_1 state for the complexes.

1



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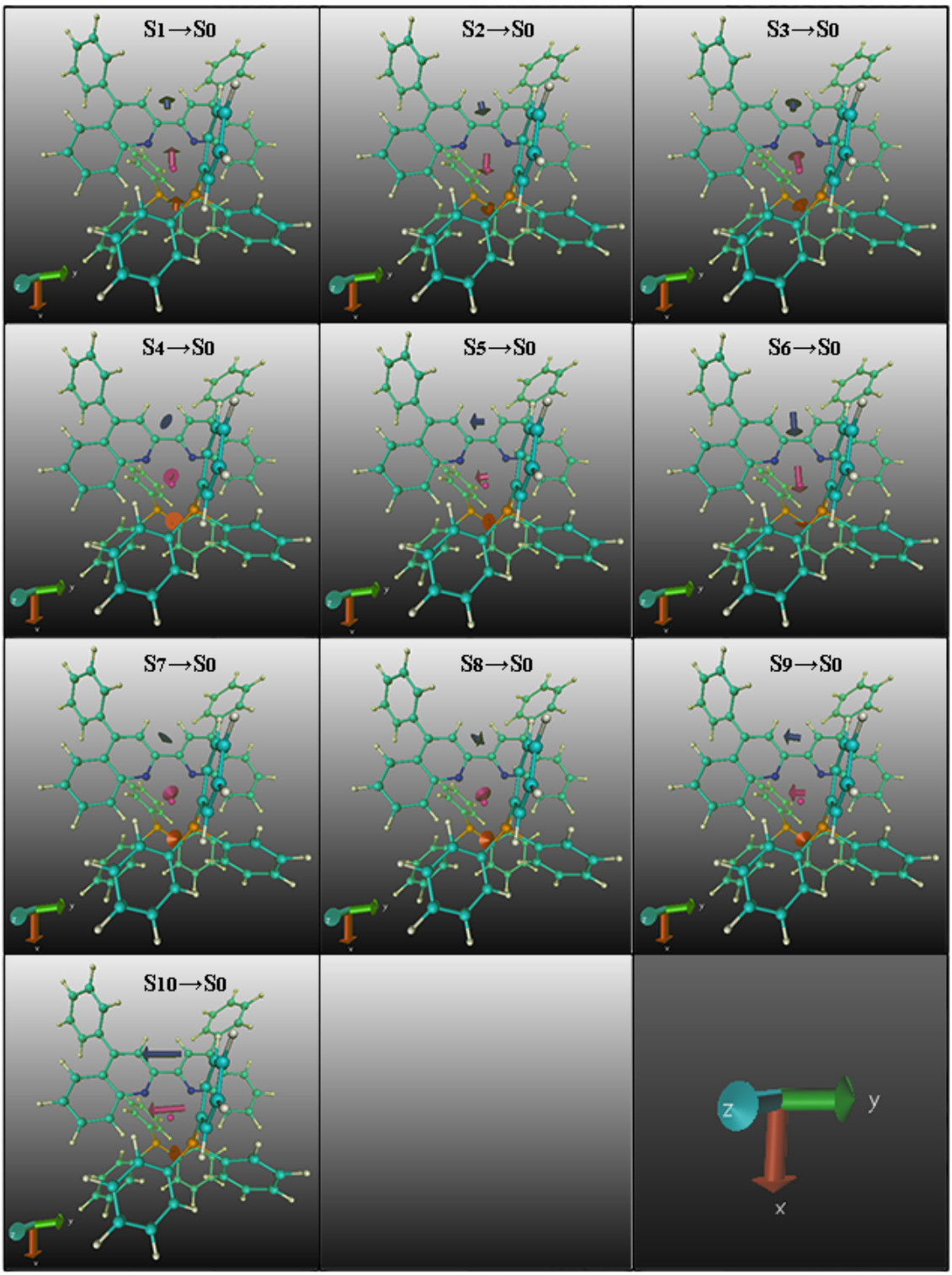


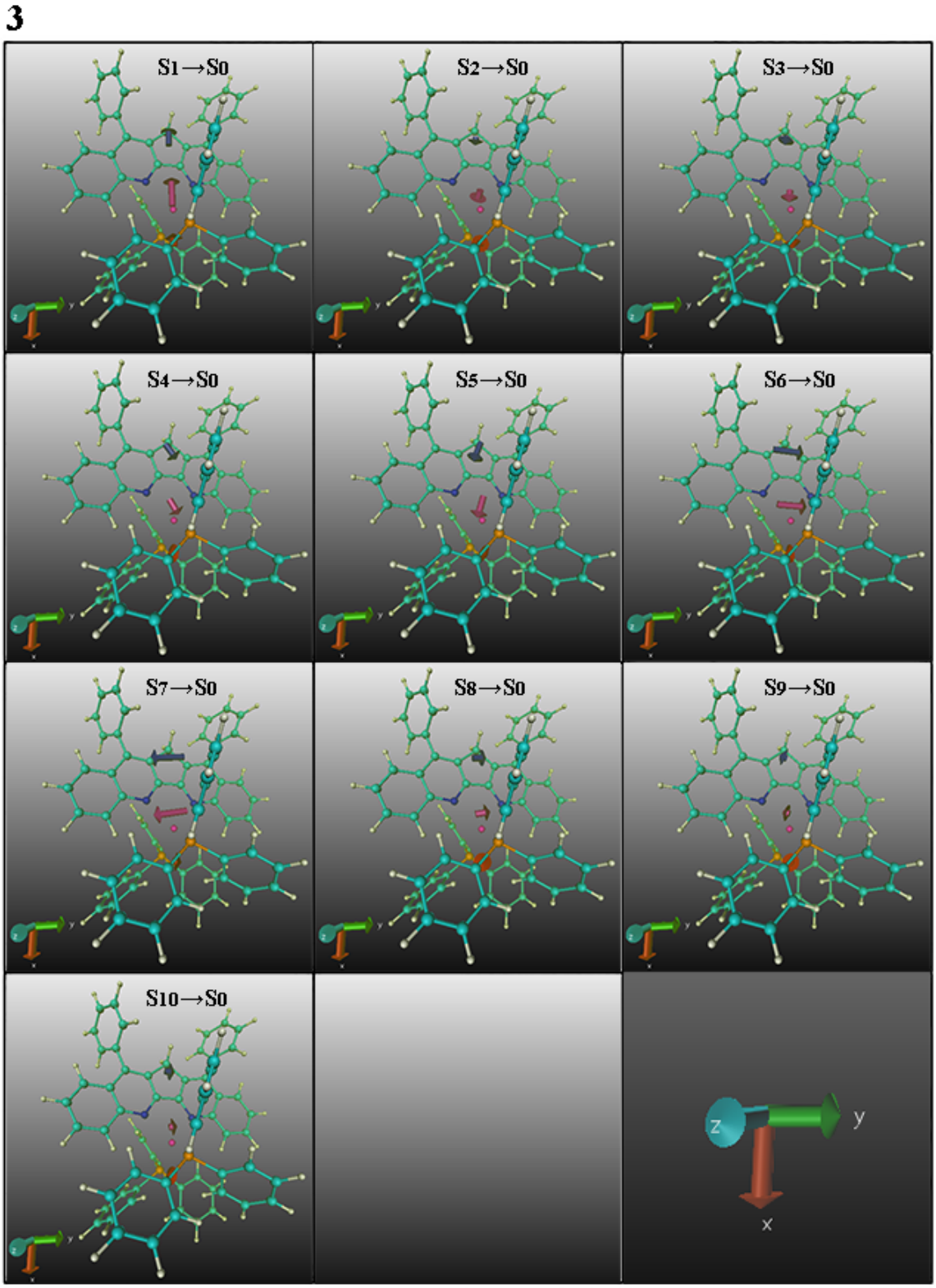
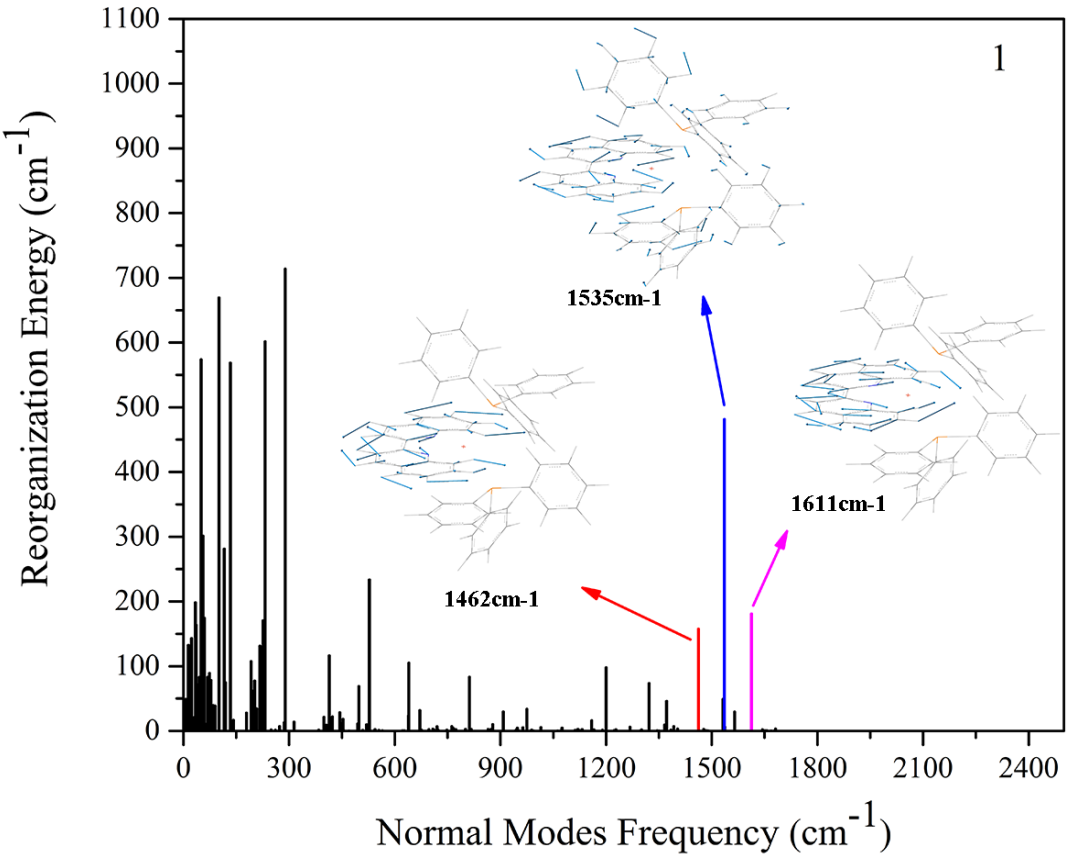


Fig. S6. The transition dipole moment vector of the contribution from N^N ligand, P^P ligand and the whole complex is described by the blue, orange and purple arrows, respectively.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1462cm-1
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Normal Modes Frequency (cm-1)
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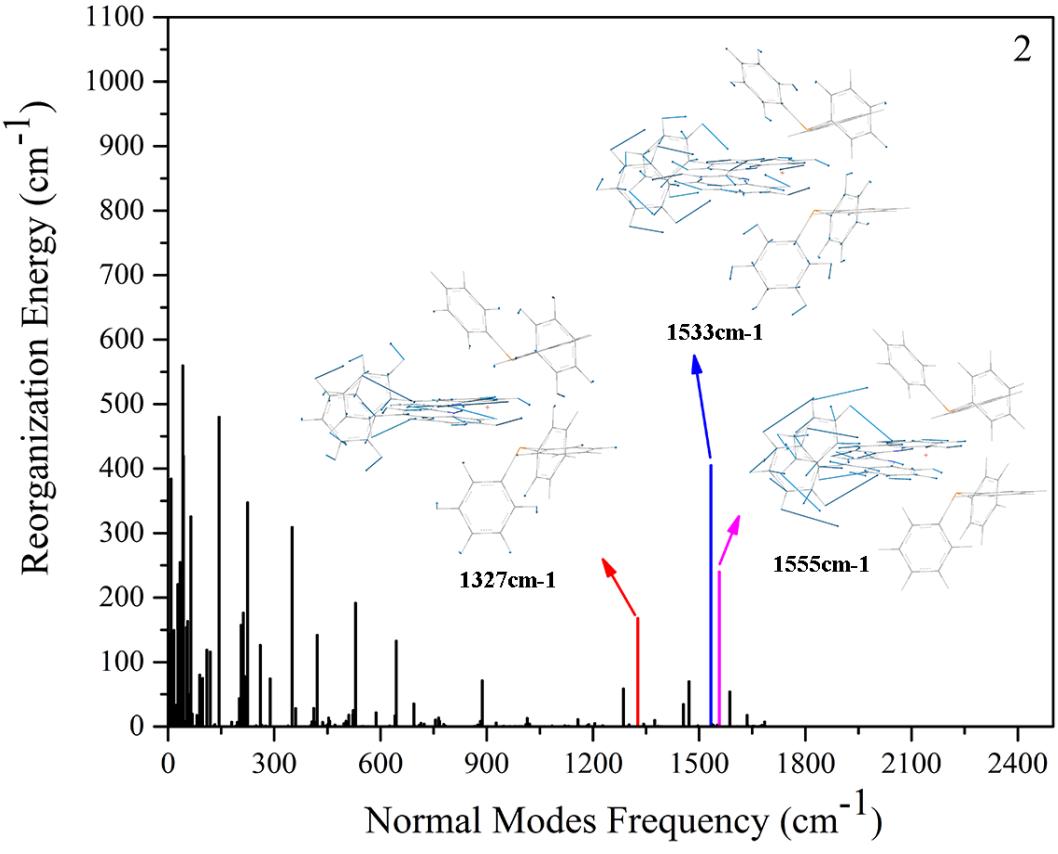
300
400
500
600
700
800
900
1000
1100
0
300
600
900
1200
1500
1800
2100
2400


2
1533cm-1
1555cm-1
1327cm-1
Reorganization Energy (cm-1)
Normal Modes Frequency (cm-1)
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500
600
700
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1200
1500
1800
2100
2400

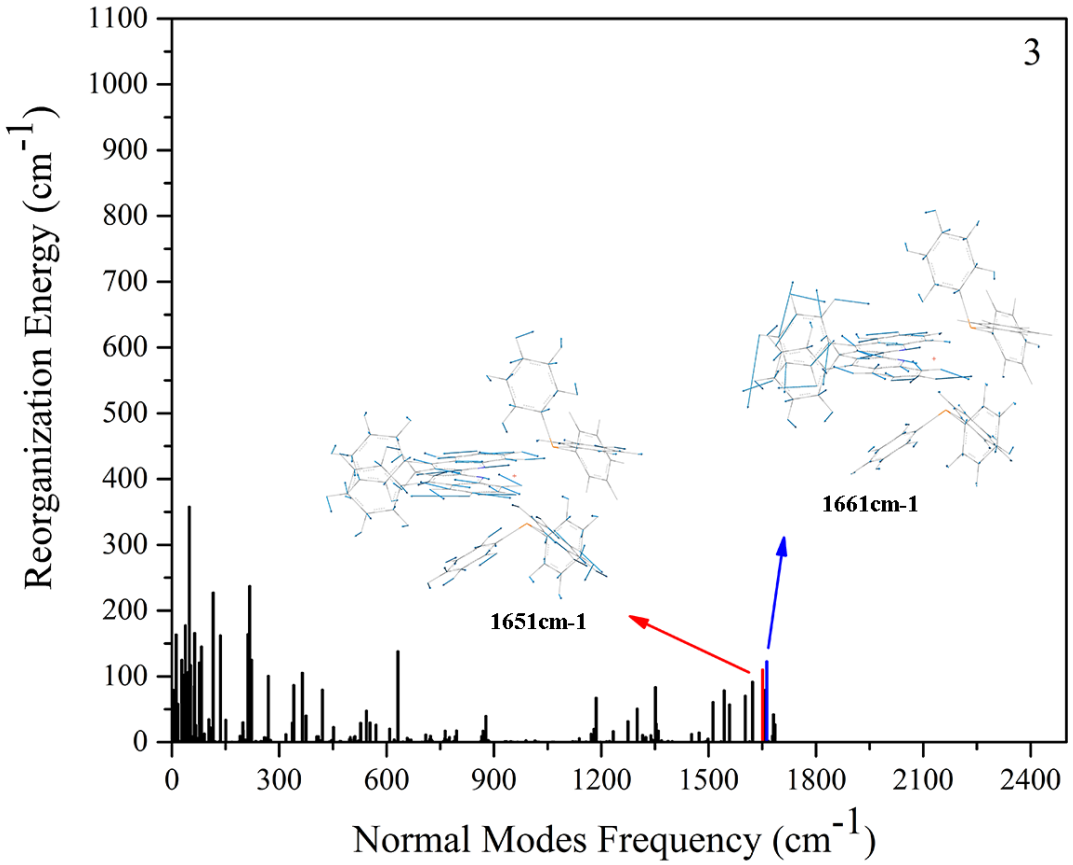
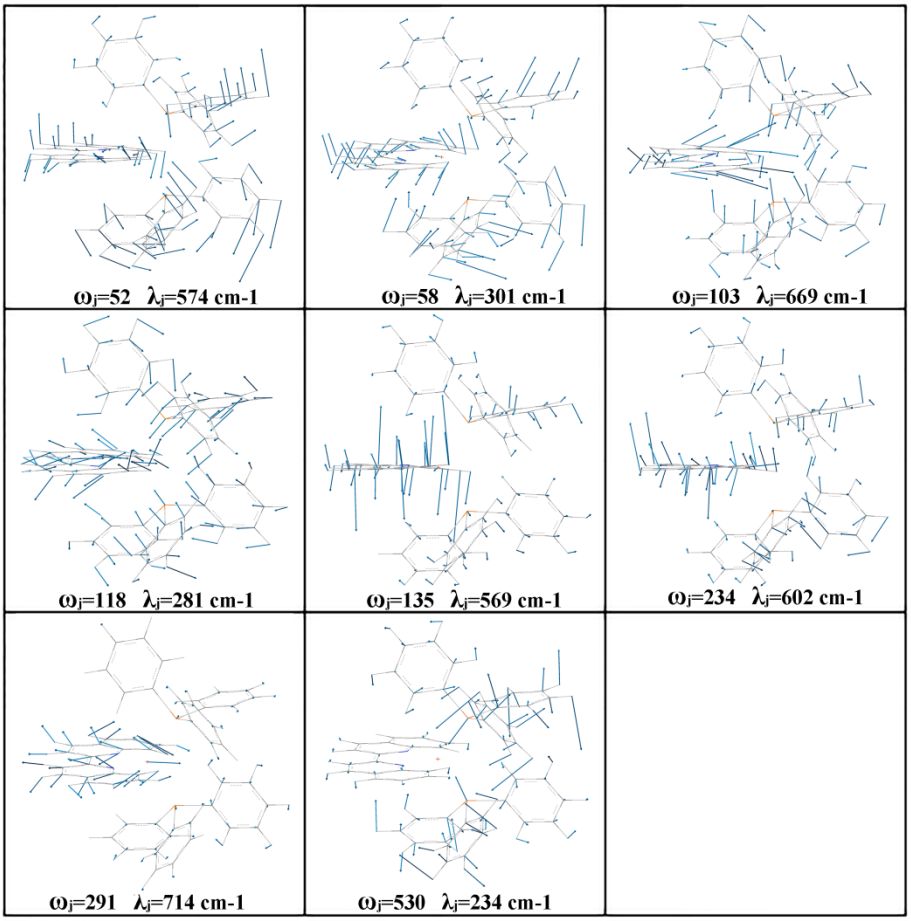


Fig. S7. Calculated reorganization energies and the displacement vectors for the normal modes with the largest reorganization energies over 100 cm^{-1} at high-frequency (inset).

1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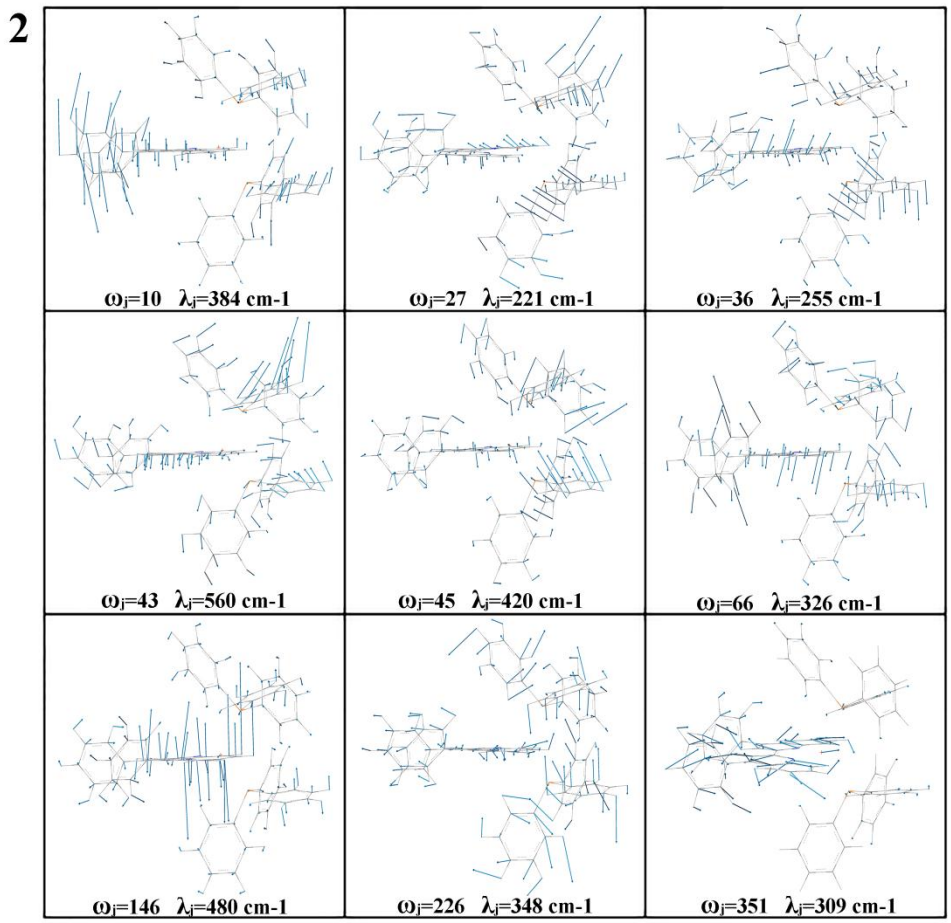
ωj=234 λj=602 cm-1
ωj=291 λj=714 cm-1
ωj=530 λj=234 cm-1



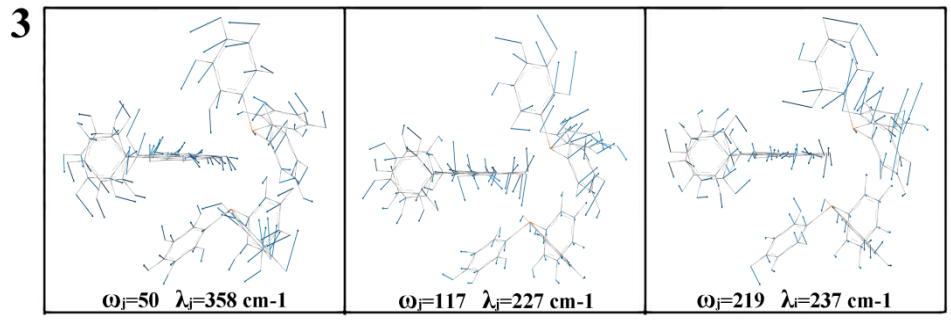


Fig. S8. Calculated reorganization energies and the displacement vectors for the normal modes with the reorganization energies over 200 cm^{-1} at low-frequency(inset).

Table S1 Partial optimized geometric structural parameters of **3** in the ground state by B3LYP, B3PW91, PBE0, M06 and M06-2X functionals, together with the observed experimentally.

	B3LYP	B3PW91	PBE0	M06	M06-2X	Expt.
$Cu\text{-}N_1$	2.2870	2.2620	2.2196	2.2216	2.2582	2.2275
$Cu\text{-}N_2$	2.2388	2.2220	2.2349	2.2116	2.2056	2.1372
$Cu\text{-}P_1$	2.4094	2.3828	2.3649	2.3297	2.3700	2.2851
$Cu\text{-}P_2$	2.3932	2.3693	2.3327	2.2768	2.4497	2.2319
$N_1\text{-}Cu\text{-}P_1$	109.25	109.13	104.93	102.35	103.24	101.95
$N_1\text{-}Cu\text{-}P2$	110.44	110.39	114.13	114.15	116.13	112.77
$N_2\text{-}Cu\text{-}P_1$	106.02	105.68	100.60	97.84	94.15	98.24
$N_2\text{-}Cu\text{-}P_2$	114.56	114.41	116.80	121.28	129.71	120.26
$N_1\text{-}Cu\text{-}N_2$	80.37	80.80	81.11	81.35	81.33	82.58
$P_1\text{-}Cu\text{-}P_2$	126.61	126.88	128.64	128.85	122.97	130.05
DHA_1	1.15	1.33	0.90	2.34	0.74	0.62

Table S2 The maximum absorption spectra $\lambda_{max(nm)}$ (oscillator strengths), emission spectra and experimental values of **3** calculated by different functionals.

	B3LYP	B3PW91	PBE0	M06	M06-2X	Expt
	λ_{max}/f	λ_{max}/f	λ_{max}/f	λ_{max}/f	$\lambda_{max(}/f$	λ_{max}
$S_0 \rightarrow S_1$	458.2/ 0.0892	463.3/ 0.0930	437.0/ 0.0975	433.7/ 0.0964	339.8/ 0.1490	421
$T_1 \rightarrow S_0$	684.6	698.4	748.8	719.2	426.9	631

Table S3 Calculated $E(S_1)$/ev using various functionals and LANL2DZ/6–31G(d) basis set in DCM solution for **3**.

	BLYP	MPWLYP1M	TPSSH	B3LYP*	B3LYP	PBE0	M06	MPW1B95	BMK	M062X
HF%	0	5	10	15	20	25	27	31	42	54
$E(S_1)$	1.9841	2.1605	2.3735	2.4763	2.7063	2.8500	2.9104	3.0813	3.4524	3.7458

Table S4 Absorption and emission values obtained by TD-DFT method with PBE0 and M06 for all, together with experimental values (unit: nm).

	PBE0		M06	
	λ^{Abs}_{max}/Expt	λ^{Em}_{max}/Expt	λ^{Abs}_{max}/Expt	λ^{Em}_{max}/Expt
1	430.2/420[a]	834.2/646[a]	429.2 /420[a]	851.5/646[a]
2	437.6/425[a]	811.9/648[a]	435.1/425[a]	742.8/648[a]
3	437.0/421[a]	705.1/625[a]	433.7/421[a]	719.2/625[a]

Table S5 Negative value of the HOMO ($-\varepsilon_{HOMO}$) and LUMO ($-\varepsilon_{LUMO}$) energies, HOMO-LUMO gaps calculated by DFT, and the lowest singlet energies (E_{S1}) calculated by TDDFT in eV for these complexes.

	$-\varepsilon_{HOMO}$	$-\varepsilon_{LUMO}$	$\Delta E_{H\text{-}L}$	E_{S1}
1	6.44	2.76	3.68	2.88
2	6.40	2.76	3.64	2.83
3	6.41	2.81	3.60	2.84

Table S6 Molecular orbital compositions of Cu at the optimized S_0 geometries in solvent DCM.

	MO	Energy(eV)	Cu contribution (%)
1	LUMO	-2.76	2.1(0.90d_{xz}+0.42d_{z^2})
	HOMO	-6.44	34.0(19.77 d_{xz}+4.25 d_{z^2}+0.86$d_{x^2-y^2}$)
	HOMO-1	-6.79	42.2(4.78 d_{xz}+0.95 d_{yz}+2.85 d_{xy}+3.03 d_{z^2}+21.45$d_{x^2-y^2}$)
	HOMO-2	-7.01	50.7 (38.61 d_{yz}+6.31 d_{xy}+0.77d_{xz}+2.09 $d_{x^2-y^2}$)
	HOMO-3	-7.08	27.4(24.64d_{yz}+0.16d_{xz}+0.25d_{z^2}+0.77$d_{x^2-y^2}$)
	HOMO-4	-7.29	2.3(0.45d_{xz}+0.20d_{yz})
2	LUMO	-2.76	2.0 (0.53d_{xz})
	HOMO	-6.40	33.3(11.07 d_{xz} +10.15 d_{z^2}+2.52$d_{x^2-y^2}$)
	HOMO-1	-6.80	41.8(5.38 d_{yz}+2.64 d_{xy}+9.63d_{xz}+13.21 d_{z^2}+1.86$d_{x^2-y^2}$)
	HOMO-2	-6.93	11.7 (7.54 d_{xy}+2.04d_{xz}+ 1.37 d_{z^2})
	HOMO-3	-7.03	51.5(3.91 d_{yz}+40.23 d_{xy}+3.49d_{xz}+0.74 d_{z^2}+0.60$d_{x^2-y^2}$)
	HOMO-4	-7.14	21.2(0.66 d_{yz}+13.87d_{xy}+1.69d_{xz}+1.06 d_{z^2}+0.65$d_{x^2-y^2}$)

3	LUMO+1	-1.66	$0.2(0.09d_{yz})$
	LUMO	-2.81	$1.4(0.61d_{xz})$
	HOMO	-6.41	$31.9(10.68d_{xz}+10.37\ d_{z^2}+1.48d_{x^2-y^2})$
	HOMO-1	-6.67	$58.2\ (18.35d_{z^2}+9.85\ d_{xz}+3.89d_{x^2-y^2})$
	HOMO-2	-6.95	$5.0(2.95\ d_{yz}+1.83\ d_{yz})$
	HOMO-3	-7.04	$3.4(1.84d_{x^2-y^2})$
	HOMO-4	-7.23	$66.4(4.92\ d_{yz}+1.15d_{xz}+58.03d_{xy}+0.05d_{z^2})$

Table S7 Molecular orbital compositions of Cu at the optimized S_0 geometries in gas phase.

	MO	Energy(eV)	Cu contribution (%)
1	LUMO	-4.66	$2.1(0.96d_{xz}+0.44d_{z^2})$
	HOMO	-8.21	$32.6(18.55\ d_{xz}+3.80\ d_{z^2}+0.62d_{x^2-y^2})$
	HOMO-1	-8.58	$39.39(3.43\ d_{xz}+2.34d_{xy}+3.05\ d_{z^2}+20.58d_{x^2-y^2})$
	HOMO-2	-8.86	$55.6\ (43.22d_{yz}+6.57d_{xy}+1.29d_{xz}+1.47d_{x^2-y^2})$
	HOMO-3	-8.94	$21.0(18.89d_{yz})$
	HOMO-4	-9.09	$1.54(0.77d_{xz})$
2	LUMO	-4.47	$2.0\ (0.54d_{xz})$
	HOMO	-8.07	$33.5(10.63\ d_{xz}+1.27d_{yz}+2.46d_{z^2}+9.80d_{x^2-y^2})$
	HOMO-1	-8.47	$40.5(5.25d_{yz}+2.26d_{xy}+9.54d_{xz}+12.49d_{z^2}+1.80d_{x^2-y^2})$
	HOMO-2	-8.61	$9.63(5.94d_{xy}+1.69d_{xz}+1.29d_{z^2})$
	HOMO-3	-8.73	$46.73(3.37d_{yz}+36.81d_{xy}+3.06d_{xz})$
	HOMO-4	-8.82	$28.7(19.97d_{xy}+2.39d_{xz}+1.36d_{z^2})$
3	LUMO+1	-3.36	$0.21(0.09d_{yz})$
	LUMO	-4.51	$1.4(0.34d_{z^2})$
	HOMO	-8.07	$31.3(10.53d_{xz}+0.63d_{xy}+9.72d_{z^2}+1.51d_{x^2-y^2})$
	HOMO-1	-8.35	$41.1(17.98d_{z^2}+9.18\ d_{xz}+1.23d_{yz}+3.65d_{x^2-y^2})$
	HOMO-2	-8.63	$4.7(2.70d_{xy}+1.80\ d_{yz})$
	HOMO-3	-8.72	$2.9(0.13d_{xy}+0.12d_{x^2-y^2})$
	HOMO-4	-8.92	$64.9(4.70\ d_{yz}+1.05d_{xz}+56.97d_{xy})$

Table S8 Molecular orbital compositions of Cu at the optimized T_1 geometries in solvent DCM.

	MO	Energy(eV)	Cu contribution (%)
1	LUMO	-3.10	3.8(0.96 d_z^2+0.87d_{yz})
	HOMO	-5.80	36.1(19.78 d_{xy}+9. 85d_{xz})
	HOMO-1	-6.76	41.3(1.23d_z^2+2.18d_{xy}+7.27 d_{xz}+2.20d_{yz}+10.91$d_{x^2-y^2}$)
	HOMO-2	-6.82	53.5 (15.60d_z^2+14.37 d_{xz}+9.80 $d_{x^2-y^2}$)
	HOMO-5	-7.41	9.5(1.79d_z^2+2.80d_{xz}+2.18d_{xy}+2.20d_{yz})
2	LUMO	-3.12	3.7(2.37 d_{xz})
	HOMO	-5.83	36.7(25.39 d_{xy} +5.55d_{xz})
	HOMO-1	-6.68	36.0(7.64d_z^2+1.35d_{xy}+0.85 d_{xz}+17.23d_{yz})
	HOMO-2	-6.76	58.4(33.26 d_{xy} +19.69 d_{xz})
	HOMO-5	-7.42	0.2(0.06 $d_{x^2-y^2}$+0.04d_{xz})
3	LUMO+1	-1.82	0.3(0.14d_{yz})
	LUMO	-3.09	2.3(1.48d_{xz})
	HOMO	-6.16	30.9 (15.39d_{xz}+6.64 d_{xy}+2.68d_z^2)
	HOMO-1	-6.63	39.3(11.58d_{yz}+1.37d_{xz}+16.75d_z^2+2.21 $d_{x^2-y^2}$)
	HOMO-2	-6.81	5.6 (0.05d_z^2)
	HOMO-5	-7.33	0.1(3.17d_{yz}+3.11d_z^2)

Table S9 Frontier molecular orbital energies(eV) and compositions (%) of different fragments in the ground state for the complexes.

MO	E/eV	MO composition (%)			Assign
		Cu	N^N	P^P	
1					
LUMO+5	-0.95	5.5	4.3	90.2	π*(P^P)
LUMO+4	-1.09	3.3	1.8	95.0	π*(P^P)
LUMO+3	-1.15	3.2	2.6	94.2	π*(P^P)
LUMO+2	-1.42	1.6	94.5	3.9	π*(N^N)
LUMO+1	-1.71	0.3	96.6	3.1	π*(N^N)
LUMO	-2.76	2.1	94.2	3.7	π*(N^N)
HOMO	-6.44	34.0	5.6	60.4	d(Cu)+π(P^P)

HOMO-1	-6.79	42.2	11.7	46.1	d(Cu)+π(N^N+P^P)
HOMO-2	-7.01	50.7	43.8	5.6	d(Cu)+π(N^N)
HOMO-3	-7.08	27.4	67.2	5.4	d(Cu)+π(N^N)
HOMO-4	-7.29	2.3	72.	25.7	π(N^N+P^P)
HOMO-5	-7.42	0.5	91.1	8.5	π(N^N)
2					
LUMO+5	-0.951	5.5	5.1	89.4	π*(P^P)
LUMO+4	-1.05	1.9	14.8	83.3	π*(N^N)+π*(P^P)
LUMO+3	-1.17	2.1	6.0	92.0	π*(P^P)
LUMO+2	-1.44	1.8	94.0	4.2	π*(N^N)
LUMO+1	-1.86	0.5	97.7	1.7	π*(N^N)
LUMO	-2.76	2.0	95.5	2.5	π*(N^N)
HOMO	-6.40	34.1	9.7	56.1	d(Cu)+π(P^P)
HOMO-1	-6.79	41.8	16.3	41.9	d(Cu)+π(N^N+P^P)
HOMO-2	-6.93	11.7	83.9	4.3	d(Cu)+π(N^N)
HOMO-3	-7.03	51.5	44.7	3.8	d(Cu)+π(N^N)
HOMO-4	-7.14	21.2	66.6	12.2	d(Cu)+π(N^N+P^P)
HOMO-5	-7.38	0.4	95.1	4.5	π(N^N)
3					
LUMO+5	-0.95	5.8	3.4	90.9	π*(P^P)
LUMO+4	-1.05	2.0	2.9	95.1	π*(P^P)
LUMO+3	-1.15	1.4	2.9	95.7	π*(P^P)
LUMO+2	-1.30	1.9	92.5	5.6	π*(N^N)
LUMO+1	-1.66	0.2	98.6	1.2	π*(N^N)
LUMO	-2.81	1.4	96.2	2.4	π*(N^N)
HOMO	-6.41	31.9	10.5	57.6	d(Cu)+π(N^N+P^P)
HOMO-1	-6.67	42.3	14.1	43.6	d(Cu)+π(N^N+P^P)
HOMO-2	-6.95	5.0	92.9	2.1	π(N^N)
HOMO-3	-7.04	3.4	84.0	12.6	π(N^N+P^P)
HOMO-4	-7.23	66.4	27.2	6.3	d(Cu)+π(N^N)
HOMO-5	-7.27	4.6	92.5	2.9	π(N^N)

Table S10 Frontier molecular orbital energies (eV) and compositions (%) of different fragments in the triplet state for the complexes.

MO	E/eV	MO composition (%)			Assign
		Cu	N^N	P^P	
1					
LUMO+5	-0.92	5.0	4.1	90.8	π*(P^P)
LUMO+4	-1.02	1.6	1.5	97.0	π*(P^P)
LUMO+3	-1.12	5.5	3.9	90.7	π*(P^P)
LUMO+2	-1.45	1.5	91.8	6.8	π*(N^N)
LUMO+1	-1.78	0.6	96.3	3.1	π*(N^N)
LUMO	-3.10	3.8	90.9	5.3	π*(N^N)
HOMO	-5.80	36.1	14.4	49.5	d(Cu)+π(N^N+P^P)
HOMO-1	-6.76	41.3	15.7	43.0	d(Cu)+π(N^N+P^P)
HOMO-2	-6.83	53.5	25.7	20.8	d(Cu)+π(N^N+P^P)
HOMO-3	-7.00	9.0	78.6	12.4	π(N^N+P^P)
HOMO-4	-7.29	7.2	63.3	29.5	π(N^N+P^P)
HOMO-5	-7.41	9.5	47.4	43.1	π(N^N+P^P)
2					
LUMO+5	-0.96	3.6	13.9	82.5	π*(N^N)+π*(P^P)
LUMO+4	-0.99	2.6	20.3	77.1	π*(N^N)+π*(P^P)
LUMO+3	-1.10	5.9	6.5	87.6	π*(P^P)
LUMO+2	-1.51	1.6	94.0	4.4	π*(N^N)
LUMO+1	-1.91	0.5	97.8	1.7	π*(N^N)
LUMO	-3.12	3.7	92.2	4.1	π*(N^N)
HOMO	-5.83	36.7	16.5	46.8	d(Cu)+π(N^N+P^P)
HOMO-1	-6.68	36.0	17.3	46.7	d(Cu)+π(N^N+P^P)
HOMO-2	-6.76	58.4	28.3	13.3	d(Cu)+π(N^N+P^P)
HOMO-3	-6.88	7.8	83.5	8.7	π(N^N)
HOMO-4	-7.13	7.2	75.7	17.1	π(N^N+P^P)
HOMO-5	-7.42	0.2	95.8	4.1	π(P^P)
3					
LUMO+5	-0.94	2.5	2.7	94.9	π*(P^P)
LUMO+4	-1.02	1.8	3.9	94.3	π*(P^P)
LUMO+3	-1.04	3.3	4.1	92.6	π*(P^P)

LUMO+2	-1.33	2.7	91.6	5.8	π*(N^N)
LUMO+1	-1.82	0.3	98.9	0.8	π*(N^N)
LUMO	-3.09	2.3	94.5	3.2	π*(N^N)
HOMO	-6.16	30.9	15.1	54.0	d(Cu)+π(N^N+P^P)
HOMO-1	-6.63	39.3	13.5	47.2	d(Cu)+π(N^N+P^P)
HOMO-2	-6.81	5.6	85.3	9.0	π(N^N)
HOMO-3	-7.01	11.3	82.0	6.7	d(Cu)+π(N^N)
HOMO-4	-7.05	65.7	26.3	8.0	d(Cu)+π(N^N)
HOMO-5	-7.33	0.1	99.5	0.5	π(N^N)

Table S11 SOC matrix elements $< T_1^{\alpha}|H_{SOC}|S_m>(cm^{-1})$, the transition dipole moment $M_{S_{m,j}}$ of **1** calculated at the T_1^{opt} optimized geometry with DCM included. The radiative decay rate constant (k_r/s^{-1}) is also given.

$E(T_1)$=11988cm^{-1}

S_m	$M_{S_{m,j}}$	$M_{S_{m,j}}$	$M_{S_{m,j}}$	$<T_1^x\|H_{SOC}\|S_m>$		$<T_1^y\|H_{SOC}\|S_m>$		$<T_1^z\|H_{SOC}\|S_m>$
				Re	Im	Re	Im	Im
S_1	0.0008	-0.6330	-0.4067	-8.0561	-30.8048	-8.0561	30.8048	8.8035
S_2	0.0773	0.5922	0.5199	127.6256	-8.6501	127.6256	8.6501	-55.9092
S_3	0.1912	-0.5392	-0.0193	57.2251	-58.3964	57.2251	58.3964	166.6064
S_4	-0.6639	-0.2856	0.1479	0.8508	-8.9057	0.8508	8.9057	-3.7694
S_5	-0.6324	-0.3100	0.3045	10.0211	-88.8470	10.0211	88.8470	-104.9409
S_6	0.0419	0.4374	0.0835	4.5139	9.8495	4.5139	-9.8495	15.8400
S_7	-0.7361	0.0936	0.4877	89.0185	174.5850	89.0185	-174.5850	426.6527
S_8	0.1658	0.2371	-0.0366	76.1690	-11.8938	76.1690	11.8938	-0.8565
S_9	-0.1707	-0.2073	0.1563	0.6071	-52.4358	0.6071	52.4358	4.0796
S_{10}	1.2138	0.9098	-0.7204	-16.4388	-9.8422	-16.4388	9.8422	6.4022
k_m^x				5985.70				
k_m^y						5985.70		
k_m^z								2568.82
k_r						**4846.74**		

a $M_{S_{m,j}}$ is the j-axis ($j \in x, y, z$)ojection of the $S_m \rightarrow S_0$ transition dipole moment .

b the superscript α denotes the spin sub-level (*x, y,* or *z*) of the T_1 excited state.

c $k_r(T_1 \rightarrow S_0) = \frac{1}{3}\sum_\alpha k_r^\alpha$

d (T_1^α) is the energy shift (cm^{-1}) of the spin sub-level α (α = *x, y,* or *z*) due to SOC with the Sm excited state. $E(T_1)$ is taken as the reference point.

Table S12 SOC matrix elements $< T_1^\alpha|H_{SOC}|S_m>$($cm^{-1}$), the transition dipole moment $M_{S_{m,j}}$ of **2** calculated at the T_1^{opt} optimized geometry with DCM included. The radiative decay rate constant (k_r/s^{-1}) is also given.

$E(T_1)$= 12371cm^{-1}

S_m	$M_{S_{m,j}}$	$M_{S_{m,j}}$	$M_{S_{m,j}}$	$<T_1^x\|H_{SOC}\|S_m>$		$<T_1^y\|H_{SOC}\|S_m>$		$<T_1^z\|H_{SOC}\|S_m>$
				Re	Im	Re	Im	Im
S_1	-1.0561	0.0438	0.0486	32.0066	4.1489	32.0066	-4.1489	2.7563
S_2	1.2269	0.0339	0.0725	15.8802	-136.1803	15.8802	136.1803	41.6169
S_3	0.5371	-0.1055	-0.3296	105.6034	21.3574	105.6034	-21.3574	-81.2957
S_4	0.1742	-0.1292	-0.2380	-2.4138	2.1208	-2.4138	-2.1208	21.2989
S_5	0.0610	-0.7402	0.0191	-39.1828	-79.6429	-39.1828	79.6429	-174.1596
S_6	-1.2169	-0.0655	-0.0502	-2.4743	-1.1103	-2.4743	1.1103	-2.4205
S_7	0.4284	-1.2015	0.2444	42.5899	42.7375	42.5899	-42.7375	514.7130
S_8	0.1043	1.0373	-0.2440	37.2695	-22.2640	37.2695	22.2640	9.3032
S_9	-0.0062	1.3071	-0.2028	-9.1107	-20.0546	-9.1107	20.0546	60.8538
S_{10}	0.1307	1.2340	-0.1321	-0.4287	-10.5200	-0.4287	10.5200	-9.6280
k_m^x				4908.30				
k_m^y						4908.30		
k_m^z								9514.32
k_r						**6443.64**		

Table S13 SOC matrix elements $< T_1^{\alpha}|H_{SOC}|S_m>$($cm^{-1}$), the transition dipole moment $M_{S_{m,j}}$ of **3** calculated at the T_1^{opt} optimized geometry with DCM included. The radiative decay rate constant (k_r/s^{-1}) is also given.

$E(T_1)$= 14182cm^{-1}

S_m	$M_{S_{m,j}}$	$M_{S_{m,j}}$	$M_{S_{m,j}}$	$<T_1^x\|H_{SOC}\|S_m>$		$<T_1^y\|H_{SOC}\|S_m>$		$<T_1^z\|H_{SOC}\|S_m>$
				Re	Im	Re	Im	Im
S_1	-1.5978	0.0092	-0.1665	88.6776	-49.0399	88.6776	49.0399	-7.9374
S_2	0.3655	-0.1326	-0.3594	12.2639	114.9570	12.2639	-144.9570	-52.7289
S_3	0.4827	-0.0437	0.0686	114.9070	-61.8399	114.9070	61.8399	18.5976
S_4	0.7062	0.4484	-0.0807	65.3256	-24.8984	65.3256	24.8984	-198.1577
S_5	1.0978	-0.4620	0.1104	12.0904	-165.7141	12.0904	165.7141	-365.5163
S_6	0.0497	2.1554	-0.4749	-2.4853	-5.6882	-2.4853	5.6882	8.3283
S_7	0.3610	-1.4467	0.3576	-2.1243	-4.1736	-2.1243	4.1736	-1.5673
S_8	0.0026	-0.0263	0.0119	-12.9428	14.8570	-12.9428	-14.8570	-23.4307
S_9	0.0550	-0.4595	0.0008	-14.0689	14.1006	-14.0689	-14.1006	11.3669
S_{10}	0.0697	-0.2017	0.1314	-9.9454	-19.9932	-9.9454	19.9932	50.9251
k_m^x				6565.84				
k_m^y						6565.84		
k_m^z								35154.51
k_r						**16095.39**		