Electronic Supplementary Material (ESI) for Materials Advances.

Effect of metal ions in the electron-transfer mechanism on the photovoltaic performance of SALPHEN-based DSSC: Experimental and theoretical studies

José Guadalupe Hernández[1], Carlos Alberto Huerta Aguilar[2], Jayanthi Narayanan[3*], Eduardo Daniel Tecuapa Flores[3], Pandiyan Thangarasu[4*], Aldo Hernández Ramírez[3], Karthika Shanmugam[5], Mayra Margarita Luna Martinez[3]

[1]Centro Tecnológico, Facultad de Estudios Superiores (FES-Aragón), Universidad Nacional Autónoma de México (UNAM), Estado de México, CP 57130, México.

[2]Instituto Tecnológico de Estudios Superiores de Monterrey (ITESM), Puebla, CP 72453, México.

[3]División de Ingeniería en Nanotecnología, Universidad Politécnica del Valle de México, Av. Mexiquense s/n esquina Av. Universidad Politécnica, Estado de México, CP 54910, México.

[4]Facultad de Química, Universidad Nacional Autónoma de México (UNAM), Ciudad Universitaria, CDMX, CP 04510, México.

[5]School of Chemical Engineering, Vellore Institute of Technology, Vellore 632014, Tamil Nadu, India.

*Corresponding authors E-mail address: jnarayanan@upvm.edu.mx; pandiyan@unam.mx

Table S1. Optical properties of SALPHEN by DGDZVP double-zeta basis set and 6-311++G(d, p) triple-zeta basis set with different functionals (B3LYP, CAM-B3LYP, B3PW91 and B3P86) at gaseous state.

FUNCTIONAL	SALPHEN	HOMO (eV)	LUMO (eV)	ΔE	μ	η	ω	χ	ω^-	ω^+
B3LYP	DGDZVP	-6.154	-2.134	4.020	4.144	2.010	-4.272	-4.144	0.640	-0.736
CAM-B3LYP	DGDZVP	-7.625	-0.838	6.787		3.394				
B3LYP	6-31G**	-5.826	-1.830	3.996	3.828	1.998	-3.667	-3.828	0.604	-0.773
B3LYP	6-311++G(d,p)	-6.204	-2.240	3.964	-4.222	1.982	-4.496	-4.222	0.657	-0.721
B3PW91	6-311++G(d,p)	-6.305	-2.307	3.998	-4.306	1.999	-4.639	-4.306	0.664	-0.717
B3P86	6-311++G(d,p)	-6.872	-2.863	4.009	-4.867	2.004	-5.910	4.867	0.732	-0.675

Where: HOMO= ionization potential (IP); LUMO= electron affinity (EA); ΔE= Relative energy; μ= chemical potential; and η=chemical hardness of the ligand; χ= electronegativity; ω= electrofphilic index, ω^-= electrodonation (a small value of ω^- makes a system a better electron donor), ω^+= electroacceptance (a large value of ω^+ makes a better charge acceptor).

ΔE=(I-A); μ=-(I+A)/2; η=(ΔE/2); ω=(I^2)+2*(IA)+(A^2)/(2*(I-A)); μ=-χ =-(I+A)/2; ω^- =2*(3I+A)/(16*(I-A)); (ω^+) ω^+=(2*(I+3A))/(16*(I-A)); ω=(μ^2/2η); ω=(I^2)+2*(IA)+(A^2)/(2*(I-A);) ω=$(I+A)^2$/(2*(I-A)).;

Table S2. Condensed–to-atom Fukui Indexes for ligand SALPHEN at gaseous state.

B3LYP/DGDZVP							B3LYP/6-31G**						Hirsfeld (B3LYP/DGDZVP)	NPA (B3LYP/6-31G**)
Gaseous state														
	Hirshfeld charge			Fukui			NPA charge			Fukui			descriptor dual (DD)=$f^{(2)}(r)$	
L^1	N	N-1	N+1	$f^{(+)}$	$f^{(-)}$	$f^{(o)}$	N	N-1	N+1	$f^{(+)}$	$f^{(-)}$	$f^{(o)}$	$f^{(2)}®$=f(+)(r)-f(-)(r)	$f^{(2)}®$=f(+)(r)-f(-)(r)
N1	-0.395	-0.391	-0.351	0.044	-0.004	0.020	-0.602	-0.655	-0.351	0.251	0.053	-0.503	0.048	0.198
N2	-0.395	-0.424	-0.351	0.044	0.029	0.037	-0.602	-0.654	-0.351	0.251	0.052	-0.503	0.015	0.199
O1	-0.55	-0.588	-0.499	0.051	0.038	0.045	-0.568	-0.608	-0.499	0.069	0.040	-0.554	0.013	0.029
O2	-0.55	-0.592	-0.499	0.051	0.042	0.047	-0.568	-0.600	-0.499	0.069	0.032	-0.550	0.009	0.037
C1	0.212	0.163	0.227	0.015	0.049	0.032	0.233	0.259	0.227	-0.006	-0.026	0.243	-0.034	0.020
C2	0.212	0.231	0.227	0.015	-0.019	-0.002	0.233	0.280	0.227	-0.006	-0.047	0.254	0.034	0.041
C3	-0.125	-0.229	-0.119	0.006	0.104	0.055	0.167	0.078	-0.119	-0.286	0.089	-0.021	-0.098	-0.375
C4	-0.125	-0.215	-0.119	0.006	0.090	0.048	0.167	0.124	-0.119	-0.286	0.043	0.003	-0.084	-0.329
C5	0.162	0.164	0.179	0.017	-0.002	0.007	0.048	0.076	0.179	0.131	-0.028	0.128	0.019	0.159
C6	0.162	0.15	0.179	0.017	0.012	0.015	0.047	0.044	0.179	0.132	0.003	0.112	0.005	0.129
C7	0.252	0.22	0.262	0.010	0.032	0.021	0.307	0.278	0.262	-0.045	0.029	0.270	-0.022	-0.074
C8	0.252	0.229	0.262	0.010	0.023	0.017	0.307	0.296	0.262	-0.045	0.011	0.279	-0.013	-0.056
N1	-	-	-	0.284	0.000	0.142	-0.533	-0.534	-0.263	0.270	0.001	0.135	0.284	0.270

	0.492	0.492	0.208											
O1	-0.392	-0.405	-0.389	0.003	0.013	0.008	-0.555	-0.585	-0.551	0.005	0.029	0.017	-0.010	-0.025
F1	-0.241	-0.251	-0.240	0.001	0.010	0.005	-0.277	-0.326	-0.276	0.001	0.049	0.025	-0.009	-0.048
F2	-0.244	-0.251	-0.243	0.001	0.007	0.004	-0.278	-0.308	-0.277	0.001	0.029	0.015	-0.006	-0.028
F3	-0.248	-0.824	-0.246	0.002	0.576	0.289	-0.274	-0.344	-0.272	0.001	0.070	0.036	-0.575	-0.069

Descriptor dual (DD)=$f^{(2)}(r)$; $f^{(2)}$®=$f^{(+)}(r)$-$f^{(-)}(r)$.

Table S3. Dipole moment (μ, Debyes), polarizability (α, esu) and hyperpolarizability (β, esu) for SALPHEN.

Functionals	B3LYP			CAM-B3LYP	B3PW91	B3P86
Parameters/basis set	dgdzvp	6-31G**	6-311++G(d,p)	dgdzvpz	6-311++G(d,p)	
$\mu t_{otal\ (D)}$	0.2305	0.1122	0.6174	0.1511	0.3968	0.4153
α_{Total}(esu.cm)	$3.6767x10^{-16}$	$3.5904x10^{-16}$	$2.7551x10^{-16}$	$3.5249x10^{-16}$	$2.6397x10^{-16}$	$2.6415x10^{-16}$
β_{total}(esu.cm)	$-5.5539x10^{-16}$	$-5.5391x10^{-16}$	$5.7937x10^{-19}$	$-7.3558x10-^{16}$	$1.5211x10^{-18}$	$1.4342x10^{-18}$
Δα (esu.cm)	$1.9051X10^{-19}$	$1.2532X10^{-19}$	4.3593e-19	$1.3080e^{-19}$	$2.8005e^{-19}$	$2.9348e^{-19}$

1Debyes=$1X10^{-18}$ esu. cm

Table S4. Components of the polarizability tensor α_{xx}, α_{yy} and α_{zz} (ua), Energy (E, in Hartree), dipole moment (μ in Debye) and Root mean-square of deviation (RMSD, Debye)

	Double.zeta basis sets				**Triple -zeta basis sets**					
Functional	**B3LYP/dgdzvp,**		**CAM-B3LYP/dgdzvp**		**B3LYP/6-311++G(d,p)**		**B3PW91/6-311++G(d,p)**		**B3P86/6-311++G(d,p)**	
Bond length complexes (Å)	**Spin**		**Spin**		**Spin**		**Spin**		**Spin**	
[Co(SALPHEN)(H_2O)]	**S=1/2**	**S=3/2**	**S=1/2**	**S=3/2**	**S=1/2**	**S=3/2**	**S=1/2**	**S=3/2**	**S=1/2**	**S=3/2**
Dipole Moment (D)	**3.3189**	**4.9670**	**7.3882**	**3.5646**	**3.3419**	**3.1410**	**3.2407**	**2.8039**	**3.2286**	**3.3847**
α_{xx}**(ua)**	**0.0190**	**-1.0888**	**-0.6558**	**0.0089**	**0.3490**	**0.0209**	**0.0258**	**0.0763**	**0.0285**	**0.1419**

α_{yy}**(ua)**	**3.3053**	**4.6340**	**7.2786**	**3.5548**	**3.3235**	**4.1409**	**3.2268**	**2.7043**	**3.2286**	**3.2278**
α_{zz}**(ua)**	**-0.2993**	**1.4186**	**1.0851**	**-0.2644**	**-0.0167**	**-0.0166**	**-0.2985**	**0.7367**	**-0.3224**	**1.0086**
Δα (D)	**2.44**	**3.51**	**5.11**	**2.61**	**2.24**	**2.22**	**2.72**	**1.67**	**2.40**	**1.95**
E_{HF}	**-2489.72**	**-2489.71**	**-2489.20**	**-2489.19**	**-2489.12**	**-2490.11**	**-2489.62**	**-2489.61**	**-2493.81**	**-2493.50**
RMSD**(D)**	**3.92e-9**	**2.91e-9**	**4.70e-9**	**4.80e-9**	**9.00e-9**	**5.45e-9**	**6.66e-9**	**5.98e-9**	**8.48e-9**	**7.97e-9**
[Fe(SALPHEN)Cl(H_2O)]	**S=1/2**	**S=3/2**	**S=1/2**	**S=3/2**	**S=1/2**	**S=3/2**	**S=1/2**	**S=3/2**	**S=1/2**	**S=3/2**
Dipole Moment (D)	**5.2562**	**4.9637**	**4.1702**	**5.0566**	**4.3298**	**5.0046**	**4.4298**	**5.2812**	**4.9036**	**4.7889**
α_{xx}**(D)**	**1.1889**	**-0.4145**	**0.1471**	**0.2849**	**0.1769**	**0.3824**	**0.1869**	**0.3117**	**1.0122**	**0.4039**
α_{yy}**(D)**	**4.2945**	**2.6711**	**3.0919**	**3.0149**	**3.4837**	**2.9916**	**3.5837**	**3.4328**	**4.1137**	**2.8271**
α_{zz}**(D)**	**-2.7879**	**-4.1627**	**-2.7945**	**-4.0499**	**-2.4973**	**-3.9937**	**-2.5973**	**-4.0013**	**-2.46**	**-3.8443**
Δα (D)	**4.19**	**4.19**	**3.60**	**4.36**	**3.69**	**4.32**	**3.79**	**5.00**	**4.03**	**4.14**
E_{HF}	**-2830.85**	**-2830.87**	**-2830.32**	**-2830.34**	**-2830.41**	**-2831.32**	**-2830.44**	**-2830.46**	**-2835.29**	**-2835.30**
RMSD**(D)**	**1.14xe-9**	**1.09xe-9**	**9.75xe-10**	**4.08xe-10**	**6.31e-9**	**1.13e-9**	**6.41e-9**	**6.18e-9**	**2.82e-9**	**1.21e-9**

[Cu(SALPHEN)]	**S=1/2**	**S=3/2**	**S=1/2**	**S=3/2**	**S=1/2**	**S=3/2**	**S=1/2**	**S=3/2**	**S=1/2**	**S=3/2**
Dipole Moment (D)	**4.7536**	**3.0711**	**5.1145**	**2.6786**	**4.6671**	**1.9045**	**5.1579**	**2.2692**	**4.5912**	**2.8782**
α_{xx}**(D)**	**-0.0002**	**0.8310**	**0.0001**	**1.6071**	**0.000**	**0.000**	**0.0001**	**0.000**	**0.0001**	**-0.8782**
α_{yy}**(D)**	**4.7530**	**2.9565**	**5.1139**	**2.1429**	**4.665**	**1.9045**	**5.1572**	**2.2692**	**4.5906**	**2.7397**
α_{zz}**(D)**	**-0.0758**	**-0.0032**	**0.0779**	**-0.0001**	**0.0748**	**0.0014**	**0.0851**	**0.0018**	**0.0734**	**0.0022**
Δα (D)	**3.39**	**1.87**	**3.59**	**1.37**	**3.27**	**1.35**	**3.62**	**1.60**	**3.22**	**2.31**
E_{HF}	**-2670.90**	**-2670.82**	**-2670.42**	**-2670.34**	**-2671.35**	**-2671.27**	**-2670.62**	**-2670.54**	**-2674.92**	**-2674.85**
RMSD**(D)**	**$2.86e^{-9}$**	**$6.38e^{-9}$**	**$1.65e^{-9}$**	**$2.13e^{-9}$**	**$7.11e^{-9}$**	**$4.65e^{-9}$**	**$4.42e^{-9}$**	**$4.61e^{-9}$**	**$7.72e^{-9}$**	**$9.45e^{-9}$**

μ=Dipole moment (Debye), Polarizability tensor α_{xx}, α_{yy} and α_{zz} (ua); Δα= Anisotropy polarizability (Debye), Hartree Fock energy (Hartree), RMSD= Root mean-square of deviation (Debye).

Table S5. Bond lengths (Å) and bond angles (°) resulted in ground state and excited state for SALPHEN and it´s complexes, using Functional B3LYP, CAM-B3LYP/DGDZVP double-zeta basis set and functionals B3LYP, B3PW91, B3P86/6-311++(d, p) triple-zeta basis set at level of theory.

Functional	**B3LYP/dgdzvp,**		**CAM-B3LYP/dgdzvp**		**B3LYP/6-311++G(d, p)**		**B3PW91/6-311++G(d,p)**		**(B3P86/6-311++G)**	
Bond length complexes (Å)	**Spin**		**Spin**		**Spin**		**Spin**		**Spin**	

[Co(SALPHEN)(H_2O)]	S=1/2	S=3/2	S=1/2	S=3/2	S=1/2	S=3/2	S=1/2	S=3/2	S=1/2	S=3/2
Co-N1	1.916	2.125	1.900	2.038	1.916	2.052	1.900	2.103	1.896	2.095
Co-N2	1.916	2.071	1.900	2.039	1.917	2.052	1.900	2.051	1.896	2.042
Co-O1	1.915	1.931	1.872	1.985	1.904	1.996	1.898	1.943	1.892	1.931
Co-O2	1.916	1.984	1.870	1.986	1.914	1.998	1.898	1.971	1.893	1.976
Co-OH2	2.348	2.218	4.137	2.225	2.383	1.304	2.348	2.212	2.314	2.135
Bond angle (°)										
N1-Co-N2	84.8	77.9	85.4	80.8	84.8	80.5	84.9	78.3	84.9	79.0
N1-Co-O1	94.0	88.4	94.7	90.8	93.9	90.5	93.9	88.4	94.0	88.1
N1-Co-O2	175.7	164.6	179.5	166.7	176.6	167.4	175.7	165.9	175.8	165.5
N1-Co-O3	101.4	95.4	133.1	109.7	102.5	107.3	100.8	98.1	101.1	100.1
N2-Co-O1	175.5	147.3	179.5	166.7	174.5	167.2	175.6	151.6	175.6	149.4
N2-Co-O2	94.0	88.6	94.8	90.8	93.7	90.4	93.9	88.1	93.9	88.3
N2-Co-O3	101.1	106.9	141.4	109.5	98.9	107.0	100.6	110.0	100.8	109.3
O1-Co-O2	86.8	107.0	85.2	95.5	87.3	96.9	87.0	105.8	86.9	106.4
O1-Co-O3	83.4	103.8	38.6	83.0	86.5	84.3	83.8	96.5	83.6	100.2
O2-Co-O3	82.9	106.9	46.8	82.7	80.7	83.6	83.5	80.8	83.1	77.3

[Fe(SALPHEN)Cl(H_2O)]	S=1/2	S=3/2	S=1/2	S=3/2	S=1/2	S=3/2	S=1/2	S=3/2	S=1/2	S=3/2
Fe-N1	1.934	1.953	1.925	1.950	1.931	1.970	1.932	1.956	1.922	1.950
Fe-N2	1.946	1.964	1.938	1.938	1.905	1.962	1.936	1.948	1.926	1.941
Fe-O1	1.883	1.887	1.864	1.866	1.843	1.888	1.863	1.875	1.861	1.872
Fe-O2	1.865	1.888	1.843	1.863	1.833	1.885	1.853	1.871	1.849	1.869
Fe-OH2	4.411	4.246	4.302	4.162	4.137	4.237	4.287	4.166	4.285	4.164
Fe-Cl	2.237	2.307	2.214	2.289	2.255	2.313	2.285	2.349	2.221	2.288
Bond angle (°)										
N1-Fe-N2	83.3	82.6	83.1	82.6	83.9	82.4	83.9	83.2	83.5	82.7
N1-Fe-O1	93.7	92.1	93.6	92.0	92.9	91.7	92.8	91.7	93.4	92.1
N1-Fe-O2	157.9	159.3	156.7	155.1	159.8	155.3	159.5	156.3	160.4	156.0
N1-Fe-O3	96.3	45.5	98.5	101.6	97.0	100.4	97.2	101.2	95.5	100.3
N1-Fe-Cl	97.3	96.4	97.0	99.4	94.5	99.6	94.8	97.9	95.5	99.1
N2-Fe-O1	167.0	155.0	167.0	159.3	165.6	158.9	165.5	160.7	165.9	160.0
N2-Fe-O2	92.3	92.1	92.2	92.0	92.5	91.7	92.0	91.7	92.6	92.1
N2-Fe-O3	43.3	101.9	42.3	44.5	42.8	46.6	43.1	44.7	43.9	45.6
N2-Fe-Cl	91.8	100.0	91.2	95.7	91.2	96.8	91.4	94.5	103.8	95.7

O1-Fe-O2	85.6	84.3	85.9	84.4	86.1	85.2	86.2	85.5	85.7	84.8
O1-Fe-O3	149.7	91.3	150.5	155.6	152.3	154.2	151.3	154.1	150.3	154.3
O1-Fe-Cl	101.1	104.9	101.7	104.9	102.7	104.1	102.9	104.6	101.8	104.2
O2-Fe-O3	95.2	154.6	93.1	91.1	92.3	92.6	93.3	91.1	94.9	92.4
O2-Fe-Cl	104.5	104.3	105.9	105.4	105.7	104.9	105.4	105.6	103.8	104.8
O3-Fe-Cl	49..3	52.7	50.3	53.3	50.6	51.6	49.6	51.8	49.1	51.6
[Cu(SALPHEN)]	**S=1/2**	**S=3/2**	**S=1/2**	**S=3/2**	**S=1/2**	**S=3/2**	**S=1/2**	**S=3/2**	**S=1/2**	**S=3/2**
Cu-N1	1.981	1.974	1.965	1.946	1.977	1.965	1.963	1.951	1.958	1.952
Cu-N2	1.981	1.974	1.965	1.954	1.977	1.965	1.963	1.951	1.958	1.950
Cu-O1	1.935	1.921	1.911	1.971	1.922	1.922	1.911	1.908	1.907	1.893
Cu-O2	1.935	1.980	1.911	1.895	1.922	1.922	1.911	1.908	1.907	1.947
Bond angle (°)										
N1-Cu-N2	83.5	84.2	83.6	84.5	83.5	84.8	84.2	85.5	83.7	84.3
N1-Cu-O1	93.6	94.1	93.5	93.4	93.2	93.8	93.0	93.7	93.5	83.9
N1-Cu-O2	177.1	177.7	177.1	178.6	176.7	178.7	177.3	179.2	177.2	177.8
N2-Cu-O1	177.1	178.2	177.1	177.8	176.7	178.7	177.3	179.2	177.2	178.2
N2-Cu-O2	93.6	93.5	93.5	94.2	93.2	93.8	90.0	93.7	93.5	93.4

O1-Cu-O2	89.3	88.3	89.4	88.0	90.1	87.5	89.8	87.2	89.3	88.3

Table S6. The optimized geometrical data of SALPHEN and its complexes with Fe(II), Co(II) and Cu(II) at gaseous state

SALPHEN	Basis set/Bond length (Å)		
Atom´s	DGDZVP	6-31G**	6-311++G(d, p)
C1-C2	1.421	1.420	1.420
N1-C1	1.416	1.413	1.413
N2-C2	1.416	1.413	1.413
N2-C3	1.292	1.293	1.293
N1-C4	1.294	1.293	1.293
C3-C5	1.453	1.449	1.449
C4-C6	1.453	1.449	1.449
C5-C7	1.424	1.424	1.424
C6-C8	1.424	1.424	1.424
C7-O2	1.350	1.341	1.341
C8-O1	1.350	1.341	1.341

Table S7. Condensed Mulliken charges of SALPHEN with its complexes Fe(III), Co(II9 and Cu(II) at gaseous state.

SALPHEN	B3LYP/DGDZVP	B3LYP/6-31G**	B3LYP/DGDZVP			
	Gaseous state		atoms	$[Fe(SALPHEN)Cl(H_2O)]^{2+}$	$[Co(SALPHEN)(H_2O)]^{2+}$	$[Cu(SALPHEN)]^{2+}$
N1	-0.395	-0.602	N1	-0.383	-0.400	-0.352
N2	-0.395	-0.602	N2	-0.345	-0.399	-0.352
O1	-0.550	-0.568	O1	-0.484	-0.518	-0.488
O2	-0.550	-0.568	O2	-0.501	-0.520	-0.488
C1	0.212	0.233	O3	-0.873	-0.813	-
C2	0.212	0.233	Cl	-0.282	-	-

C3	-0.125	0.167	M	0.623	0.720	0.583
C4	-0.125	0.167	C1	0.382	0.367	0.360
C5	0.162	0.047	C2	0.361	0.367	0.360
C6	0.162	0.048	C3	-0.147	-0.170	-0.129
C7	0.252	0.307	C4	0.140	-0.170	-0.129
C8	0.252	0.307	C5	0.429	0.119	0.088
			C6	-0.099	0.119	0.088
			C7	0.137	0.381	0.411
			C8	0.407	0.381	0.411

Table S8. Electronic properties of the ligand SALPHEN and it´s complexes at gaseous state.

Gaseous state		**Spin**	**E_{HF}**	**HOMO (eV)**	**LUMO (eV)**	**ΔE (eV)**	**Hardness (η, eV)**	**Softness (σ, eV)**	**Oscilltor Strength (f)**
		Functiona/Double-zeta basis set							
SALPHEN	B3LYP/DGDZVP	GS	-1031.81	-6.154	-2.134	4.020	2.010	0.497	0.4016
	B3LYP/6-31G**	GS	-1031.75	-5.826	-1.830	3.996	1.998	0.500	0.2845
$[Fe(SALPHEN)Cl(H_2O)]^{2+}$	B3LYP/DGDZVP	GS	-2830.85	-6.020	-2.764	3.256	1.628	0.614	0.0651
		ES	-2830.87	-6.217	-3.372	2.844	1.422	0.703	0.0565
$[Co(SALPHEN)(H_2O)]^{2+}$		GS	-2489.72	-5.476	-2.375	3.101	1.551	0.645	0.1950
		ES	-2489.71	-5.498	-2.290	3.208	1.604	0.624	0.1741
$[Cu(SALPHEN)]^{2+}$		GS	-2670.90	-5.742	-2.980	2.762	1.381	0.724	0.6320
		ES	-2670.82	-5.683	-4.499	1.184	0.592	1.689	0.2934

		Functional/Triple-zeta basis set							
SALPHEN	B3PW91/6-311++G(d,p)	GS	-1031.28	-6.305	-2.307	3.998	1.999	0.503	0.2941
$[Fe(SALPHEN)Cl(H_2O)]^{2+}$		GS	-2830.44	-6.066	-2.739	3.327	1.664	0.601	0.0922
		ES	-2830.46	-6.314	-3.198	3.116	1.558	0.642	0.0607
$[Co(SALPHEN)(H_2O)]^{2+}$		GS	-2489.62	-5.482	-2.441	3.041	1.521	0.658	0.1452
		ES	-2489.62	-5.606	-2.339	3.267	1.633	0.612	0.1365
$[Cu(SALPHEN)]^{2+}$		GS	-2670.62	-5.787	-2.529	3.258	1.629	0.614	0.3343
		ES	-2670.54	-5.558	-4.872	0.686	0.343	2.914	0.3113

Table S9. TD-DFT spectral data of electronic transitions SALPHEN at gaseous state and it is complexes, with oscillator strength f > 0.0001. using B3LYP/DGDZVP **double-zeta basis set**.

Wevelength (nm)	Osc. Strength (f)	Contribution percentage B3LYP/DGDZVP Double-zeta basis set	Character	Theory (nm)	Experimental (nm)
		[Fe(SALPHEN)Cl(H$_2$O)], S=1/2			Agregar los valores UV experimentales obtenidos
1234.2	0.0004	HOMO->LUMO+1 (15%) HOMO-2->LUMO+1 (11%) HOMO-2->LUMO (8%)	MLCT		

		HOMO-6->LUMO (7%) HOMO-3->LUMO (7%) HOMO-3->LUMO+1 (7%) HOMO-11->LUMO (6%) HOMO-3->LUMO (6%)			
1154.1	0.0013	HOMO-3->LUMO (15%) HOMO-2->LUMO (13%) HOMO-1->LUMO (11%) HOMO->LUMO (11%) HOMO-5->LUMO (7%) HOMO-4->LUMO (7%) HOMO-12->LUMO (6%) HOMO-3->LUMO (4%)	MLCT		
1014.4	0.0111	HOMO->LUMO (45%) HOMO-5->LUMO (8%) HOMO-3->LUMO (7%) HOMO-6->LUMO (6%) HOMO-13->LUMO (5%) HOMO-1->LUMO (4%)	MLCT	997	
768.8	0.0013	HOMO-1->LUMO (61%) HOMO->LUMO (6%) HOMO-2->LUMO (5%) HOMO-1->LUMO+1 (5%) HOMO->LUMO+1 (5%) HOMO-3->LUMO (4%)	MLCT		
731.8	0.0001	HOMO-6->LUMO (40%) HOMO-5->LUMO (8%) HOMO-4->LUMO+1 (8%) HOMO-3->LUMO+1 (7%) HOMO-11->LUMO (4%) HOMO-3->LUMO (4%)	MLCT		

627.2	0.0026	HOMO-5->LUMO (26%) HOMO->LUMO (25%) HOMO-6->LUMO (8%) HOMO->LUMO (6%) HOMO-1->LUMO+1 (5%)	MLCT		
577.7	0.0001	HOMO->LUMO+4 (11%) HOMO->LUMO+2 (10%) HOMO-2->LUMO+4 (9%) HOMO-3->LUMO+3 (8%) HOMO-5->LUMO (7%) HOMO->LUMO+3 (6%) HOMO-1->LUMO+3 (5%) HOMO-3->LUMO+4 (4%) HOMO->LUMO+1 (4%) HOMO-11->LUMO+3 (4%)	MLCT		
548.5	0.0018	HOMO->LUMO+1 (18%) HOMO-1->LUMO (17%) HOMO->LUMO+2 (17%) HOMO-1->LUMO+1 (13%) HOMO-1->LUMO+2 (13%) HOMO->LUMO+2 (5%)	MLCT		
540.3	0.0008	HOMO->LUMO+2 (22%) HOMO->LUMO+1 (13%) HOMO->LUMO (10%) HOMO-1->LUMO (7%) HOMO-1->LUMO+1 (5%) HOMO-1->LUMO+2 (5%)	MLCT		
506.0	0.0019	HOMO-2->LUMO (33%)	MLC	507	

		HOMO-3->LUMO (31%) HOMO->LUMO+1 (7%) HOMO->LUMO+1 (5%)	T		
494.4	0.0083	HOMO-1->LUMO (35%) HOMO->LUMO+1 (14%) HOMO->LUMO+1 (8%) HOMO-1->LUMO+2 (7%) HOMO-2->LUMO+1 (5%) HOMO-1->LUMO+1 (5%) HOMO-1->LUMO+3 (4%)	MLC T		
481.4	0.0072	HOMO->LUMO (17%) HOMO-1->LUMO (14%) HOMO-3->LUMO (10%) HOMO->LUMO+3 (8%) HOMO-2->LUMO+1 (5%) HOMO-1->LUMO (5%) HOMO-2->LUMO+2 (5%) HOMO->LUMO+2 (5%)	MLC T		
473.5	0.0139	HOMO-1->LUMO+1 (41%) HOMO->LUMO+1 (14%) HOMO-2->LUMO+1 (10%) HOMO-1->LUMO+1 (5%)	MLC T		
459.8	0.0026	HOMO-6->LUMO+3 (11%) HOMO->LUMO+2 (10%) HOMO-1->LUMO+1 (8%) HOMO->LUMO+1 (3%) H0MO-4->LUMO+4 (6%) HOMO-3->LUMO+4 (6%)	MLC T		

		HOMO-1->LUMO+1 (4%)			
458.7	0.0078	HOMO-6->LUMO+3 (10%) HOMO-2->LUMO+1 (16%) HOMO-1->LUMO+1 (9%) HOMO-2->LUMO+2 (6%) HOMO-1->LUMO+2 (5%) HOMO-3->LUMO+4 (5%) HOMO->LUMO+2 (4%)	MLCT		
427.1	0.036	HOMO-4->LUMO (22%) HOMO-1->LUMO+1 (10%) HOMO->LUMO+3 (8%) HOMO-5->LUMO (7%) HOMO->LUMO+2 (7%) HOMO-1->LUMO+1 (6%) HOMO-2->LUMO+2 (5%) HOMO->LUMO+3 (4%)	MLCT	423	
413.9	0.0651	HOMO-4->LUMO (15%) HOMO->LUMO+2 (11%) HOMO-2->LUMO+1 (7%) HOMO-1->LUMO+1 (7%) HOMO-1->LUMO+2 (6%) HOMO-3->LUMO+2 (4%)	MLCT		
378.0	0.0205	HOMO-10->LUMO (34%) HOMO-12->LUMO (7%) HOMO-4->LUMO (4%) HOMO-3->LUMO+1 (6%) HOMO-2->LUMO+1 (4%)	MLCT		
366.3	0.046	HOMO-1->LUMO+3	MLC		

		(39%) HOMO-1->LUMO+3 (5%) HOMO-5->LUMO+2 (5%) HOMO-12->LUMO (4%) HOMO-1->LUMO+2 (4%)	T		
356.8	0.052	HOMO-4->LUMO+2 (29%) HOMO-4->LUMO+1 (8%) HOMO-12->LUMO (7%) HOMO-2->LUMO+2 (7%) HOMO-6->LUMO (5%) HOMO-3->LUMO+2 (5%) HOMO-1->LUMO+3 (4%)	MLCT	358	248, 295, 336
		[Fe(SALPHEN)Cl(H_2O)], S=3/2			
1530.3	0.0002	HOMO-3->LUMO+1 (67%) HOMO-12->LUMO+1 (12%) HOMO-5->LUMO+1 (14%)			
865.9	0.0002	HOMO-5->LUMO+2 (14%) HOMO-3->LUMO+2 (66%) HOMO-12->LUMO+2 (9%)			
687.2	0.003	HOMO-1->LUMO (75%) HOMO->LUMO (14%)			
661.2	0.0002	HOMO-3->LUMO+5			

		(34%) HOMO-7->LUMO (13%) HOMO-12->LUMO (11%) HOMO-12->LUMO+5 (7%) HOMO-5->LUMO+5 (7%) HOMO->LUMO (5%)			
595.1	0.0011	HOMO-1->LUMO (79%) HOMO-1->LUMO+1 (5%)			
572.0	0.0113	HOMO-1->LUMO+1 (73%) HOMO->LUMO+1 (10%) HOMO->LUMO+1 (6%)			
556.9	0.0089	HOMO->LUMO+1 (46%) HOMO-1->LUMO+3 (14%) HOMO->LUMO+1 (7%) HOMO->LUMO (5%) HOMO-1->LUMO+1 (4%)			
539.0	0.0029	HOMO->LUMO+1 (47%) HOMO->LUMO+2 (11%) HOMO-1->LUMO+1 (10%) HOMO-1->LUMO+1 (8%) HOMO->LUMO+3 (6%)			
511.4	0.0106	HOMO->LUMO+1 (15%) HOMO->LUMO+3 (15%) HOMO-1->LUMO+1 (15%)			

		HOMO->LUMO+2 (14%) HOMO-1->LUMO+2 (12%) HOMO->LUMO+2 (8%) HOMO-1->LUMO+4 (4%)			
495.6	0.0008	HOMO-2->LUMO (34%) HOMO-1->LUMO+2 (23%) HOMO->LUM+2 (11%) HOMO->LUMO+2 (9%)			
482.7	0.007	HOMO->LUMO+2 (18%) HOMO-7->LUMO (12%) HOMO-3->LUMO+5 (11%) HOMO-3->LUMO (8%) HOMO-1->LUMO+3 (8%) HOMO-2->LUMO (5%) HOMO-6->LUMO (4%)			
467.2	0.0092	HOMO-1->LUMO+2 (44%) HOMO-2->LUMO (18%) HOMO->LUMO+1 (11%) HOMO-5->LUMO (6%) HOMO-1->LUMO+1 (3%)			
446.2	0.0073	HOMO-5->LUMO (36%) HOMO->LUMO+2 (9%) HOMO-2->LUMO+1 (6%) HOMO-1->LUMO+1 (6%)			

		HOMO-3->LUMO (6%) HOMO-2->LUMO+3 (4%)			
441.4	0.0222	HOMO->LUMO+1 (16%) HOMO-6->LUMO (9%) HOMO-5->LUMO (8%) HOMO-1->LUMO+3 (7%) HOMO-6->LUMO (6%) HOMO-1->LUMO+1 (5%) HOMO-2->LUMO (5%) HOMO-3->LUMO (4%) HOMO-1->LUMO (4%) HOMO-2->LUMO (4%)			
435.9	0.0089	HOMO-5->LUMO (17%) HOMO-6->LUMO (15%) HOMO->LUMO+2 (13%) HOMO-1->LUMO+1 (8%) HOMO->LUMO (6%) HOMO->LUMO+3 (6%) HOMO-2->LUMO (5%) HOMO-5->LUMO (4%)			
431.6	0.0216	HOMO-6->LUMO (37%) HOMO-5->LUMO (9%) HOMO-1->LUMO+1 (5%) HOMO-1->LUMO+2 (5%) HOMO->LUMO+1 (5%) HOMO-1->LUMO+3 (5%) HOMO->LUMO+3 (4%)			
427.6	0.0196	HOMO-6->LUMO (19%)			

		HOMO-1->LUMO+3 (13%) HOMO->LUMO+3 (10%) HOM-5->LUMO (10%) HOMO-1->LUMO (9%) HOMO-3->LUMO (4%) HOMO-1->LUMO+1 (4%)			
425.5	0.0394	HOMO->LUMO+2 (14%) HOMO-1->LUMO+3 (14%) HOMO->LUMO+3 (13%) HOMO-6->LUMO (11%) HOMO-2->LUMO (6%) HOMO-6->LUMO (5%) HOMO-5->LUMO (5%) HOMO-1->LUMO+2 (4%) HOMO->LUMO (4%)			
408.8	0.0197	HOMO-2->LUMO+1 (18%) HOMO-1->LUMO+1 (15%) HOMO->LUMO+3 (12%) HOMO-1->LUMO+3 (8%) HOMO-6->LUMO (6%) HOMO-4->LUMO (5%) HOMO-3->LUMO (4%) HOMO-2->LUMO+2 (4%)			
392.5	0.0182	HOMO-5->LUMO+1 (21%)			

		HOMO-2->LUMO+1 (18%) HOMO-2->LUMO (12%) HOMO-5->LUMO+2 (8%) HOMO-3->LUMO+1 (6%) HOMO-5->LUMO (4%)			
389.2	0.0256	HOMO-2->LUMO (21%) HOMO-3->LUMO (12%) HOMO-2->LUMO+1 (12%) HOMO-2->LUMO+1 (11%) HOMO-5->LUMO+1 (10%) HOMO-5->LUMO (5%)			
381.2	0.0565	HOMO-4->LUMO (32%) HOMO-1->LUMO+2 (16%) HOMO-2->LUMO+3 (10%) HOMO-6->LUMO (8%) HOMO-2->LUMO+1 (7%) HOMO-1->LUMO+3 (6%) HOMO-2->LUMO+1 (4%)			
365.2	0.0461	HOMO-2->LUMO+2 (43%) HOMO-11->LUMO (9%) HOMO-1->LUMO+4 (7%)			

		HOMO-4->LUMO+1 (6%) HOMO-6->LUMO+2 (4%)			
351.6	0.0018	HOMO-12->LUMO (20%) HOMO-4->LUMO (14%) HOMO-10->LUMO (9%) HOMO-3->LUMO (7%) HOMO-3->LUMO+3 (6%) HOMO-5->LUMO (5%) HOMO-3->LUMO+4 (5%) HOMO-11->LUMO (4%)			
		[Co(SALPHEN)(H_2O)], S=1/2			
605.0	0.0003	HOMO->LUMO (49%) HOMO->LUMO (30%) HOMO-1->LUMO+1 (9%) HOMO-1->LUMO+1 (8%)	MLCT		
510.9	0.0006	HOMO-3->LUMO+2 (38%) HOMO-3->LUMO+4 (16%) HOMO-1->LUMO+2 (12%) HOMO-11->LUMO+2 (9%) HOMO-5->LUMO+2 (4%)	MLCT		
499.3	0.0341	HOMO->LUMO (37%) HOMO->LUMO (30%) HOMO->LUMO+4 (9%) HOMO->LUMO+2 (6%)	MLCT		

		HOMO-4->LUMO+4 (4%)			
486.4	0.0009	HOMO-2->LUMO (25%) HOMO->LUMO+1 (16%) HOMO-5->LUMO+2 (15%) HOMO-2->LUMO (14%) HOMO-1->LUMO (5%) HOMO-3->LUMO+4 (5%)	MLCT	488	
485.8	0.0018	HOMO-5->LUMO+2 (37%) HOMO-3->LUMO+4 (11%) HOMO-2->LUMO (10%) HOMO-2->LUMO (10%) HOMO->LUMO+1 (9%) HOMO-11->LUMO+2 (4%)	MLCT		Experimental (nm)
457.7	0.0116	HOMO->LUMO+4 (21%) HOMO->LUMO+2 (20%) HOMO->LUMO (14%) HOMO->LUMO (11%) HOMO-4->LUMO+4 (8%) HOMO-6->LUMO+4 (7%) HOMO-7->LUMO+2 (6%) HOMO-1->LUMO+1 (5%)			458
456.9	0.0003	HOMO->LUMO+1 (40%) HOMO-1->LUMO (31%) HOMO-2->LUMO (10%) HOMO-4->LUMO+1 (4%)	MLCT		
453.7	0.0001	HOMO-1->LUMO+1 (27%)	MLCT		

		HOMO-2->LUMO+1) (20%) HOMO-2->LUMO+1 (16%) HOMO-1->LUMO+1 (14%) HOMO->LUMO (7%) HOMO-4->LUMO (4%)			
448.4	0.0588	HOMO-1->LUMO (49%) HOMO-1->LUMO (31%) HOMO-2->LUMO (6%)	MLCT		
431.5	0.0028	HOMO->LUMO+1 (65%) HOMO->LUMO+1 (13%) HOMO-5->LUMO+2 (4%) HOMO-1->LUMO (4%)	MLCT		
427.6	0.0009	HOMO-1->LUMO+1 (19%) HOMO-2->LUMO+1 (19%) HOMO-1->LUMO+1 (16%) HOMO-2->LUMO+1 (11%) HOMO->LUMO (9%) HOMO-4->LUMO (8%) HOMO-4->LUMO (7%)	MLCT		
425.1	0.0352	HOMO-2->LUMO+4 (29%) HOMO-6->LUMO+2 (16%) HOMO-2->LUMO+2	MLCT	416	

		(15%) HOMO-5->LUMO+4 (13%) HOMO-1->LUMO (4%) HOMO-1->LUMO (4%)			
389.9	0.195	HOMO-1->LUMO+1 (49%) HOMO-1->LUMO+1 (39%)	MLCT		393
381.6	0.0818	HOMO-3->LUMO (38%) HOMO-2->LUMO (26%) HOMO-5->LUMO (10%) HOMO-2->LUMO (8%)	MLCT		
372.6	0.0913	HOMO-3->LUMO (55%) HOMO-2->LUMO (14%) HOMO-5->LUMO (9%) HOMO-2->LUMO (8%)	MLCT	375	
366.8	0.0057	HOMO-2->LUMO+1 (31%) HOMO-4->LUMO (23%) HOMO-5->LUMO+1 (11%) HOMO-4->LUMO (10%) HOMO-3->LUMO+1 (5%) HOMO-6->LUMO+1 (4%)	MLCT		250, 331
		[Co(SALPHEN)(H_2O)], S=3/2			
1156.9	0.0004	HOMO-4->LUMO+3 (12%) HOMO-3->LUMO+3 (30%)	MLCT		

		HOMO-3->LUMO+1 (8%) HOMO-5->LUMO+2 (5%) HOMO->LUMO+3 (4%)			
1019.8	0.0001	HOMO-5->LUMO+3 (31%) HOMO-5->LUMO+2 (10%) HOMO-3->LUMO+2 (7%) HOMO-2->LUMO+3 (6%) HOMO-5->LUMO+4 (4%) HOMO-3->LUMO+4 (4%) HOMO-2->LUMO+2 (4%)	MLCT		
583.2	0.0004	HOMO-3->LUMO+4 (30%) HOMO-4->LUMO+4 (12%) HOMO->LUMO+4 (8%) HOMO-5->LUMO+2 (5%) HOMO-5->LUMO+3 (5%) HOMO-1->LUMO+4 (5%)			
557.7	0.0002	HOMO-1->LUMO (25%) HOMO-1->LUMO (25%) HOMO->LUMO+1 (21%) HOMO->LUMO0+1 (16%)			
513.9	0.0003	HOMO-5->LUMO+4 (38%) HOMO-2->LUMO+4 (10%) HOMO-6->LUMO+4 (4%),			
495.6	0.024	HOMO->LUMO (37%) HOMO->LUMO (27%)			

		HOMO-2->LUMO (10%) HOMO-1->LUMO (5%) HOMO->LUMO+1 (5%)			
474.4	0.019	HOMO->LUMO+1 (24%) HOMO->LUMO+2 (23%) HOMO->LUMO+1 (12%) HOMO-1->LUMO+1 (8%) HOMO-2->LUMO (5%) HOMO-2->LUMO (5%) HOMO->LUMO (4%)			
468.9	0.0076	HOMO->LUMO (20%) HOMO->LUMO+1 (14%) HOMO->LUMO+1 (14%) HOMO-1->LUMO (10%) HOMO-1->LUMO (8%) HOMO-3->LUMO (6%) HOMO-5->LUMO+4 (5%) HOMO-2->LUMO (4%)			
453.1	0.0063	HOMO-2->LUMO (18%) HOMO-3->LUMO (13%) HOMO->LUMO+1 (13%) HOMO-1->LUMO+1 (8%) HOMO-3->LUMO+1 (5%) HOMO-1->LUMO+1 (5%) HOMO->LUMO+1 (5%) HOMO-1->LUMO (4%) HOMO-2->LUMO+1 (4%)			
439.4	0.0016	HOMO-2->LUMO (26%) HOMO->LUMO (14%) HOMO-1->LUMO (12%) HOMO->LUMO+2 (11%)			

		HOMO-2->LUMO+1 (7%) HOMO->LUMO+1 (6%) HOMO-1->LUMO+1 (5%)			
429.7	0.037	HOMO->LUMO+2 (25%) HOMO-2->LUMO (16%) HOMO-2->LUMO+1 (10%) HOMO->LUMO+1 (7%) HOMO-1->LUMO+1 (6%) HOMO-3->LUMO+1 (5%) HOMO-2->LUMO+1 (4%)			
421.5	0.0263	HOMO-1->LUMO (17%) HOMO-1->LUMO+1 (35%) HOMO-1->LUMO (7%) HOMO-1->LUMO+2 (8%)			
412.2	0.0356	HOMO-2->LUMO (25%) HOMO-1->LUMO+1 (11%) HOMO-1->LUMO (8%) HOMO->LUMO+2 (6%) HOMO-2->LUMO+1 (6%) HOMO-4->LUMO (5%) HOMO-3->LUMO+1 (5%) HOMO->LUMO (5%) HOMO-3->LUMO (4%)			
410.7	0.0608	HOMO-1->LUMO (24%) HOMO-1->LUMO (15%)			

		HOMO-1->LUMO+1 (14%) HOMO-1->LUMO+2 (12%) HOMO-2->LUMO+1 (5%) HOMO-1->LUMO+1 (5%)			
396.8	0.0765	HOMO-1->LUMO+1 (20%) HOMO-2->LUMO+1 (18%) HOMO->LUMO+2 (11%) HOMO->LUMO+3 (9%) HOMO->LUMO+1 (7%) HOMO-2->LUMO (6%) HOMO->LUMO+1 (5%) HOMO-1->LUMO) (4%) HOMO-1->LUMO (4%)			
389.2	0.0103	HOMO->LUMO+3 (60%) HOMO-1->LUMO+1 (14%) HOMO-1->LUMO+3 (4%)			
375.0	0.0682	HOMO-2->LUMO+1 (27%) HOMO-1->LUMO+1 (20%) HOMO-1->LUMO+2 (21%) HOMO-1->LUMO+1 (9%) HOMO->LUMO+3 (5%)			

		HOMO->LUMO+1 (4%)			
350.7	0.0825	HOMO-2->LUMO (35%) HOMO-4->LUMO (14%) HOMO-3->LUMO (10%) HOMO-3->LUMO (5%) HOMO-2->LUMO+1 (5%)			
346.6	0.0163	HOMO-2->LUMO+1 (14%) HOMO-3->LUMO (9%) HOMO-2->LUMO+2 (5%) HOMO-7->LUMO (5%) HOMO-6->LUMO+1 (5%) HOMO->LUMO+5 (4%)			
341.3	0.1741	HOMO-3->LUMO (20%) HOMO-2->LUMO+1 (18%) HOMO-2->LUMO (13%) HOMO-4->LUMO (10%) HOMO-3->LUMO (5%) HOMO-5->LUMO (4%)			
329.2	0.0111	HOMO-5->LUMO (32%) HOMO-4->LUMO (15%) HOMO-3->LUMO+1 (11%) HOMO-2->LUMO+2 (9%) HOMO-4->LUMO+1 (4%) HOMO-2->LUMO+1 (4%)			

327.3	0.034	HOMO-5->LUMO (19%) HOMO-2->LUMO+2 (15%) HOMO-3->LUMO+1 (10%) HOMO-4->LUMO (8%) HOMO-3->LUMO (6%) HOMO-4->LUMO+1 (4%) HOMO->LUMO+5 (4%)			
320.5	0.0195	HOMO-3->LUMO+1 (16%) HOMO-5->LUMO (13%) HOMO-5->LUMO (10%) HOMO->LUMO+4 (10%) HOMO-3->LUMO+1 (9%) HOMO-4->LUMO (6%) HOMO-3->LUMO+2 (4%)			
314.3	0.0217	HOMO->LUMO+3 (9%) HOMO->LUMO+5 (7%) HOMO-1->LUMO+4 (6%) HOMO->LUMO+6 (6%) HOMO-5->LUMO (5%) HOMO-2->LUMO+3 (5%) HOMO->LUMO+8 (5%) HOMO-3->LUMO+1 (4%) HOMO-4->LUMO+1 (4%)			
313.7	0.0928	HOMO-6->LUMO+1 (23%) HOMO-5->LUMO (13%) HOMO-6->LUMO+2 (9%)			

		HOMO->LUMO+2 (6%) HOMO-5->LUMO+1 (6%) HOMO-4->LUMO (4%)			
309.2	0.0155	HOMO-4->LUMO (12%) HOMO->LUMO+2 (11%) HOMO-5->LUMO+1 (9%) HOMO->LUMO+5 (8%) HOMO-5->LUMO+1 (5%) HOMO-5->LUMO+2 (5%)			
307.3327872	0.0317	HOMO->LUMO+4 (30%) HOMO-4->LUMO (11%) HOMO-5->LUMO+1 (6%) HOMO-1->LUMO+4 (5%) HOMO-7->LUMO (4%)			
304.9	0.0579	HOMO-4->LUMO (11%) HOMO-5->LUMO+1 (10%) HOMO-4->LUMO (6%) HOMO->LUMO+2 (5%) HOMO-8->LUMO (5%) HOMO-6->LUMO+1 (5%) HOMO-3->LUMO+1 (4%) HOMO-5->LUMO+1 (4%)			
		[Cu(SALPHEN)], S=1/2			
597.6	0.0001	HOMO-1->LUMO+1 (35%) HOMO->LUMO (33%) HOMO-1->LUMO+1	MLCT		618, 657

		(14%) HOMO->LUMO+2 (14%)			
585.2	0.0001	HOMO->LUMO+1 (35%) HOMO-1->LUMO (32%) HOMO->LUMO+1 (16%) HOMO-1->LUMO+2 (15%)	MLCT		574
536.8	0.009	HOMO-4->LUMO (56%) HOMO-14->LUMO (14%) HOMO-21->LUMO (9%) HOMO-9->LUMO (8%) HOMO-1->LUMO+1 (5%) HOMO->LUMO (4%)	MLCT		
458.6	0.0013	HOMO-9->LUMO (76%) HOMO-14->LUMO (9%) HOMO-15->LUMO (6%)	MLCT	463	
458.1	0.0004	HOMO-1->LUMO+2 (26%) HOMO->LUMO+1 (22%) HOMO->LUMO+1 (15%) HOMO-3->LUMO+1 (11%) HOMO-2->LUMO+2 (11%) HOMO-1->LUMO (5%) HOMO-4->LUMO (4%) HOMO-3->LUMO+1 (4%)	MLCT		452
439.9	0.0372	HOMO-1->LUMO (49%) HOMO->LUMO+1 (40%) HOMO->LUMO+1 (4%)	MLCT		
436.3	0.1468	HOMO-1->LUMO+1	MLC		

		(44%) HOMO->LUMO (41%) HOMO-14->LUMO (7%) HOMO-21->LUMO (4%)	T		
433.3	0.0001	HOMO-2->LUMO (94%)	MLCT		
420.2	0.0008	HOMO->LUMO+2 (34%) HOMO->LUMO (13%) HOMO-1->LUMO+1 (10%) HOMO-3->LUMO (9%) HOMO-2->LUMO+1 (9%) HOMO-1->LUMO+1 (8%) HOMO-4->LUMO+1 (6%) HOMO-3->LUMO+2 (6%)	MLCT		
403.1	0.1727	HOMO-1->LUMO+2 (50%) HOMO->LUMO+1 (29%) HOMO-6->LUMO (8%)	MLCT		
400.9	0.0101	HOMO->LUMO+1 (22%) HOMO-4->LUMO (15%) HOMO-3->LUMO+1 (15%) HOMO-2->LUMO+2 (13%) HOMO-3->LUMO+1 (11%) HOMO-1->LUMO (5%) HOMO->LUMO+1 (5%)	MLCT		
341.6	0.1339	HOMO-2->LUMO+1 (43%)	MLCT	346	345

		HOMO-3->LUMO (39%) HOMO-14->LUMO (6%) HOMO-4->LUMO (5%)			
323.5	0.5008	HOMO-4->LUMO (33%) HOMO-14->LUMO (23%) HOMO-21->LUMO (16%) HOMO-3->LUMO (7%) HOMO-2->LUMO+1 (7%)	MLCT		
323.2	0.0264	HOMO-6->LUMO (36%) HOMO-3->LUMO+1 (25%) HOMO-4->LUMO (14%) HOMO-2->LUMO+2 (9%) HOMO-3->LUMO+1 (6%)	MLCT	314	
294.6	0.632	HOMO-4->LUMO (28%) HOMO-3->LUMO+1 (27%) HOMO-6->LUMO (20%) HOMO-2->LUMO+2 (7%) HOMO-3->LUMO+1 (6%)	CT		298
		[Cu(SALPHEN)], S=3/2			
588.7	0.0001	HOMO->LUMO+1 (31%) HOMO->LUMO (29%) HOMO-1->LUMO+1 (14%) HOMO-1->LUMO+2 (14%)	MLCT		
554.1	0.0001	HOMO-1->LUMO+1 (27%) HOMO-1->LUMO (26%)	MLCT		

		HOMO->LUMO+1 (20%) HOMO->LUMO+2 (20%)			
533.0	0.0003	HOMO->LUMO (87%) HOMO-9->LUMO (7%)	MLCT		
522.5	0.0092	HOMO-4->LUMO (36%) HOMO-10->LUMO (22%) HOMO-22->LUMO (17%) HOMO-21->LUMO (8%) HOMO-14->LUMO (5%) HOMO-13->LUMO (5%)	MLCT		
475.3	0.0047	HOMO-10->LUMO (50%) HOMO-18->LUMO (17%) HOMO-21->LUMO (12%) HOMO-14->LUMO (12%) HOMO-4->LUMO (5%)	MLCT		
451.0	0.0001	HOMO-2->LUMO+1 (25%) HOMO-2->LUMO (24%) HOMO-4->LUMO+1 (8%) HOMO-3->LUMO+2 (8%) HOMO-1->LUMO+1 (6%) HOMO-1->LUMO+2 (6%)	MLCT		
396.8	0.1305	HOMO->LUMO (33%) HOMO->LUMO+1 (31%) HOMO-1->LUMO+1 (13%) HOMO-1->LUMO+2 (12%) HOMO-22->LUMO (4%)	MLCT		

Table S10. TD-DFT spectral data of electronic transitions SALPHEN and it is complexes at gaseous state with oscillator strength f > 0.0001 using B3PW91/6-311++G(d, p) **basis set triple-zeta.**

Wevelength (nm)	Osc. Strength (f)	Contribution percentage B3PW91/6-311++G(d, p)	Character	Theory (nm)
		[Fe(SALPHEN)Cl(H_2O)], S=1/2		
1217.2	0.0003	HOMO-3->LUMO (10%) HOMO-2->LUMO (10%) HOMO-4->LUMO+2 (8%) HOMO->LUMO+2 (8%) HOMO-2->LUMO+2 (7%) HOMO-11->LUMO (5%) HOMO->LUMO+1 (5%) HOMO->LUMO+3 (5%)	MLCT	
973.9	0.001	HOMO-1->LUMO (15%) HOMO-3->LUMO (11%) HOMO-5->LUMO (8%) HOMO-2->LUMO (8%) HOMO->LUMO (7%) HOMO-3->LUMO+1 (6%) HOMO-12->LUMO (5%) HOMO-3->LUMO+3 (5%) HOMO-3->LUMO (4%) HOMO->LUMO+2 (4%)	MLCT	
864.5	0.0098	HOMO->LUMO (40%) HOMO-13->LUMO (6%) HOMO-6->LUMO (8%) HOMO-5->LUMO (5%)	MLCT	997

		HOMO-3->LUMO (6%)		
742.6	0.0001	HOMO-6->LUMO (29%) HOMO-5->LUMO (15%) HOMO-12->LUMO (4%) HOMO-3->LUMO+1 (7%) HOMO-3->LUMO+2 (4%) HOMO-3->LUMO+3 (6%) HOMO-3->LUMO+4 (4%)	MLCT	
647.6	0.0024	HOMO-1->LUMO (59%) HOMO-3->LUMO (7%) HOMO-2->LUMO (6%) HOMO-1->LUMO+2 (4%)	MLCT	
581.8	0.003	HOMO->LUMO (17%) HOMO->LUMO+1 (7%) HOMO->LUMO+4 (7%) HOMO-6->LUMO (5%) HOMO-5->LUMO (5%) HOMO-3->LUMO+3 (4%) HOMO->LUMO+1 (5%) HOMO-1->LUMO+1 (4%)	MLCT	
570.6	0.0033	HOMO->LUMO (24%) HOMO->LUMO+1 (21%) HOMO-1->LUMO+1 (9%) HOMO-1->LUMO (8%) HOMO->LUMO+2 (5%)	MLCT	
532.0	0.0016	HOMO-5->LUMO (10%) HOMO->LUMO+1 (19%)	MLCT	

		HOMO-1->LUMO (16%) HOMO->LUMO (13%) HOMO->LUMO+2 (5%)		
490.7	0.0064	HOMO->LUMO (26%) HOMO-2->LUMO (12%) HOMO-1->LUMO (6%) HOMO->LUMO+3 (6%) HOMO-2->LUMO+3 (5%) HOMO->LUMO+1 (5%) HOMO-1->LUMO (4%)	MLCT	
478.5	0.0079	HOMO->LUMO+2 (9%) HOMO-1->LUMO+1 (7%) HOMO-2->LUMO (7%) HOMO->LUMO+1 (6%) HOMO->LUMO+2 (5%) HOMO-6->LUMO+3 (5%) HOMO-3->LUMO+4 (5%) HOMO-1->LUMO (5%) HOMO-2->LUMO+1 (4%) HOMO-1->LUMO+1 (4%) HOMO-1->LUMO+2 (4%) HOMO->LUMO+1 (4%)	MLCT	507
458.5	0.0057	HOMO-1->LUMO+1 (18%) HOMO-1->LUMO+1 (14%) HOMO-1->LUMO (12%) HOMO->LUMO+2 (11%)	MLCT	

		HOMO-2->LUMO+2 (5%) HOMO-1->LUMO+3 (4%)		
454.7	0.0113	HOMO-3->LUMO (30%) HOMO-2->LUMO (22%) HOMO-2->LUMO+1 (7%) HOMO->LUMO+1 (7%) HOMO-2->LUMO+1 (6%) HOMO->LUMO (4%)	MLCT	
447.8	0.0063	HOMO->LUMO+2 (17%) HOMO-1->LUMO+2 (9%) HOMO-1->LUMO+1 (8%) HOMO-1->LUMO+1 (7%) HOMO->LUMO+2 (6%) HOMO-2->LUMO+2 (5%) HOMO-3->LUMO (4%) HOMO->LUMO+1 (4%) HOMO-1->LUMO+3 (4%)	MLCT	
431.7	0.038	HOMO-1->LUMO (16%) HOMO->LUMO+3 (11%) HOMO->LUMO+1 (10%) HOMO->LUMO (10%) HOMO-2->LUMO (6%) HOMO-2->LUMO+1 (4%) HOMO-1->LUMO+2 (4%)	MLCT	
420.8	0.0922	HOMO-1->LUMO+1 (12%) HOMO-1->LUMO+1	MLCT	

		(12%) HOMO->LUMO+3 (10%) HOMO->LUMO (9%) HOMO-1->LUMO+2 (6%) HOMO->LUMO+1 (6%)		
415.1	0.0187	HOMO->LUMO+1 (13%) HOMO->LUMO+2 (10%) HOMO-1->LUMO+1 (10%) HOMO->LUMO+3 (9%) HOMO-1->LUMO (6%) HOMO-2->LUMO (4%) HOMO-2->LUMO+1 (4%) HOMO-1->LUMO+2 (4%)	MLCT	423
410.8	0.0139	HOMO->LUMO+3 (11%) HOMO-2->LUMO+2 (9%) HOMO-1->LUMO+2 (8%) HOMO->LUMO+3 (7%) HOMO-2->LUMO+1 (7%) HOMO->LUMO+1 (6%) HOMO-1->LUMO (6%) HOMO-4->LUMO+1 (4%) HOMO-1->LUMO+1 (4%)	MLCT	
403.7	0.0177	H0M0-1->LUMO+1 (23%) HOMO->LUMO+2 (20%) HOMO->LUMO+4 (5%) HOMO-1->LUMO+3 (4%) HOMO->LUMO+3 (4%)	MLCT	

		HOMO-2->LUMO (4%)		
388.7	0.0315	HOMO->LUMO+3 (25%) HOMO-4->LUMO (21%) HOMO-1->LUMO+2 (8%) HOMO-3->LUMO (7%) HOMO-4->LUMO+1 (6%) HOMO-5->LUMO (4%) HOMO-4->LUMO (4%)	MLCT	
384.9	0.026	HOMO-1->LUMO+2 (45%) HOMO-1->LUMO+1 (7%) HOMO-11->LUMO (5%) HOMO-2->LUMO+3 (4%) HOMO-1->LUMO (4%)	MLCT	358
364.3	0.0157	HOMO-4->LUMO (30%) HOMO-2->LUMO+1 (15%) HOMO-1->LUMO+3 (10%) HOMO-1->LUMO+3 (7%) HOMO->LUMO+4 (4%)	MLCT	
360.5	0.0212	HOMO-1->LUMO+3 (44%) HOMO-1->LUMO+3 (10%) HOMO-3->LUMO+1 (6%) HOMO-2->LUMO+1 (5%)	MLCT	

		HOMO-4->LUMO+1 (5%)		
359.3	0.0387	HOMO-3->LUMO+1 (13%) HOMO-2->LUMO+1 (13%) HOMO-1->LUMO+3 (18%) HOMO-2->LUMO (14%) HOMO-4->LUMO (8%)	MLCT	
346.2	0.0219	HOMO-4->LUMO+2 (13%) HOMO-3->LUMO+1 (12%) HOMO-3->LUMO+3 (7%) HOMO-2->LUMO+2 (7%) HOMO-1->LUMO+3 (5%) HOMO-3->LUMO+1 (4%)	MLCT	
343.9	0.0174	HOMO-1->LUMO+3 (21%) HOMO-2->LUMO+2 (6%) HOMO-5->LUMO (6%) HOMO-5->LUMO+1 (6%) HOMO-4->LUMO+2 (5%) HOMO-7->LUMO+2 (4%) HOMO-2->LUMO+1 (4%)	MLCT	
		[Fe(SALPHEN)Cl(H_2O)],		

		S=3/2		
936.4	0.0001	HOMO-2->LUMO+3 (77%) HOMO-12->LUMO+3 (6%) HOMO-2->LUMO+4 (4%)	MLCT	
747.5	0.0002	HOMO-2->LUMO+5 (32%) HOMO-12->LUMO+1 (8%) HOMO-7->LUMO+1 (7%) HOMO-12->LUMO (6%) HOMO-7->LUMO (6%) HOMO->LUMO (5%) HOMO-2->LUMO+11 (4%)	MLCT	
717.6	0.0002	HOMO->LUMO (45%) HOMO->LUMO+1 (27%) HOMO-2->LUMO+5 (4%)	MLCT	
605.9	0.0011	HOMO-1->LUMO (49%) HOMO->LUMO+1 (11%) HOMO-1->LUMO (9%) HOMO->LUMO (9%) HOMO-1->LUMO+1 (6%) HOMO->LUMO (6%)	MLCT	
591.5	0.0015	HOMO->LUMO (56%) HOMO-1->LUMO (11%)	MLCT	

		HOMO->LUMO+1 (9%) HOMO->LUMO+2 (8%) HOMO-1->LUMO (6%)		
548.7	0.0031	HOMO-1->LUMO (41%) HOMO-1->LUMO+1 (30%) HOMO->LUMO (7%) HOMO-1->LUMO (4%)	MLCT	
532.4	0.0033	HOMO->LUMO (19%) HOMO->LUMO+1 (18%) HOMO->LUMO (14%) HOMO-1->LUMO (14%) HOMO->LUMO+2 (8%) HOMO-1->LUMO+1 (4%)	MLCT	
499.3	0.016	HOMO-1->LUMO+1 (19%) HOMO->LUMO+1 (16%) HOMO->LUMO+2 (14%) HOMO-1->LUMO (13%) HOMO-1->LUMO (7%) HOMO-1->LUMO+1 (4%)	MLCT	
471.5	0.0033	HOMO-1->LUMO+2 (26%) HOMO->LUMO+2 (22%) HOMO-3->LUMO+1 (9%) HOMO-2->LUMO (5%) HOMO->LUMO+1 (5%)	MLCT	

		HOMO-1->LUMO+1 (5%)		
442.1	0.014	HOMO-1->LUMO+1 (10%) HOMO->LUMO+1 (9%) HOMO->LUMO+2 (7%) HOMO-3->LUMO (7%) HOMO-3->LUMO+1 (7%) HOMO-1->LUMO (7%) HOMO-1->LUMO+1 (6%) HOMO-2->LUMO+1 (5%) HOMO-12->LUMO+1 (4%) HOMO-2->LUMO (4%) HOMO->LUMO (7%) HOMO->LUMO+1 (4%) HOMO-3->LUMO (4%)	MLCT	
429.9	0.019	HOMO-3->LUMO (8%) HOMO-1->LUMO+1 (8%) HOMO-1->LUMO+2 (8%) HOMO->LUMO+1 (8%) HOMO-3->LUMO (7%) HOMO-2->LUMO (6%) HOMO->LUMO+2 (6%) HOMO-3->LUMO+1 (5%) HOMO-2->LUMO+1 (5%) HOMO->LUMO+1 (5%)	MLCT	
420.0	0.0151	HOMO->LUMO+2 (23%) HOMO-1->LUMO+1	MLCT	

		(20%) HOMO->LUMO+3 (13%) HOMO-1->LUMO (8%) HOMO-3->LUMO (7%) HOMO-1->LUMO+1 (5%) HOMO-4->LUMO (4%)		
416.0	0.0202	HOMO-4->LUMO (20%) HOMO-5->LUMO (13%) HOMO-2->LUMO (9%) HOMO-3->LUMO (8%) HOMO->LUMO+3 (6%) HOMO-2->LUMO+1 (5%) HOMO->LUMO+1 (5%)	MLC T	
410.3	0.0347	HOMO->LUMO+1 (26%) HOMO-4->LUMO (14%) HOMO-1->LUMO+1 (8%) HOMO-5->LUMO (5%) HOMO->LUMO+3 (5%) HOMO-1->LUMO (5%) HOMO-4->LUMO (4%) HOMO-4->LUMO+1 (4%) HOMO->LUMO+2 (4%)	MLC T	
399.6	0.0328	HOMO->LUMO+3 (44%) HOMO-1->LUMO+1 (9%) HOMO-4->LUMO (8%) HOMO-6->LUMO (7%)	MLC T	
388.9	0.0119	HOMO-1->LUMO+3	MLC	

		(30%) HOMO-6->LUMO (10%) HOMO-5->LUMO (10%) HOMO-1->LUMO+2 (9%) HOMO-4->LUMO (4%)	T	
386.4	0.0173	HOMO-4->LUMO (12%) HOMO-1->LUMO+3 (12%) HOMO-1->LUMO+1 (7%) HOMO-6->LUMO (7%) HOMO-4->LUMO+1 (6%) HOMO-1->LUMO+1 (7%) HOMO-2->LUMO (4%) HOMO->LUMO+1 (4%)	MLC T	
365.6	0.0177	HOMO-2->LUMO+4 (28%) HOMO-2->LUMO (16%) HOMO-3->LUMO (7%) HOMO-12->LUMO (6%) HOMO-4->LUMO (6%) HOMO-2->LUMO+1 (5%)	MLC T	
363.3	0.0269	HOMO-3->LUMO (22%) HOMO-2->LUMO+1 (19%) HOM-4->LUMO (14%) HOMO-2->LUMO (12%) HOMO-2->LUMO+2 (6%)	MLC T	

355.2	0.0607	HOMO-6->LUMO (23%) HOMO-5->LUMO (22%) HOMO-2->LUMO+1 (8%) HOMO-4->LUMO (8%) HOMO-3->LUMO+1 (8%) HOMO-2->LUMO (5%)	MLCT	
346.9	0.0344	HOMO-3->LUMO+1 (30%) HOMO-3->LUMO (16%) HOMO-2->LUMO (9%) HOMO-3->LUMO+1 (4%)	MLCT	
		[Co(SALPHEN)(H_2O)], S=1/2		
517.5	0.0382	HOMO->LUMO (53%) HOMO->LUMO (27%) HOMO->LUMO+4 (4%)	MLCT	
510.2	0.0007	HOMO-3->LUMO+2 (30%) HOMO-3->LUMO+4 (16%) HOMO-11->LUMO+2 (9%) HOMO-1->LUMO+2 (8%) HOMO-3->LUMO+9 (6%)	MLCT	
488.3	0.0069	HOMO-5->LUMO+2 (31%) HOMO->LUMO+1 (26%)	MLCT	

		HOMO->LUMO+1 (8%) HOMO-1->LUMO (7%) HOMO-3->LUMO+4 (5%)		
459.3	0.0055	HOMO-2->LUMO+1 (27%) HOMO->LUMO+2 (13%) HOMO->LUMO+4 (11%) HOMO-2->LUMO+1 (9%) HOMO->LUMO (5%) HOMO-4->LUMO+4 (4%)	MLCT	
446.6	0.0301	HOMO-1->LUMO (47%) HOMO-1->LUMO (26%) HOMO-2->LUMO (9%)	MLCT	
423.9	0.0552	HOMO-3->LUMO (18%) HOMO-2->LUMO+4 (13%) HOMO-2->LUMO+2 (12%) HOMO-2->LUMO (11%) HOMO-2->LUMO (9%) HOMO-6->LUMO+2 (8%) HOMO-2->LUMO+9 (4%)	MLCT	
392.8	0.0549	HOMO-3->LUMO+1 (50%) HOMO-1->LUMO+1 (20%) HOMO-1->LUMO+1	MLCT	

		(15%)		
391.2	0.1452	HOMO-2->LUMO (24%) HOMO-3->LUMO (16%) HOMO-2->LUMO (15%) HOMO-5->LUMO (14%) HOMO-4->LUMO+1 (4%)	MLCT	
370.3	0.1336	HOMO-3->LUMO+1 (31%) HOMO-1->LUMO+1 (20%) HOMO-1->LUMO+1 (17%) HOMO-4->LUMO (7%) HOMO-2->LUMO+1 (7%) HOMO-3->LUMO+1 (5%)	MLCT	488
352.6	0.1203	HOMO-3->LUMO (29%) HOMO-2->LUMO (22%) HOMO-6->LUMO (15%) HOMO-5->LUMO (8%) HOMO-4->LUMO+1 (4%)	MLCT	
333.44	0.0297	HOMO-3->LUMO+1 (61%) HOMO-2->LUMO+1 (9%) HOMO-4->LUMO (6%) HOMO-3->LUMO+1 (4%)	MLCT	
332.1	0.0115	HOMO-5->LUMO (87%)	MLC	

			T	
318.8	0.0305	HOMO-5->LUMO (45%) HOMO-4->LUMO+1 (12%) HOMO-1->LUMO+2 (9%) HOMO-4->LUMO+1 (7%) HOMO->LUMO+3 (5%) HOMO->LUMO+3 (4%)	MLCT	
		[Co(SALPHEN)(H_2O)], S=3/2	MLCT	
974.0	0.0002	HOMO-2->LUMO+3 (30%) HOMO-4->LUMO+3 (26%) HOMO-2->LUMO+2 (6%) HOMO-4->LUMO+2 (4%) HOMO-3->LUMO+5 (4%)	MLCT	
587.2	0.0001	HOMO->LUMO (35%) HOMO->LUMO (27%) HOMO->LUMO+1 (9%) HOMO->LUMO+1 (6%) HOMO-1->LUMO+1 (5%) HOMO-1->LUMO (5%)	MLCT	
562.0	0.0005	HOMO-3->LUMO+5 (15%) HOMO-1->LUMO (9%) HOMO->LUMO+5 (8%) HOMO-3->LUMO+11	MLCT	416

		(6%) HOMO-4->LUMO+3 (5%) HOMO-2->LUMO+3 (5%)		
544.4	0.0001	HOMO-1->LUMO (24%) HOMO-1->LUMO (20%) HOMO->LUMO+1 (19%) HOMO->LUMO+1 (13%) HOMO-1->LUMO+1 (4%)	MLCT	
500.9	0.0007	HOMO-2->LUMO+5 (18%) HOMO-4->LUMO+5 (16%) HOMO-2->LUMO (8%) HOMO-2->LUMO+11 (7%) HOMO-4->LUMO+11 (6%)	MLCT	
480.4	0.0284	HOMO->LUMO (41%) HOMO-2->LUMO (25%) HOMO->LUMO (20%) HOMO-1->LUMO (6%)	MLCT	375
462.6	0.0025	HOMO-3->LUMO (13%) HOMO->LUMO+1 (13%) HOMO->LUMO+1 (12%) HOMO->LUMO (11%) HOMO-2->LUMO (9%) HOMO-1->LUMO+1 (5%)	MLCT	

		HOMO-4->LUMO (4%)		
452.2	0.0048	HOMO-2->LUMO (16%) HOMO->LUMO (14%) HOMO-3->LUMO (10%) HOMO->LUMO+1 (10%) HOMO-1->LUMO+1 (7%) HOMO-1->LUMO+1 (6%) HOMO-3->LUMO+1 (5%) HOMO-2->LUMO+1 (4%)	MLCT	
433.9	0.054	HOMO-2->LUMO (27%) HOMO->LUMO+1 (10%) HOMO-2->LUMO+1 (9%) HOMO->LUMO+1 (8%) HOMO-1->LUMO (7%) HOMO->LUMO (6%) HOMO-3->LUMO+1 (5%) HOMO->LUMO (4%) HOMO-2->LUMO+1 (4%)	MLCT	
417.0	0.0341	HOMO-2->LUMO (20%) HOMO-1->LUMO (20%) HOMO-2->LUMO+1 (12%) HOMO-3->LUMO+1 (7%) HOMO-2->LUMO+1 (7%) HOMO-1->LUMO (6%) HOMO-1->LUMO+2 (4%) HOMO->LUMO+1 (4%)	MLCT	

412.0	0.032	HOMO-1->LUMO+1 (24%) HOMO-1->LUMO (21%) HOMO-1->LUMO (15%) HOMO->LUMO+1 (11%) HOMO-2->LUMO (6%)	MLCT	
397.4	0.0131	HOMO-1->LUMO+1 (26%) HOMO-2->LUMO+1 (20%) HOMO->LUMO+1 (10%) HOMO-2->LUMO (5%) HOMO-1->LUMO+1 (5%) HOMO->LUMO+1 (5%) HOMO-4->LUMO (4%) HOMO->LUMO (4%)	MLCT	
394.6	0.1035	HOMO-1->LUMO+1 (24%) HOMO->LUMO+2 (19%) HOMO-1->LUMO+2 (12%) HOMO-1->LUMO (12%) HOMO-2->LUMO (6%) HOMO-1->LUMO (4%) HOMO->LUMO+1 (4%)	MLCT	
371.7	0.0866	HOMO->LUMO+2 (25%) HOMO-1->LUMO+1 (20%) HOMO-2->LUMO+1	MLCT	

		(18%) HOMO-1->LUMO+1 (7%) HOMO->LUMO+1 (5%)		
366.5	0.0844	HOMO-2->LUMO (35%) HOMO-4->LUMO (23%) HOMO-3->LUMO (6%) HOMO-3->LUMO (6%)	MLCT	
359.5	0.0291	HOMO-1->LUMO+2 (42%) HOMO-3->LUMO (19%) HOMO-3->LUMO+1 (12%) HOMO-3->LUMO+2 (5%	MLCT	
350.2	0.0149	HOMO-3->LUMO (45%) HOMO-5->LUMO (7%) HOMO-4->LUMO (6%) HOMO-3->LUMO+1 (6%)	MLCT	
334.2	0.0324	HOMO->LUMO+3 (30%) HOMO-3->LUMO (13%) HOMO-1->LUMO+3 (12%) HOMO-4->LUMO (5%) HOMO-3->LUMO (4%)	MLCT	
329.1	0.1348	HOMO-3->LUMO+1 (24%) HOMO-4->LUMO (19%) HOMO-3->LUMO (18%)	MLCT	

		HOMO-5->LUMO (5%) HOMO-3->LUMO+2 (6%) HOMO-2->LUMO (4%)		
326.7	0.0395	HOMO-4->LUMO (24%) HOMO-3->LUMO+1 (18%) HOMO-3->LUMO+2 (6%) HOMO-1->LUMO+3 (5%) HUMO-2->LUMO (4%)	MLCT	
313.9	0.0361	HOMO-4->LUMO+1 (42%) HOMO-3->LUMO+1 (22%) HOMO-4->LUMO (9%) HOMO-5->LUMO (5%)	MLCT	
299.1	0.1259	HOMO-5->LUMO (23%) HOMO-4->LUMO+2 (18%) HOMO-4->LUMO (17%) HOMO-2->LUMO+2 (17%)	MLCT	
291.6	0.1365	HOMO-8->LUMO (9%) HOMO-6->LUMO (8%) HOMO-4->LUMO (8%) HOMO-2->LUMO+2 (8%) HOMO->LUMO+2 (7%) HOMO-4->LUMO+2 (7%)	CT	

		HOMO-6->LUMO (6%) HOMO-5->LUMO (6%) HOMO-5->LUMO (4%)		
		[Cu(SALPHEN)] S=1/2		
595.8	0.0001	HOMO-1->LUMO (33%) HOMO-1->LUMO (31%) HOMO->LUMO+1 (15%) HOMO->LUMO+1 (16%)	MLCT	
590.7	0.0001	HOMO->LUMO (38%) HOMO->LUMO (34%) HOMO-1->LUMO+1 (13%) HOMO-1->LUMO+1 (12%)	MLCT	
527.8	0.0043	HOMO-3->LUMO+2 (49%) HOMO-13->LUMO+2 (28%) HOMO-8->LUMO+2 (9%) HOMO-20->LUMO+2 (6%)	MLCT	
466.3	0.0019	HOMO-8->LUMO+2 (78%) HOMO-13->LUMO+2 (13%)	MLCT	
456.9	0.0002	HOMO-1->LUMO+2	MLC	

		(35%) HOMO-10->LUMO+2 (26%) HOMO-2->LUMO+2 (17%) HOMO-2->LUMO+1 (10%) HOMO-11->LUMO+2 (7%)	T	
452.1	0.0021	HOMO-1->LUMO+1 (28%) HOMO-1->LUMO+1 (20%) HOMO->LUMO (17%) HOMO-2->LUMO+1 (11%) HOMO-3->LUMO+1 (10%) HOMO-4->LUMO (4%) HOMO-4->LUMO (4%)	MLCT	
442.5	0.0388	HOMO->LUMO (51%) HOMO->LUMO (35%) HOMO-1->LUMO+1 (8%)	MLCT	
432.7	0.1246	HOMO-1->LUMO (51%) HOMO-1->LUMO (40%)	MLCT	
421.5	0.0045	HOMO->LUMO+1 (37%) HOMO-1->LUMO (20%)	MLCT	

		HOMO-3->LUMO (8%) HOMO-2->LUMO (8%) HOMO-1->LUMO (7%) HOMO->LUMO+1 (6%) HOMO-4->LUMO+1 (5%) HOMO-4->LUMO+1 (5%)		
409.4	0.0017	HOMO->LUMO+1 (63%) HOMO->LUMO+1 (30%)	MLCT	
386.2	0.2528	HOMO-1->LUMO+1 (43%) HOMO-1->LUMO+1 (43%)	MLCT	
348.2	0.0001	HOMO-3->LUMO (91%) HOMO-5->LUMO+1 (4%)	MLCT	
334.5	0.3113	HOMO-2->LUMO (53%) HOMO-3->LUMO (40%)	MLCT	
330.4	0.008	HOMO-4->LUMO+1 (23%) HOMO-4->LUMO+1 (21%) HOMO-3->LUMO (20%) HOMO-2->LUMO (5%)	MLCT	
320.5	0.0177	HOMO-3->LUMO+1 (41%) HOMO-2->LUMO+1 (41%) HOMO-4->LUMO (8%)	MLCT	

		HOMO-4->LUMO (6%)		
305.7	0.0018	HOMO->LUMO+6 (11%) HOMO->LUMO+6 (11%) HOMO-4->LUMO+1 (9%) HOMO-1->LUMO+3 (7%) HOMO-4>LUMO+1 (7%) HOMO-1->LUMO+4 (7%) HOMO-7->LUMO (6%) HOMO-7->LUMO (6%) HOMO-1->LUMO+7 (5%) HOMO-1->LUMO+8 (5%) HOMO->LUMO+3 (5%) 3HOMO->LUMO+2 (4%)	MLCT	
302.9	0.0998	HOMO-4->LUMO (27%) HOMO-5->LUMO+2 (25%) HOMO-4->LUMO (25%) HOMO-4->LUMO+2 (11%)	MLCT	463
290.9	0.3343	HOMO-3->LUMO+2 (46%) HOMO-13->LUMO+2 (34%) HOMO-20->LUMO+2 (8%)	MLCT	
284.9	0.0313	HOMO-4->LUMO+1 (49%)	MLCT	

		HOMO-4->LUMO+1 (45%)		
284.8	0.2623	HOMO-5->LUMO+2 (34%) HOMO-1->LUMO+2 (10%) HOMO-4->LUMO (6%) HOMO-4->LUMO (7%) HOMO-1->LUMO+3 (7%) HOMO-6->LUMO (5%)	MLCT	
284.3	0.1569	HOMO-5->LUMO+2 (21%) HOMO-1->LUMO+3 (15%) HOMO-1->LUMO+2 (10%) HOMO-6->LUMO (9%) HOMO-6->LUMO (6%) HOMO-4->LUMO (5%) HOMO-4->LUMO (4%)	MLCT	
281.6	0.0161	HOMO-5->LUMO (75%) HOMO-3->LUMO+1 (15%) HOMO-5->LUMO+2 (5%)	MLCT	
267.3	0.0015	HOMO->LUMO+3 (24%) HOMO-1->LUMO+3 (14%) HOMO-1->LUMO+4 (12%)	MLCT	

		HOMO-6->LUMO+1 (7%) HOMO-6->LUMO+1 (5%) HOMO->LUMO+2 (4%)		
		[Cu(SALPHEN)], S=3/2	MLCT	
1314.5	0.0606	HOMO-1->LUMO (76%) HOMO->LUMO (14%) HOMO-2->LUMO (4%)	MLCT	346
797.5	0.0129	HOMO-2->LUMO (91%) HOMO-1->LUMO (4%)	MLCT	
611.5	0.009	HOMO->LUMO+1 (92%)	MLCT	314
588.9	0.0022	HOMO->LUMO+1 (46%) HOMO-1->LUMO (43%) HOMO-4->LUMO (4%)	CT	
506.4	0.0426	HOMO->LUMO+2 (37%) HOMO-3->LUMO+2 (19%) HOMO-4->LUMO (9%) HOMO-8->LUMO+2 (6%) HOMO-13->LUMO+2 (6%) HOMO-1->LUMO (4%) HOMO-9->LUMO (4%) HOMO->LUMO+1 (4%)	MLCT	
485.3	0.0018	HOMO-5->LUMO (53%) HOMO-4->LUMO (26%)	MLCT	

		HOMO-3->LUMO+2 (5%) HOMO->LUMO+3 (4%) HOMO-13->LUMO+2 (4%)		
474.3	0.1394	HOMO->LUMO+2 (35%) HOMO-13->LUMO+2 (10%) HOMO-5->LUMO (10%) HOMO-3->LUMO+2 (14%) HOMO-8->LUMO+2 (5%)	MLCT	
459.1	0.0289	HOMO-1->LUMO+1 (32%) HOMO-3->LUMO (29%) HOMO-2->LUMO+1 (10%) HOMO-4->LUMO (8%)	MLCT	
446.5	0.0004	HOMO-8->LUMO (97%)	MLCT	
437.6	0.0267	HOMO->LUMO+3 (36%) HOMO-1->LUMO (18%) HOMO->LUMO+1 (18%) HOMO-7->LUMO (7%) HOMO-8->LUMO+2 (4%)	MLCT	
423.9	0.0548	HOMO->LUMO+3 (36%) HOMO-7->LUMO (30%) HOMO->LUMO+1 (5%) HOMO->LUMO+3 (5%) HOMO->LUMO+6 (4%)	MLCT	

		HOMO-1->LUMO+3 (4%)		
419.7	0.0983	HOMO-9->LUMO (53%) HOMO-1->LUMO (10%) HOMO->LUMO+1 (10%) HOMO-7->LUMO (7%)	MLCT	
408.9	0.0779	HOMO-7->LUMO (27%) HOMO-9->LUMO (26%) HOMO->LUMO+3 (9%) HOMO-1->LUMO (8%) HOMO->LUMO+1 (7%) HOMO->LUMO+10 (5%)	MLCT	
390.6	0.1037	HOMO->LUMO+10 (24%) HOMO->LUMO+6 (20%) HOMO->LUMO+3 (19%) HOMO-7->LUMO (17%) HOMO-1->LUMO+3 (5%)	MLCT	
375.6	0.0589	HOMO->LUMO+6 (65%) HOMO->LUMO+10 (12%) HOMO->LUMO+3 (8%)	MLCT	
367.3	0.0713	HOMO->LUMO+3 (57%) HOMO->LUMO+10 (25%)	MLCT	
358.4	0.1779	HOMO-1->LUMO+1 (49%) HOMO-3->LUMO (21%) HOMO->LUMO+10 (9%) HOMO-2->LUMO+1 (5%)	MLCT	

353.3	0.0152	HOMO-4->LUMO (26%) HOMO-3->LUMO (16%) HOMO-2->LUMO+1 (15%) HOMO-5->LUMO (7%) HOMO-1->LUMO+3 (7%) HOMO-2->LUMO+3 (6%) HOMO-1->LUMO+1 (5%)	MLCT	
340.9	0.0085	HOMO-7->LUMO (11%) HOMO-10->LUMO (11%) HOMO-1->LUMO+6 (10%) HOMO-5->LUMO+1 (7%) HOMO->LUMO+13 (6%) HOMO-12->LUMO (5%) HOMO-4->LUMO+1 (5%) HOMO->LUMO+8 (5%) HOMO-3->LUMO (4%) HOMO->LUMO+9 (6%)	MLCT	
335.4	0.0172	HOMO-12->LUMO (48%) HOMO-10->LUMO (20%)	MLCT	
328.1	0.1252	HOMO-4->LUMO (10%) HOMO-1->LUMO+3 (55%) HOMO-3->LUMO (9%)	MLCT	
323.9	0.0001	HOMO-3->LUMO+1	MLC	

		(75%) HOMO-13->LUMO (8%) HOMO->LUMO+11 (7%)	T	

Table S11. Coordinates of the structures obtained by DFT for Co-SALPHEN (Ground states)

Stoichiometry C20H16CoN2O3(2)
Framework group C1[X(C20H16CoN2O3)]
Deg. of freedom 120 (No. Of vibrational modes)
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.246845	5.587868	-0.177983
2	6	0	-0.700189	4.648973	-0.199256
3	6	0	0.709532	2.217798	-0.207898
4	6	0	-1.397922	3.442224	-0.192052
5	6	0	0.699973	4.649029	-0.197952
6	6	0	1.397759	3.442316	-0.189609
7	6	0	-0.709625	2.217731	-0.208956
8	1	0	-2.481939	3.464906	-0.145098

9	1	0	1.246519	5.587966	-0.175573
10	1	0	2.481690	3.464986	-0.140692
11	7	0	1.320726	0.941696	-0.168425
12	7	0	-1.320730	0.941595	-0.169989
13	6	0	-2.599927	0.780347	-0.422976
14	1	0	-3.183346	1.652263	-0.729944
15	6	0	2.599948	0.780533	-0.421548
16	1	0	3.183211	1.652667	-0.728172
17	6	0	3.337130	-0.437364	-0.348472
18	6	0	4.945000	-2.739974	-0.185089
19	6	0	2.743281	-1.693888	0.039452
20	6	0	4.729446	-0.387649	-0.656184
21	6	0	5.527084	-1.509318	-0.581555
22	6	0	3.600106	-2.832379	0.117621
23	1	0	5.161451	0.567113	-0.951935
24	1	0	6.585529	-1.454453	-0.819087
25	1	0	3.148877	-3.773330	0.419071
26	1	0	5.568936	-3.628914	-0.119084
27	6	0	-3.336824	-0.437589	-0.349236
28	6	0	-4.944123	-2.740420	-0.184186
29	6	0	-4.728988	-0.388561	-0.657760
30	6	0	-2.742832	-1.693443	0.040574
31	6	0	-3.599398	-2.832081	0.119531
32	6	0	-5.526337	-1.510380	-0.582386
33	1	0	-5.161102	0.565758	-0.954790
34	1	0	-3.148097	-3.772534	0.422407
35	1	0	-6.584657	-1.456084	-0.820611
36	1	0	-5.567835	-3.629474	-0.117586
37	8	0	1.481363	-1.831792	0.319588
38	8	0	-1.481115	-1.830618	0.322026
39	27	0	-0.000152	-0.614749	0.098094
40	8	0	-0.001923	1.027929	3.239005

41	1	0	-0.770068	0.900223	2.661466
42	1	0	0.766642	0.906620	2.660642

Table S12. Coordinates of the structures obtained by DFT for Co-SALPHEN (Excited state)

Stoichiometry C20H16CoN2O3(4)
Framework group C1[X(C20H16CoN2O3)]
Deg. of freedom 120
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.222424	5.674150	-0.048340
2	6	0	-0.668962	4.738800	-0.055868
3	6	0	0.760666	2.310867	-0.028498
4	6	0	-1.356877	3.526930	-0.115672
5	6	0	0.729538	4.745230	0.026305
6	6	0	1.434926	3.542089	0.049060
7	6	0	-0.659424	2.306485	-0.117598
8	1	0	-2.442801	3.533902	-0.127513
9	1	0	1.268589	5.686662	0.093865
10	1	0	2.516130	3.570479	0.143222
11	7	0	1.363875	1.037469	-0.005233
12	7	0	-1.270882	1.036315	-0.128262
13	6	0	-2.498402	0.858723	-0.548431
14	1	0	-3.016970	1.697607	-1.024407
15	6	0	2.643626	0.866305	-0.197859

16	1	0	3.285223	1.740676	-0.348916
17	6	0	3.321716	-0.394347	-0.275593
18	6	0	4.808228	-2.768175	-0.546541
19	6	0	2.629861	-1.660663	-0.328497
20	6	0	4.740681	-0.369452	-0.377302
21	6	0	5.485209	-1.526558	-0.499565
22	6	0	3.428272	-2.834056	-0.473244
23	1	0	5.244389	0.596099	-0.351561
24	1	0	6.568723	-1.485686	-0.565443
25	1	0	2.904976	-3.785185	-0.519694
26	1	0	5.381219	-3.687870	-0.648039
27	6	0	-3.263443	-0.348302	-0.441903
28	6	0	-4.964551	-2.578941	-0.206293
29	6	0	-4.570830	-0.343927	-1.006468
30	6	0	-2.798158	-1.525742	0.256178
31	6	0	-3.703180	-2.623118	0.360355
32	6	0	-5.414264	-1.432267	-0.903378
33	1	0	-4.905172	0.550870	-1.529707
34	1	0	-3.353443	-3.505445	0.889495
35	1	0	-6.406673	-1.409213	-1.344358
36	1	0	-5.620437	-3.442585	-0.115541
37	8	0	1.334474	-1.780481	-0.286196
38	8	0	-1.615376	-1.619091	0.797560
39	27	0	-0.014267	-0.544525	0.332173
40	8	0	0.222957	-0.560813	2.536927
41	1	0	-0.577753	-1.099364	2.691321
42	1	0	0.066449	0.294362	2.969960

Table S13. Coordinates of the structures obtained by DFT for Fe-SALPHEN (Ground states)

Stoichiometry C20H16ClFeN2O3(2)

Framework group C1[X(C20H16ClFeN2O3)]
Deg. of freedom 123
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.516958	5.474622	-0.628319
2	6	0	-0.904352	4.578313	-0.581425
3	6	0	0.674031	2.267345	-0.438592
4	6	0	-1.515915	3.328420	-0.531737
5	6	0	0.493707	4.681706	-0.555473
6	6	0	1.279317	3.534456	-0.475294
7	6	0	-0.733563	2.163744	-0.471186
8	1	0	-2.597993	3.273601	-0.522221
9	1	0	0.970050	5.657929	-0.585845
10	1	0	2.357649	3.643571	-0.433569
11	7	0	1.348925	1.025424	-0.338832
12	7	0	-1.222110	0.836908	-0.416693
13	6	0	-2.504251	0.568020	-0.477326
14	1	0	-3.207128	1.392629	-0.569708
15	6	0	2.663129	0.946460	-0.355652
16	1	0	3.230421	1.864769	-0.505414
17	6	0	3.438421	-0.232331	-0.206892
18	6	0	5.079414	-2.503555	0.025087
19	6	0	2.838216	-1.535298	-0.078582
20	6	0	4.860006	-0.114119	-0.217526
21	6	0	5.672739	-1.220180	-0.100676
22	6	0	3.708139	-2.660657	0.032630

23	1	0	5.299598	0.876793	-0.317208
24	1	0	6.753815	-1.115419	-0.104564
25	1	0	3.246082	-3.638799	0.128064
26	1	0	5.717469	-3.379718	0.118371
27	6	0	-3.077353	-0.735891	-0.446990
28	6	0	-4.307500	-3.259085	-0.531353
29	6	0	-4.493906	-0.855226	-0.464313
30	6	0	-2.268840	-1.921303	-0.462009
31	6	0	-2.926074	-3.180359	-0.518527
32	6	0	-5.107606	-2.091703	-0.499662
33	1	0	-5.093336	0.052318	-0.437723
34	1	0	-2.303691	-4.070150	-0.537585
35	1	0	-6.190929	-2.170453	-0.502334
36	1	0	-4.786120	-4.235510	-0.561667
37	8	0	1.555709	-1.742265	-0.091803
38	8	0	-0.960402	-1.900319	-0.457975
39	26	0	0.164960	-0.473990	-0.035802
40	17	0	-0.081656	-0.200996	2.170700
41	8	0	-2.863273	1.758681	2.265962
42	1	0	-2.138838	1.107102	2.339368
43	1	0	-2.591443	2.489723	2.841501

Table S14. Coordinates of the structures obtained by DFT for Fe-SALPHEN (Excited state)

Stoichiometry C20H16ClFeN2O3(2)
Framework group C1[X(C20H16ClFeN2O3)]
Deg. of freedom 123 (No. Of vibrational modes)
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.239313	5.586010	-0.953945
2	6	0	-0.696201	4.702326	-0.621501
3	6	0	0.705814	2.428470	0.218255
4	6	0	-1.396934	3.567289	-0.208901
5	6	0	0.696708	4.702344	-0.621563
6	6	0	1.397002	3.567007	-0.208859
7	6	0	-0.705969	2.427667	0.217931
8	1	0	-2.481659	3.595074	-0.241375
9	1	0	1.238702	5.585483	-0.954073
10	1	0	2.481542	3.594754	-0.241486
11	7	0	1.364083	1.316906	0.616720
12	7	0	-1.363445	1.316890	0.616342
13	6	0	-2.681795	1.121303	0.650977
14	1	0	-3.356588	1.918822	1.015826
15	6	0	2.681237	1.121440	0.651302
16	1	0	3.355705	1.917816	1.015438
17	6	0	3.329304	-0.126568	0.237826
18	6	0	4.764059	-2.381124	-0.573550
19	6	0	2.965342	-0.813190	-0.918705
20	6	0	4.435219	-0.553447	0.979205
21	6	0	5.142884	-1.688872	0.577940
22	6	0	3.679954	-1.937871	-1.331731
23	1	0	4.765526	-0.008873	1.860410
24	1	0	6.003062	-2.027856	1.153555
25	1	0	3.404592	-2.468870	-2.240697
26	1	0	5.328802	-3.257360	-0.889351
27	6	0	-3.330180	-0.126642	0.238570
28	6	0	-4.764628	-2.380989	-0.573663

29	6	0	-4.435383	-0.553042	0.979002
30	6	0	-2.965439	-0.813339	-0.919513
31	6	0	-3.679994	-1.938230	-1.331280
32	6	0	-5.143187	-1.688767	0.577822
33	1	0	-4.765476	-0.007960	1.860491
34	1	0	-3.405209	-2.468858	-2.239881
35	1	0	-6.003640	-2.027193	1.153571
36	1	0	-5.328739	-3.256969	-0.889567
37	8	0	1.936374	-0.372540	-1.714808
38	8	0	-1.935821	-0.373175	-1.714884
39	26	0	0.000146	-0.822903	-0.194969
40	17	0	0.000259	-2.923643	0.776371
41	8	0	-0.000058	-0.106281	2.316417
42	1	0	0.791295	0.494016	2.309662
43	1	0	-0.792093	0.494163	2.309700

Table S15. Coordinates of the structures obtained by DFT for Cu-SALPHEN (Ground states)

Stoichiometry C20H14CuN2O2(2)
Framework group C1[X(C20H14CuN2O2)]
Deg. of freedom 111 (No. Of vibrational modes)
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	1	0	1.248695	5.668669	0.015685
2	6	0	0.700581	4.730343	0.010860
3	6	0	-0.710498	2.297235	0.002241
4	6	0	1.397241	3.524308	0.007483
5	6	0	-0.700502	4.730350	0.011175
6	6	0	-1.397176	3.524321	0.008095
7	6	0	0.710551	2.297223	0.001932
8	1	0	2.481744	3.552141	0.011545
9	1	0	-1.248608	5.668679	0.016260
10	1	0	-2.481677	3.552168	0.012616
11	7	0	-1.319438	1.022552	0.000799
12	7	0	1.319474	1.022539	0.000316
13	6	0	2.620081	0.849104	-0.019536
14	1	0	3.262337	1.732395	-0.041482
15	6	0	-2.620054	0.849131	-0.018711
16	1	0	-3.262313	1.732435	-0.040020
17	6	0	-3.314024	-0.392288	-0.015713
18	6	0	-4.848485	-2.751161	-0.006473
19	6	0	-2.643634	-1.674007	0.009715
20	6	0	-4.741453	-0.347183	-0.037459
21	6	0	-5.505068	-1.492851	-0.033283
22	6	0	-3.472088	-2.841711	0.014402
23	1	0	-5.227103	0.627348	-0.057506
24	1	0	-6.589684	-1.438399	-0.049726
25	1	0	-2.966711	-3.803042	0.034439
26	1	0	-5.441810	-3.663432	-0.002528
27	6	0	3.314053	-0.392312	-0.016074
28	6	0	4.848436	-2.751208	-0.005618
29	6	0	4.741455	-0.347258	-0.038711
30	6	0	2.643637	-1.673988	0.010932
31	6	0	3.472038	-2.841705	0.016174
32	6	0	5.505038	-1.492958	-0.033977

33	1	0	5.227135	0.627233	-0.059933
34	1	0	2.966671	-3.803015	0.037399
35	1	0	6.589645	-1.438542	-0.051138
36	1	0	5.441721	-3.663502	-0.001207
37	8	0	-1.359335	-1.831232	0.027593
38	8	0	1.359339	-1.831093	0.029801
39	29	0	-0.000038	-0.454775	0.017376

Table S16. Coordinates of the structures obtained by DFT for Cu-SALPHEN (Excited states)

Stoichiometry C20H14CuN2O2(4)
Framework group C1[X(C20H14CuN2O2)]
Deg. of freedom 111
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.208039	5.681204	0.000375
2	6	0	0.666568	4.738551	0.000406
3	6	0	-0.747956	2.305822	0.000920
4	6	0	1.372316	3.544599	-0.000522
5	6	0	-0.739985	4.737651	0.001655
6	6	0	-1.434574	3.525951	0.001968
7	6	0	0.691075	2.294092	-0.000338
8	1	0	2.455438	3.577341	-0.000997
9	1	0	-1.289400	5.674923	0.002559
10	1	0	-2.519583	3.550029	0.003179

11	7	0	-1.350342	1.032447	0.001049
12	7	0	1.294743	1.063438	-0.001005
13	6	0	2.648670	0.901719	-0.003902
14	1	0	3.277938	1.787347	-0.007741
15	6	0	-2.646924	0.834460	0.000040
16	1	0	-3.304843	1.706446	-0.000613
17	6	0	-3.315057	-0.424260	-0.000551
18	6	0	-4.796025	-2.816958	-0.002331
19	6	0	-2.617606	-1.689353	-0.000946
20	6	0	-4.741667	-0.411714	-0.001135
21	6	0	-5.480098	-1.575866	-0.001978
22	6	0	-3.415351	-2.874084	-0.001828
23	1	0	-5.249782	0.551438	-0.000876
24	1	0	-6.565800	-1.545106	-0.002371
25	1	0	-2.888036	-3.823836	-0.002139
26	1	0	-5.366921	-3.743366	-0.003027
27	6	0	3.330026	-0.339633	-0.002426
28	6	0	4.861405	-2.796509	0.001717
29	6	0	4.747543	-0.346390	-0.005603
30	6	0	2.672065	-1.664279	0.002640
31	6	0	3.478686	-2.849426	0.004765
32	6	0	5.490271	-1.526889	-0.003629
33	1	0	5.271235	0.606972	-0.009595
34	1	0	2.940412	-3.793216	0.008685
35	1	0	6.576321	-1.466024	-0.006197
36	1	0	5.454826	-3.705825	0.003275
37	8	0	-1.324402	-1.817080	-0.000713
38	8	0	1.392219	-1.814311	0.005129
39	29	0	-0.010120	-0.416666	0.001597

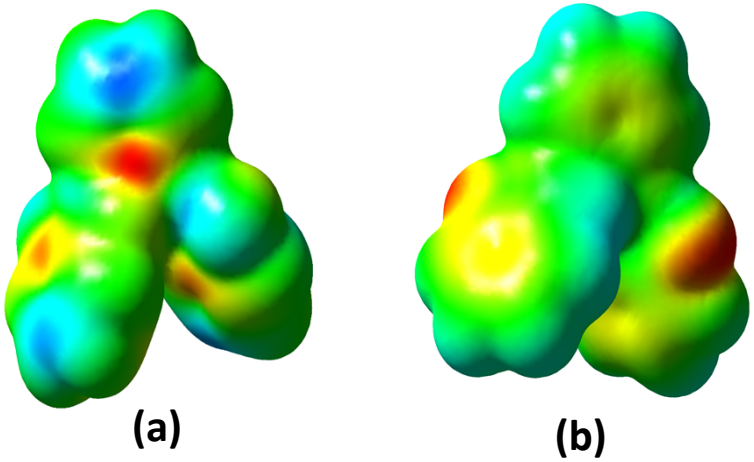


Figure S1. Electrostatic potential plotted on a 0.0004 electron density isosurface of SALPHEN: a) B3LYP/dgdzvp and b) B3LYP/6-31G** at gaseous state. In the electrostatic potential: blue color=negative electric charge; red color= positive electric charge; yellow=potential close to zero. All the plots were calculated at the DFT level of theory. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.

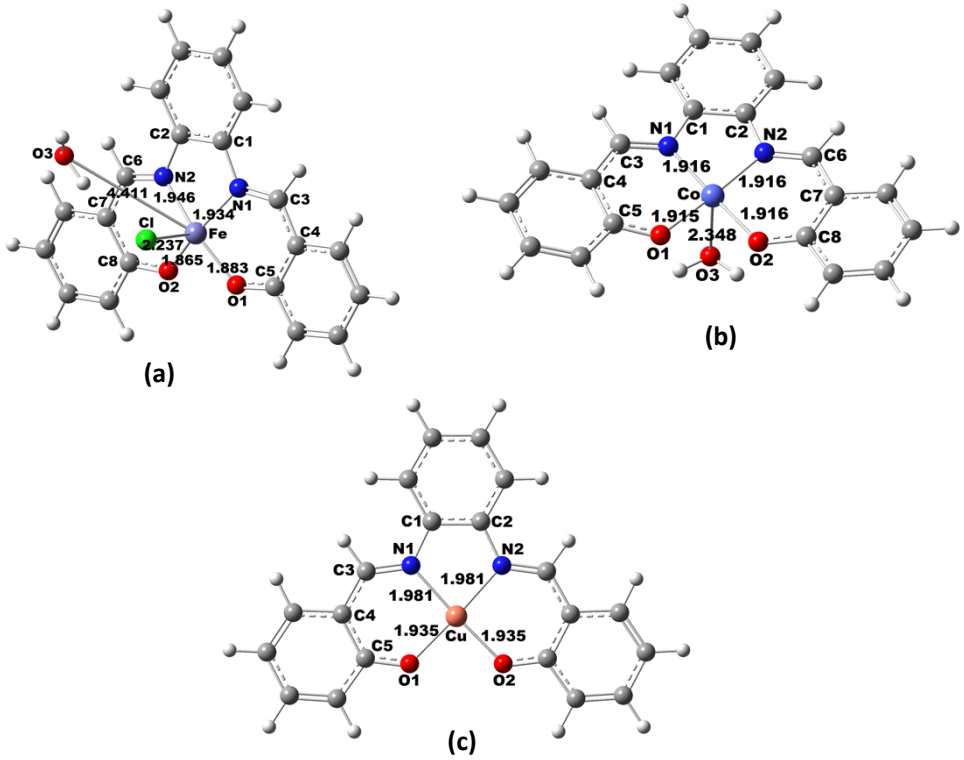
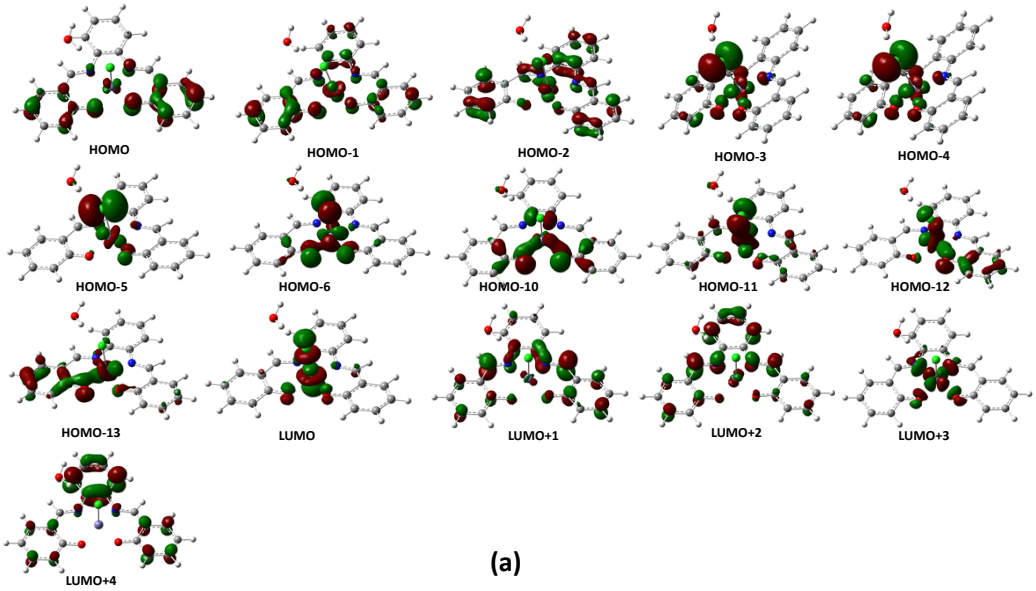
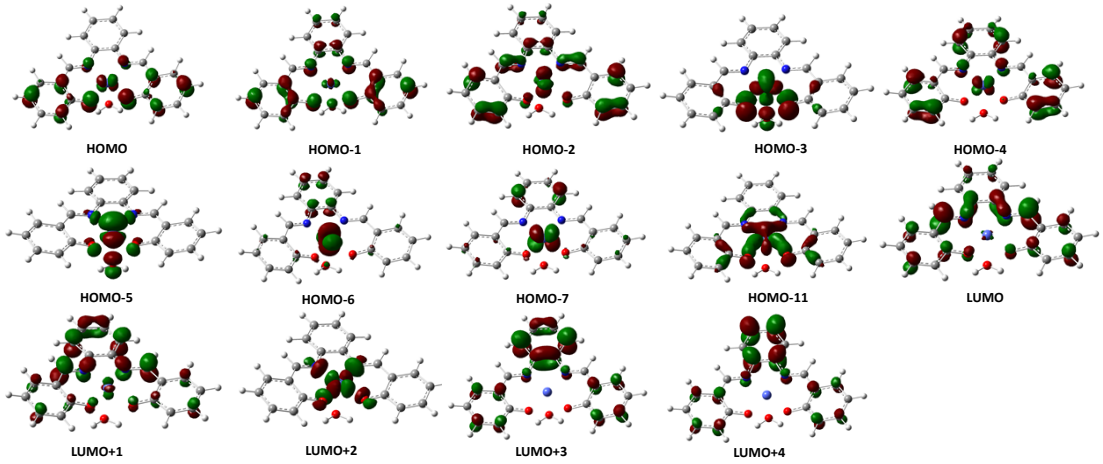


Figure S2. Optimized structure of different complexes: a) $[Fe(SALPHEN)Cl(H_2O)]^{2+}$; b) $[Co(SALPHEN)Cl(H_2O)]^{2+}$ and c) $[Cu(SALPHEN)]^{2+}$ with ligand (SALPHEN).


HOMO
HOMO-1
HOMO-2
HOMO-3
HOMO-4
HOMO-5
HOMO-6
HOMO-10
HOMO-11
HOMO-12
HOMO-13
LUMO
LUMO+1
LUMO+2
LUMO+3
LUMO+4

(a)


HOMO
HOMO-1
HOMO-2
HOMO-3
HOMO-4
HOMO-5
HOMO-6
HOMO-7
HOMO-11
LUMO
LUMO+1
LUMO+2
LUMO+3
LUMO+4

(b)

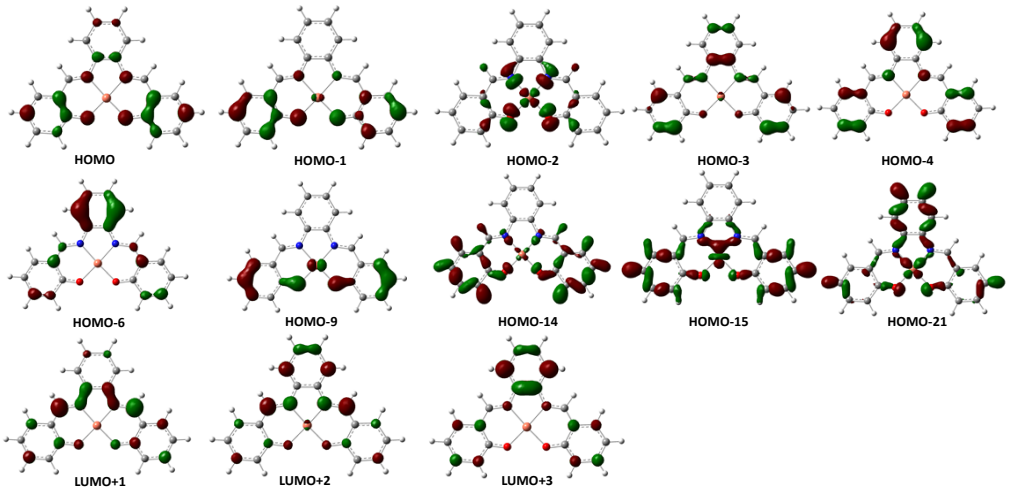


Figure S3. Molecular orbital: a) $[Fe(SALPHEN)Cl(H_2O)]^{2+}$, b) $[Co(SALPHEN)(H_2O)]^{2+}$ and c) $[Cu(SALPHEN)]^{2+}$ at gaseous state.

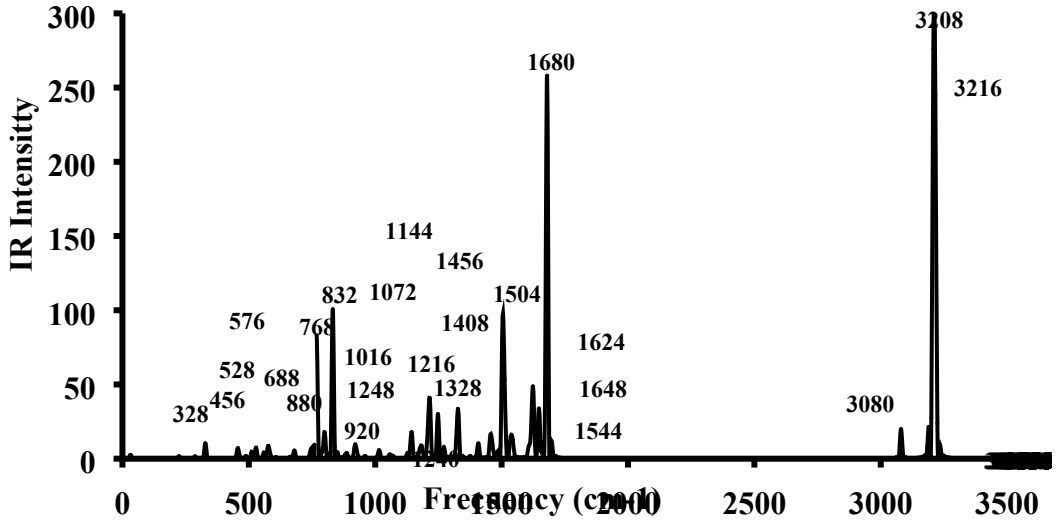


Figure S4. FTIR spectra of SALPHEN obtained using B3LYP/DGDZVP at gaseous state.

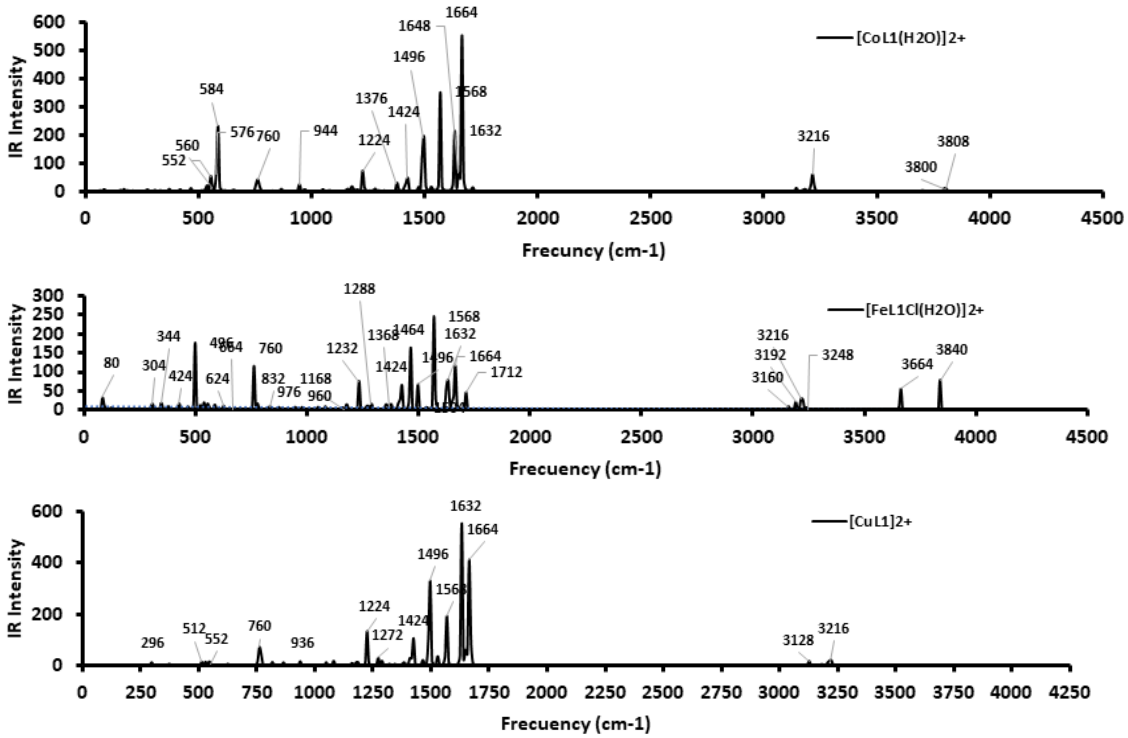


Figure S5. Theoretical FTIR spectra of $[Co(SALPHEN)(H_2O)]^{2+}$, $[Fe(SALPHEN)Cl(H_2O)]^{2+}$ and $[Cu(SALPHEN)]^{2+}$; (L = SALPHEN).

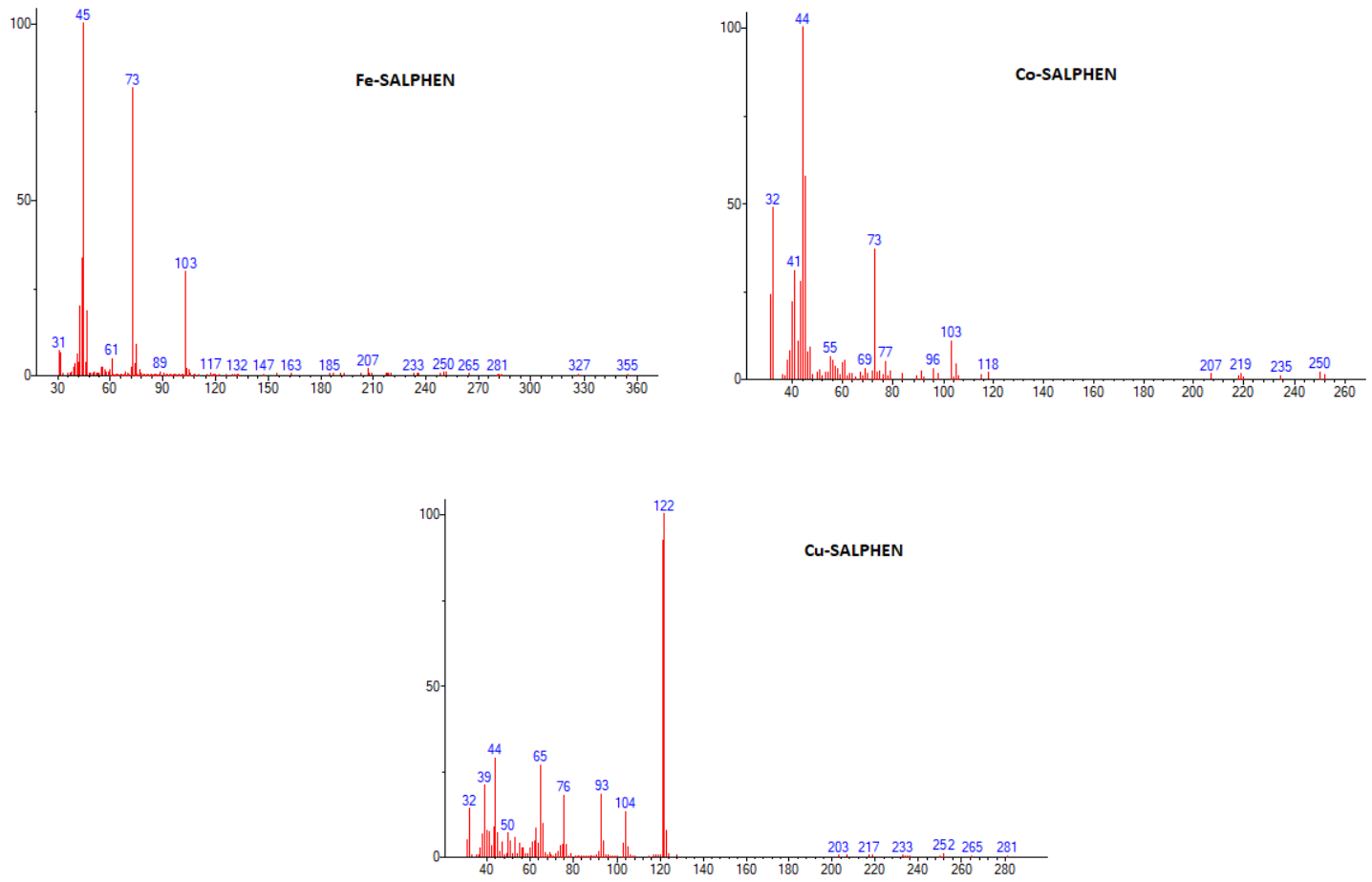
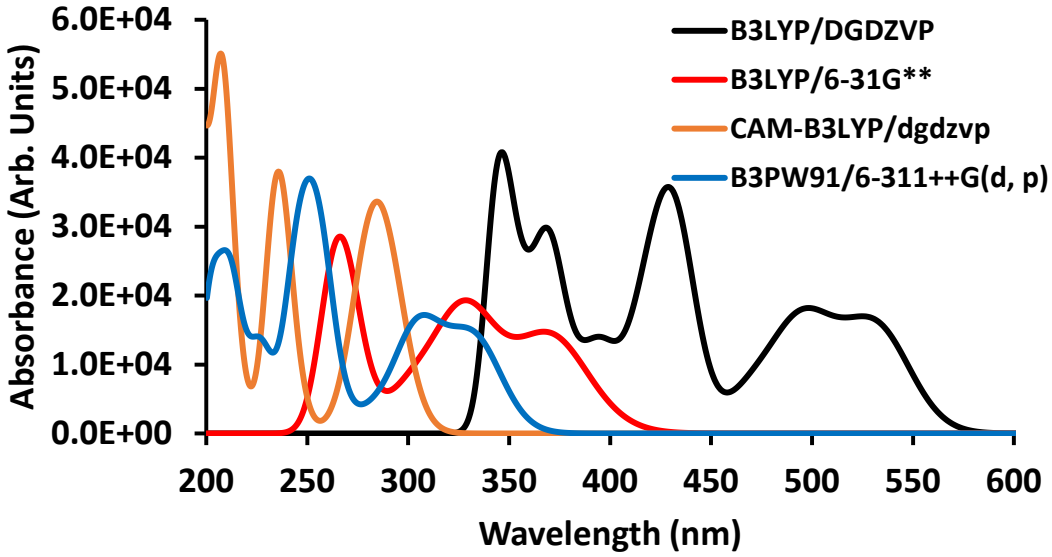
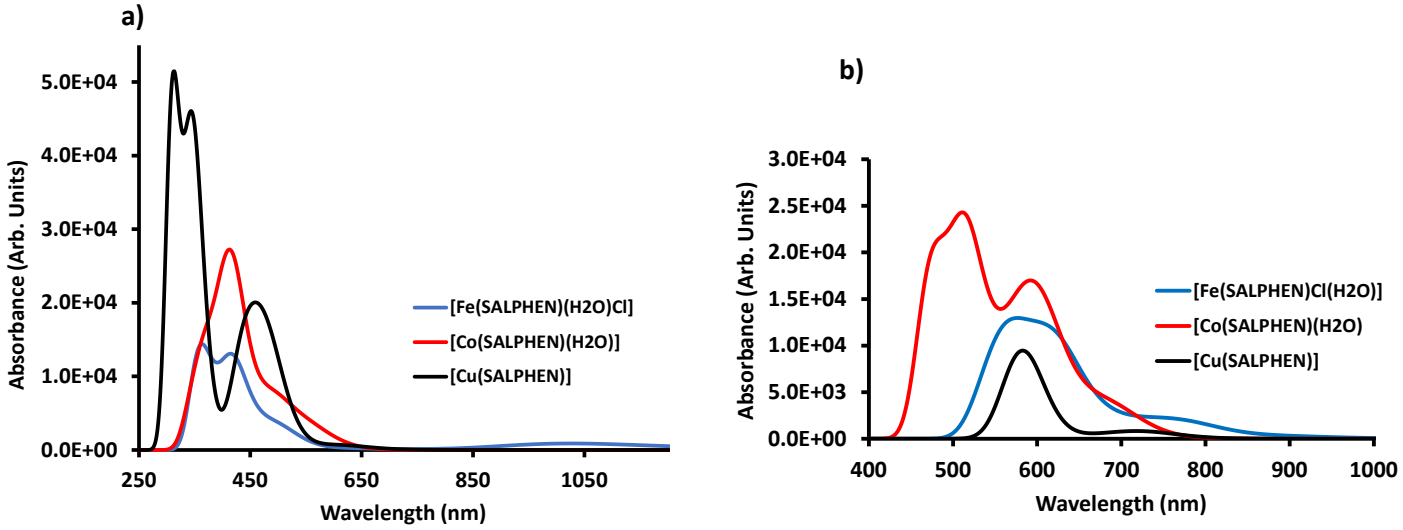


Figure S6. Mass spectrum of the metal complexes of SALPHEN.



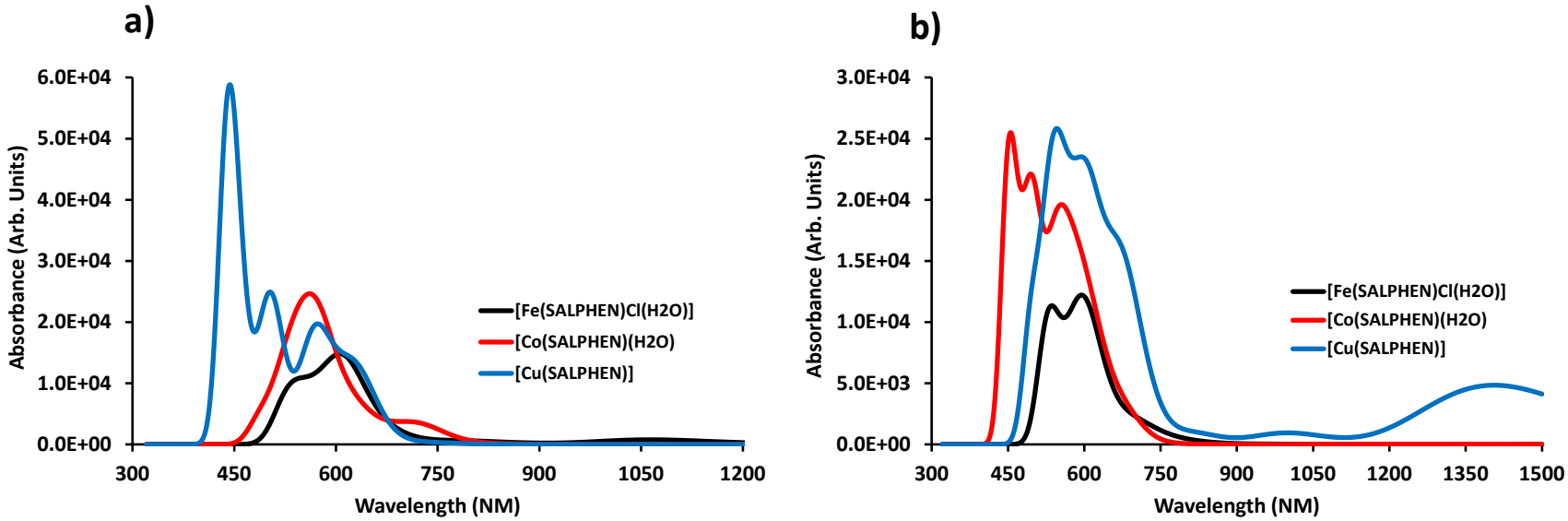
Basis set	λ1	λ2	λ3	λ4	λ5	λ6
DGDZVP	348	370	396	429	500	528
6-31G**	267	331	371			
CAM-B3LYP/6-311++G(d, P)	207	236	287			
B3PW91/6-311++G(d, p)	210	228	252	310	331	

Figure S7. TD-DFT spectra of SALPHEN using different functionals at gaseous state.



Basis set		GS	ES
B3LYP/DGDZVP	Fe(SALPHEN)Cl(H2O)]	369, 430, 475, 1019	566, 625, 763
	[Co(SALPHEN)(H2O)]	506, 570, 667	481, 513, 594, 683
	[Cu(SALPHEN)]	455, 493, 615	585, 720

Figure S8. TD-DFT spectra of SALPHEN and its complexes using functional B3LYP/DGDZVP basis set at gaseous state, a) in ground state and b) Excited state.



Basis set		GS	ES
B3PW91/6-311++G(d, p)		540, 603, 778	
	Fe(SALPHEN)Cl(H2O)]	570, 725	539, 612, 720
	[Co(SALPHEN)(H2O)]	444, 506, 575, 625	456, 498, 563, 849
	[Cu(SALPHEN)]		499, 550, 599, 668

Figure S9. TD-DFT spectra of SALPHEN using functional B3PW91/6-311++G(d, p) basis set at gaseous state, **a**) in ground state and **b**) Excited state.