Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Redox induced oxidative C-C coupling of non-innocent bis(heterocyclo)methanides

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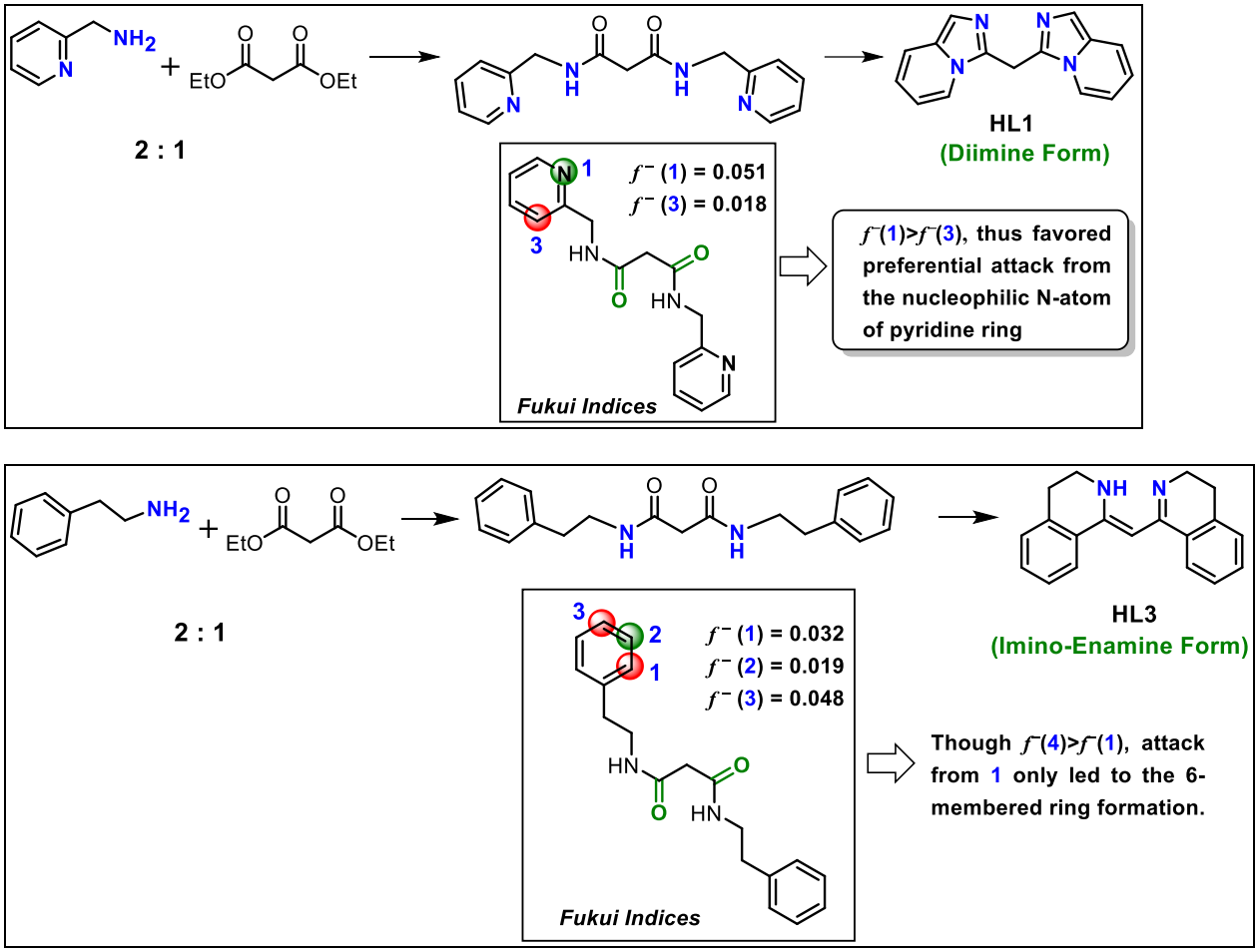


Scheme S1 Fukui indices calculation and positional selectivity.

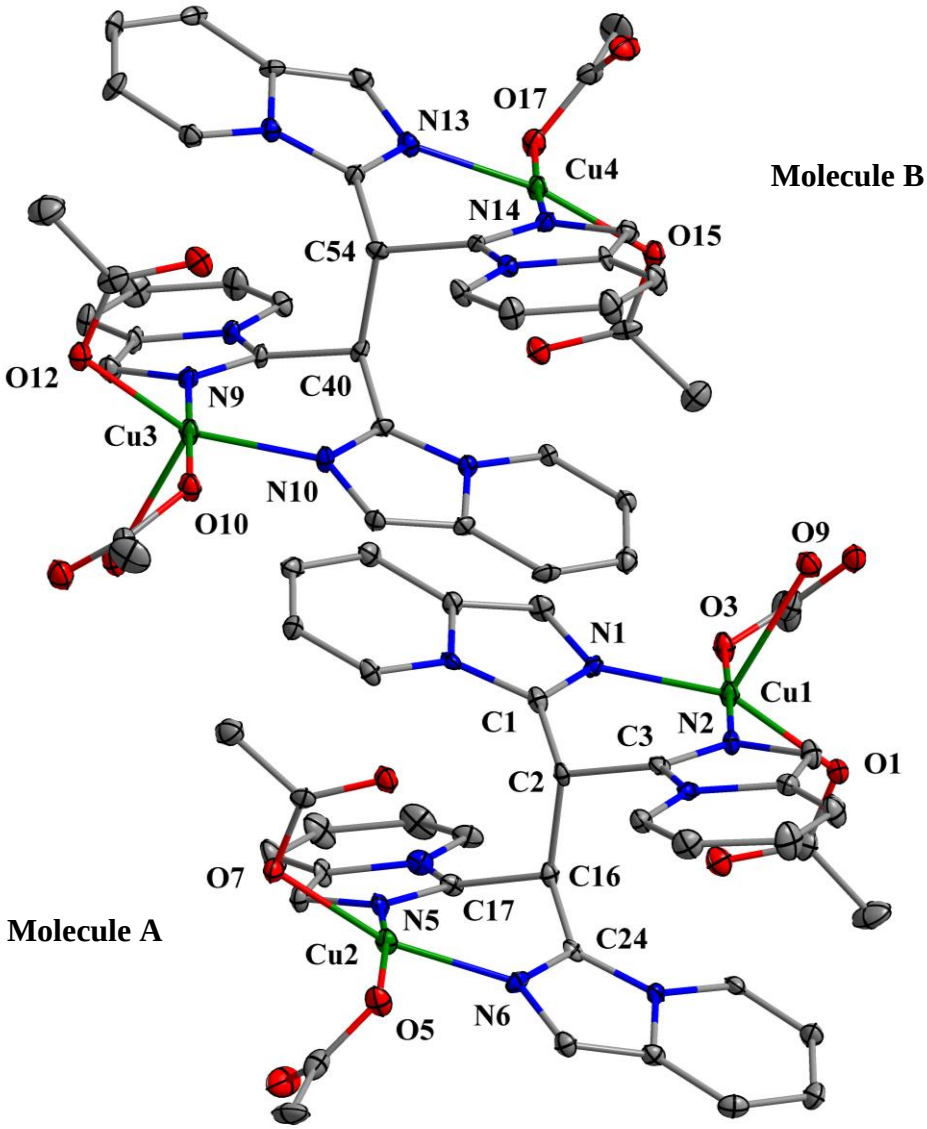


Fig. S1a Perspective view of the asymmetric unit of **1a**. Ellipsoids are drawn at 20% probability level. Hydrogen atoms are removed for clarity.

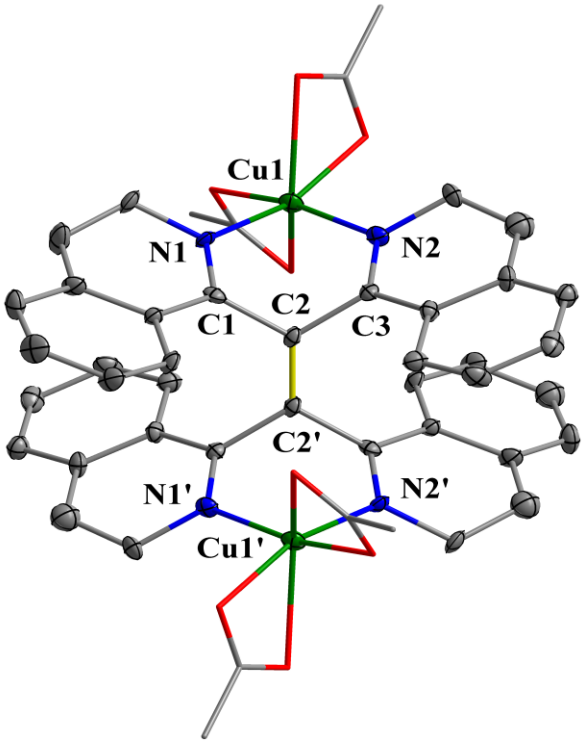


Fig. S1b Perspective view of the asymmetric unit of **1c**. Ellipsoids are drawn at 25% probability level. Hydrogen atoms are removed for clarity.

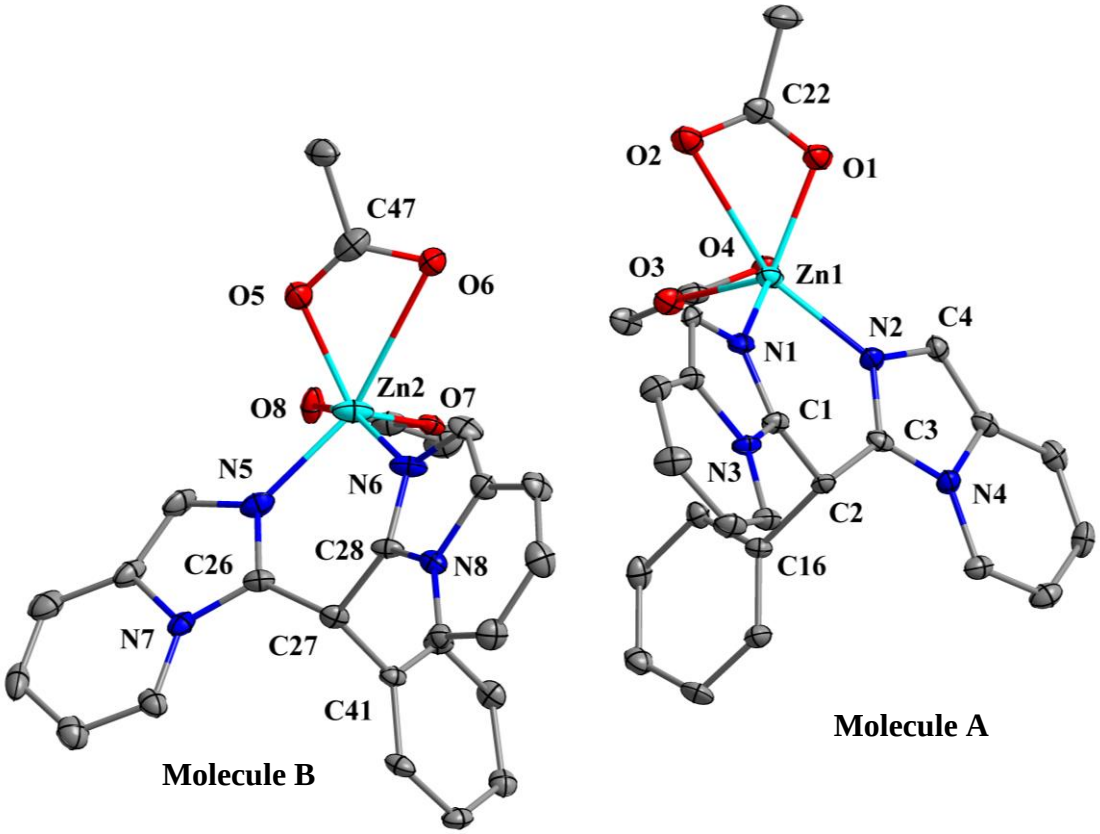


Fig. S1c Perspective view of the asymmetric unit of **2**. Ellipsoids are drawn at 20% probability level. Hydrogen atoms are removed for clarity.

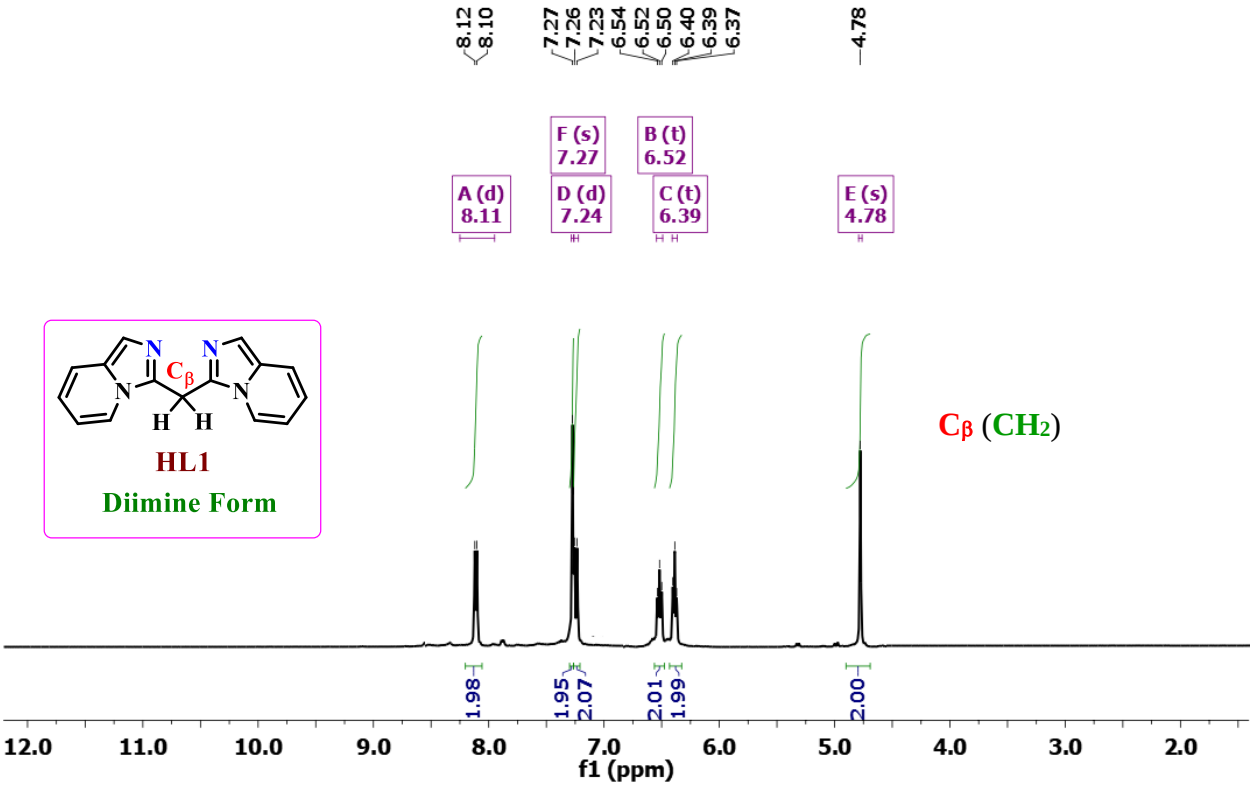


Fig. S2a ^{1}H NMR of **HL1** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

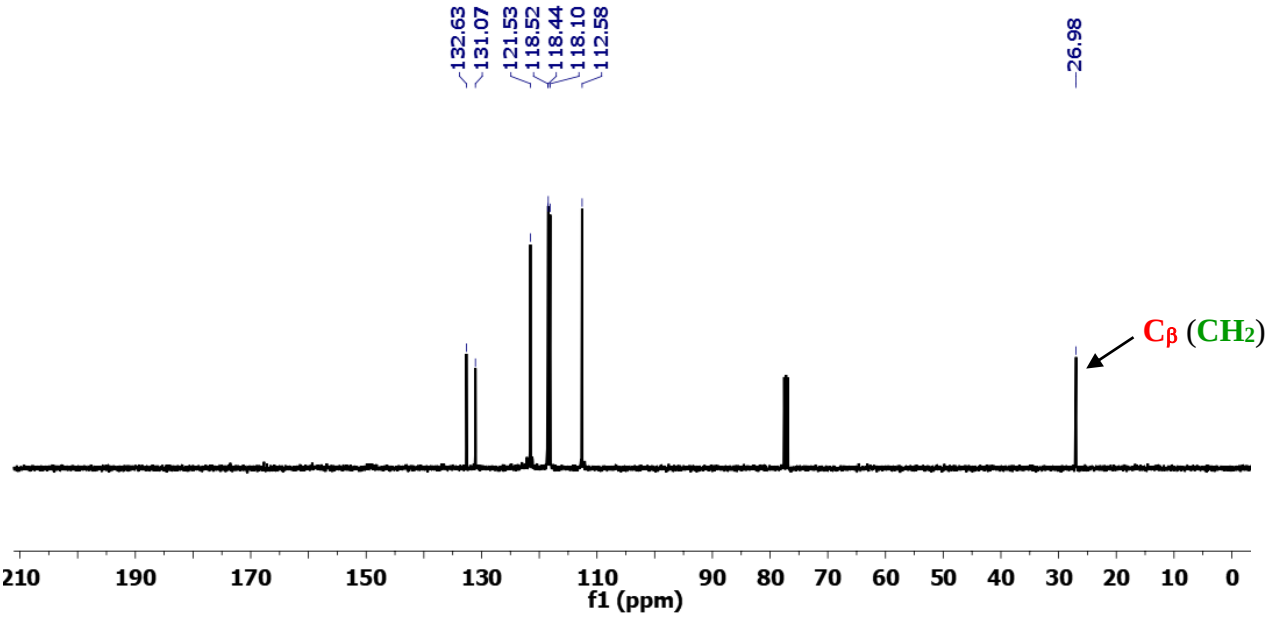


Fig. S2b ^{13}C NMR of **HL1** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

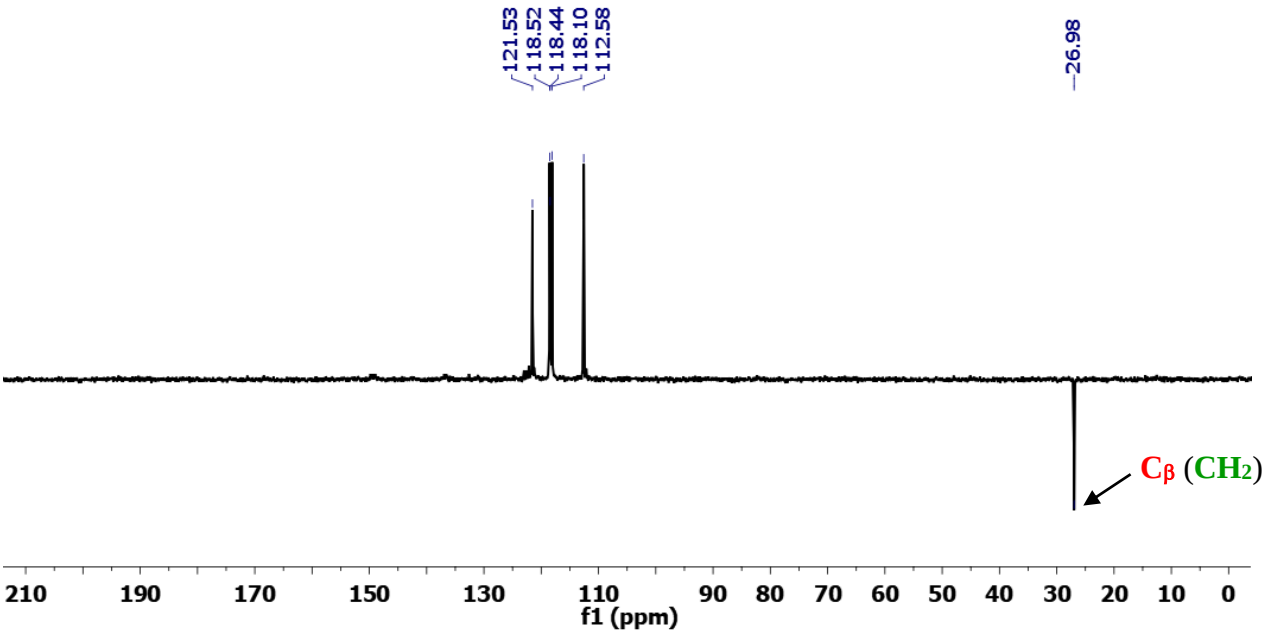


Fig. S2c DEPT-135 NMR of **HL1** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

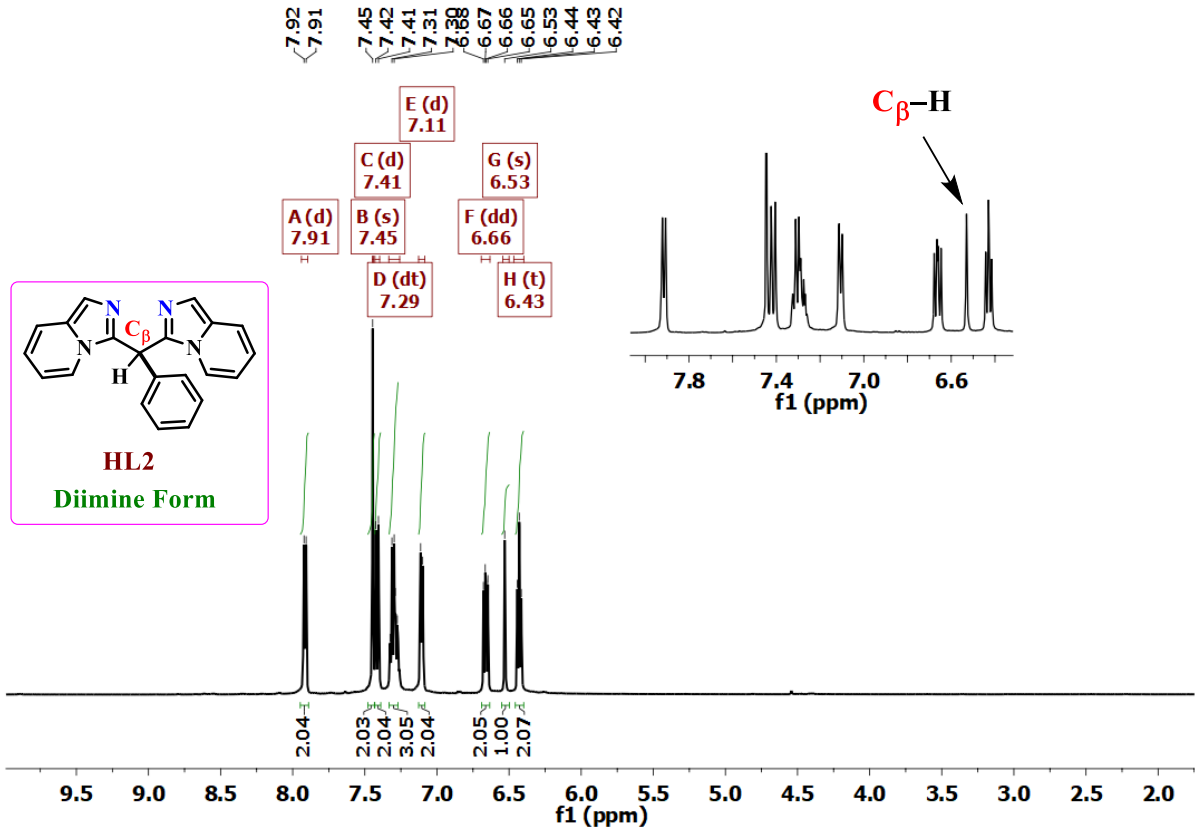


Fig. S2d ^{1}H NMR of **HL2** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

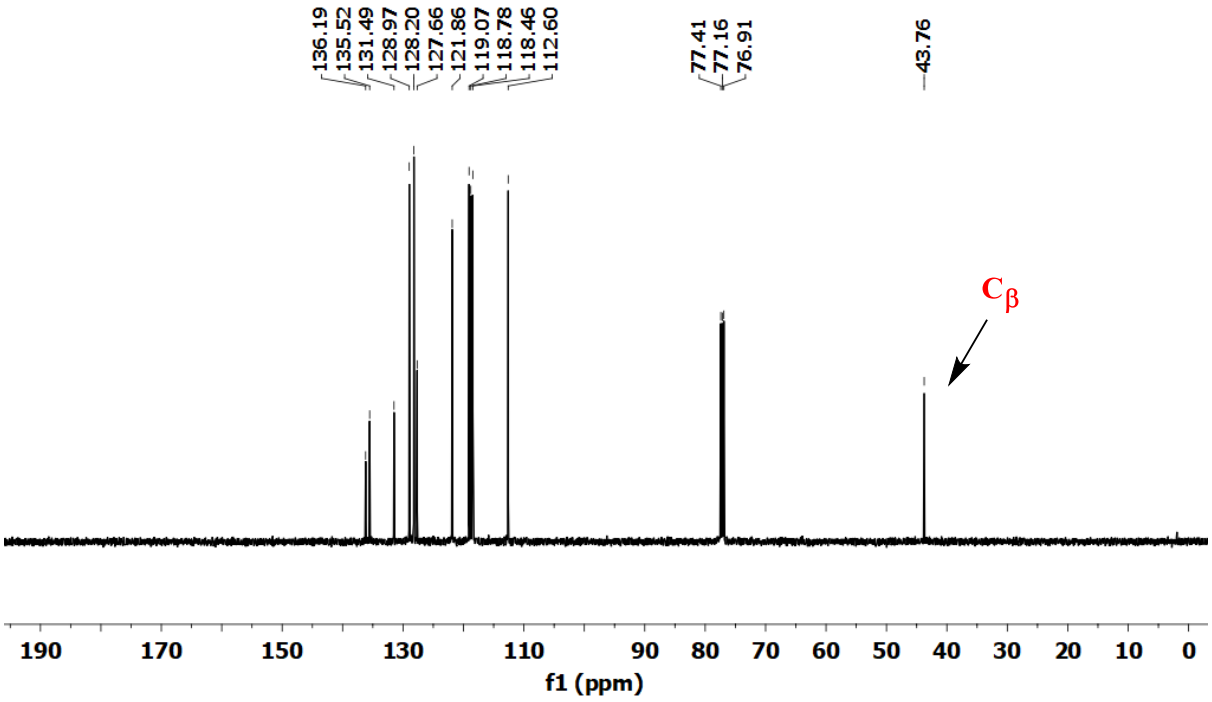


Fig. S2e ^{13}C NMR of **HL2** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

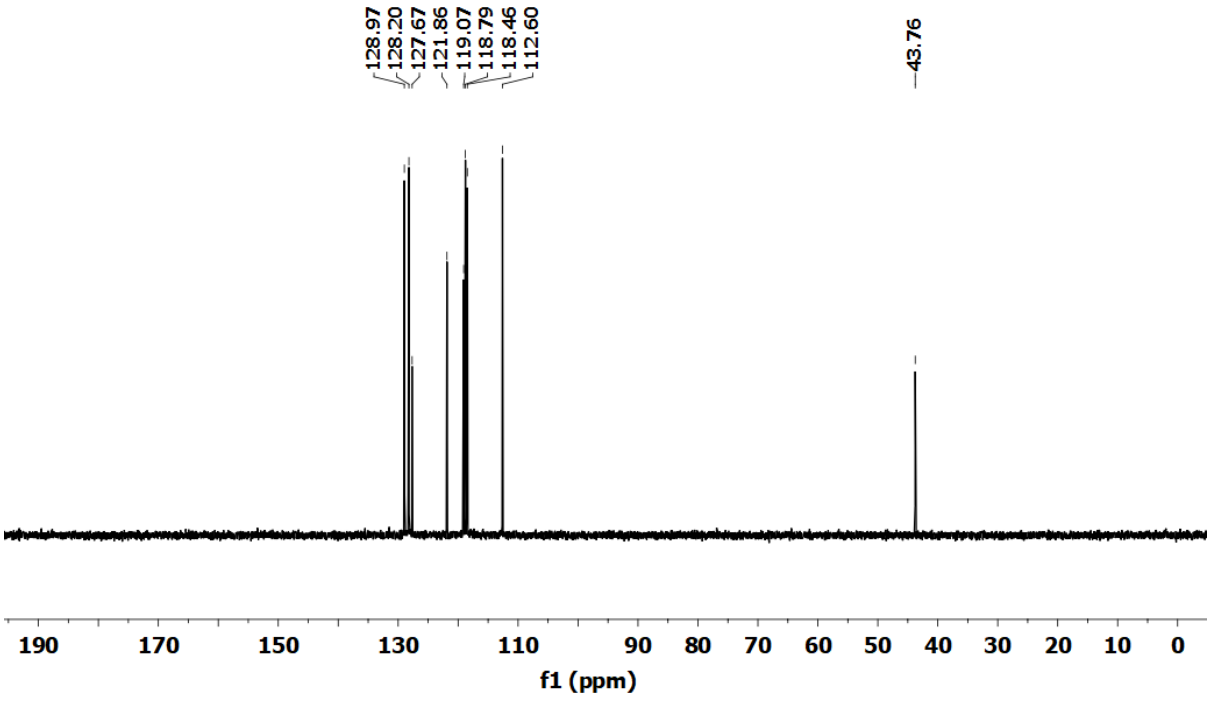


Fig. S2f DEPT-135 NMR of **HL2** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

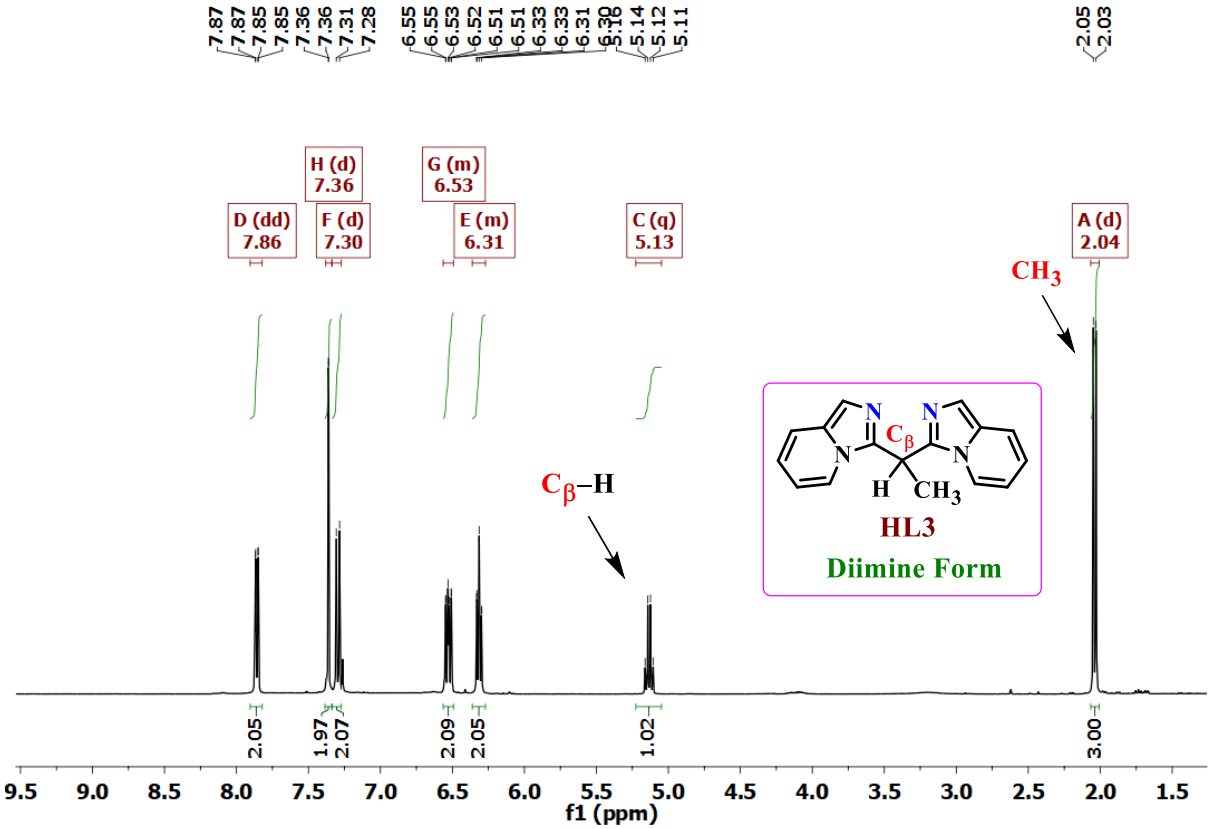


Fig. S2g ^{1}H NMR of **HL3** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

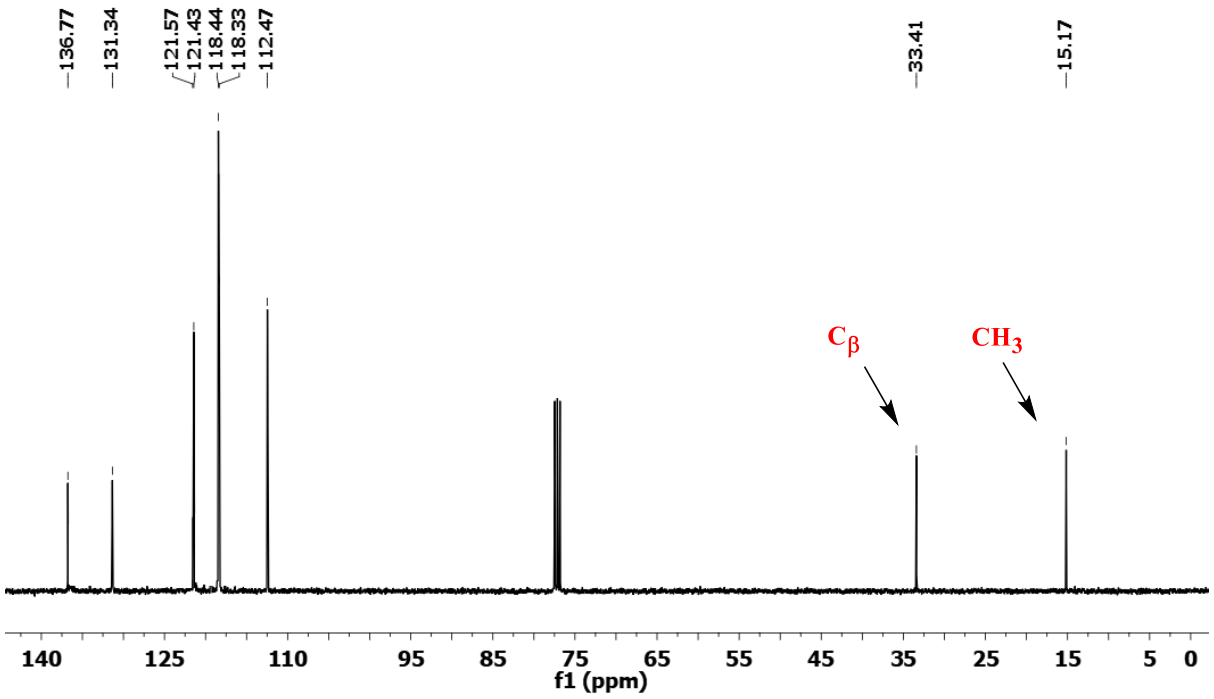


Fig. S2h ^{13}C NMR of **HL3** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

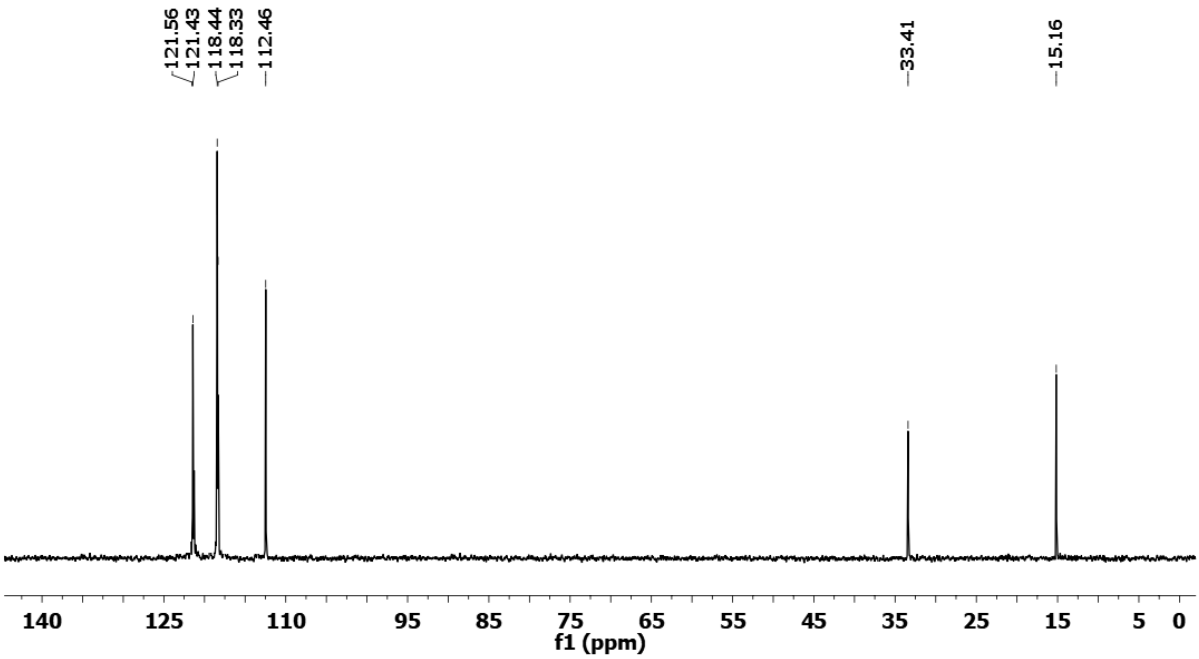


Fig. S2i DEPT-135 NMR of **HL3** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

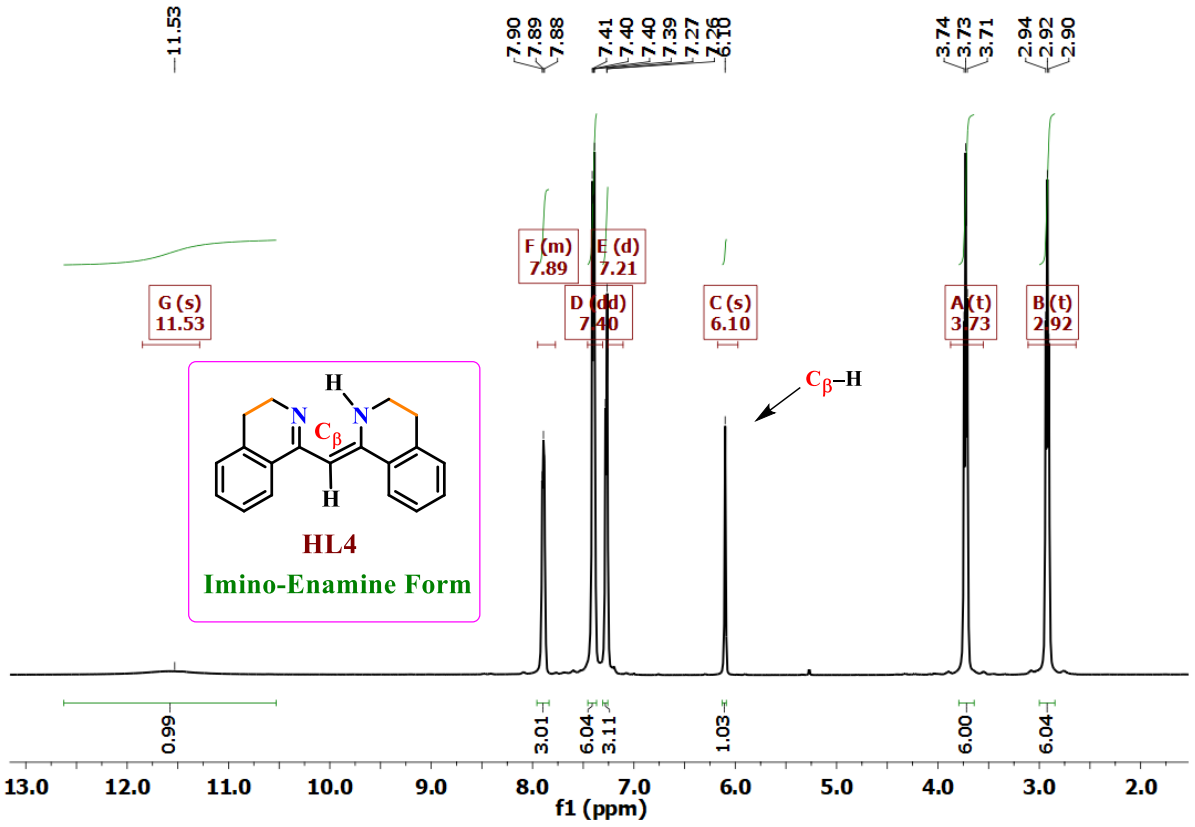


Fig. 2j ^{1}H NMR of **HL4** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

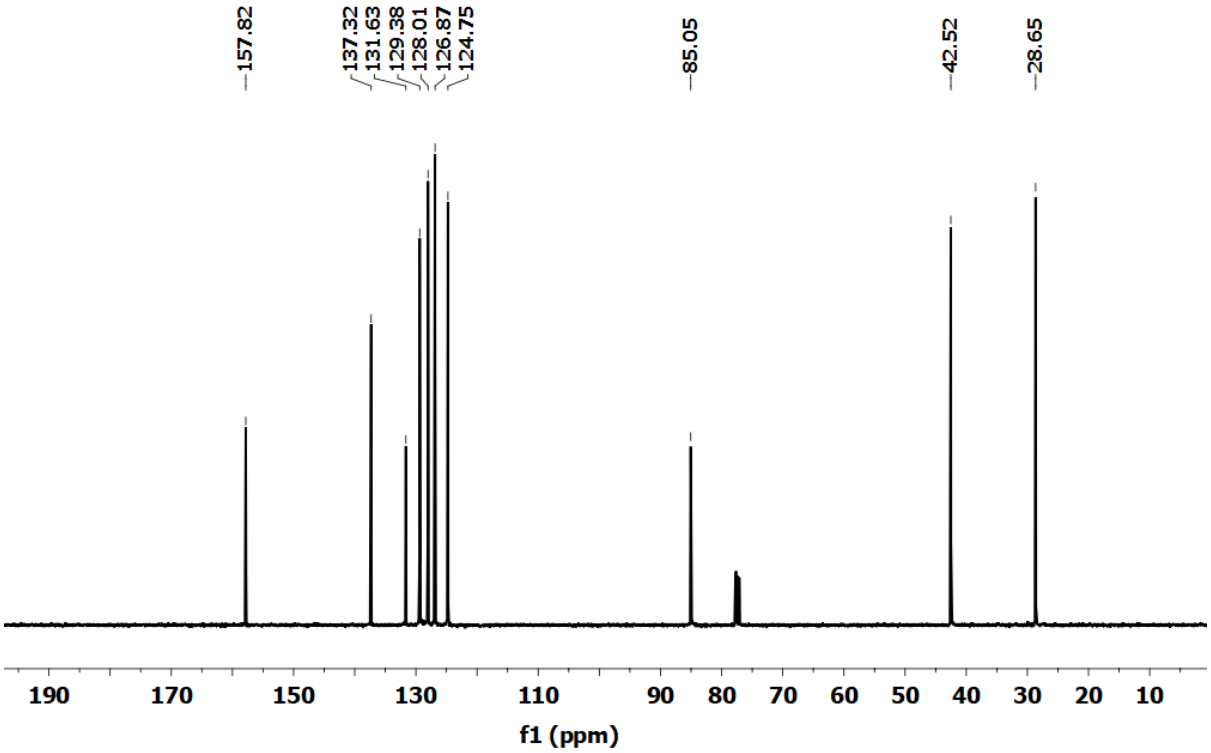


Fig. S2k ^{13}C NMR of **HL4** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

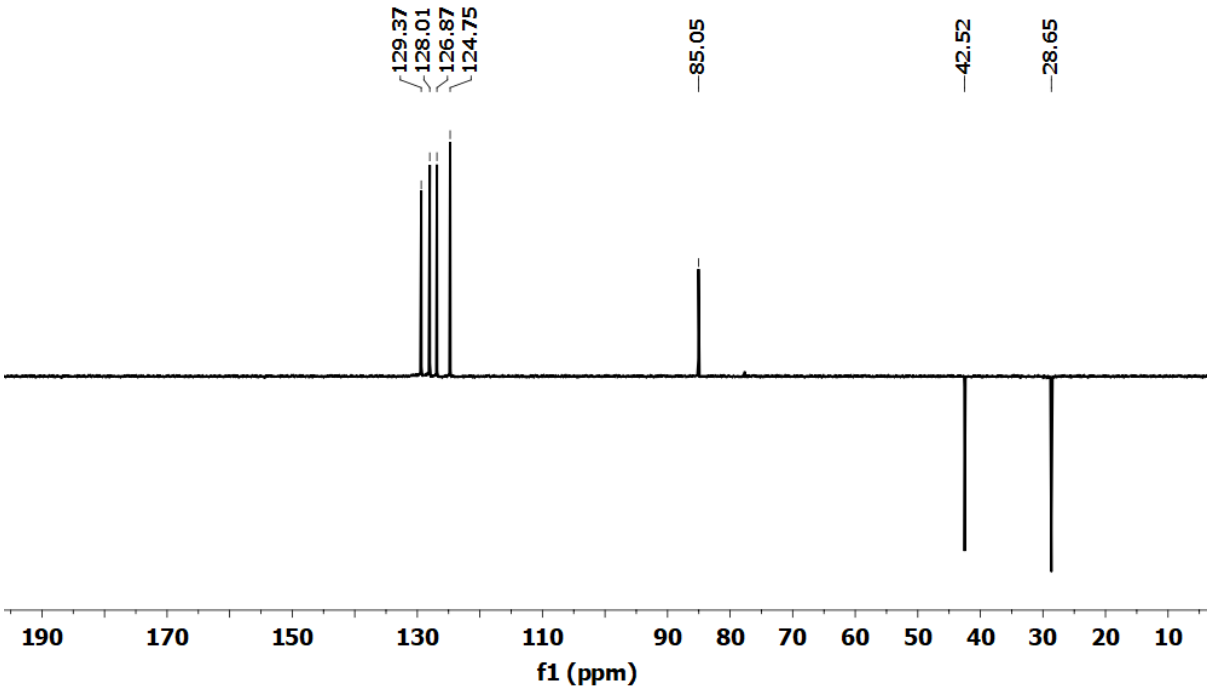


Fig. S2l DEPT-135 NMR of **HL4** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

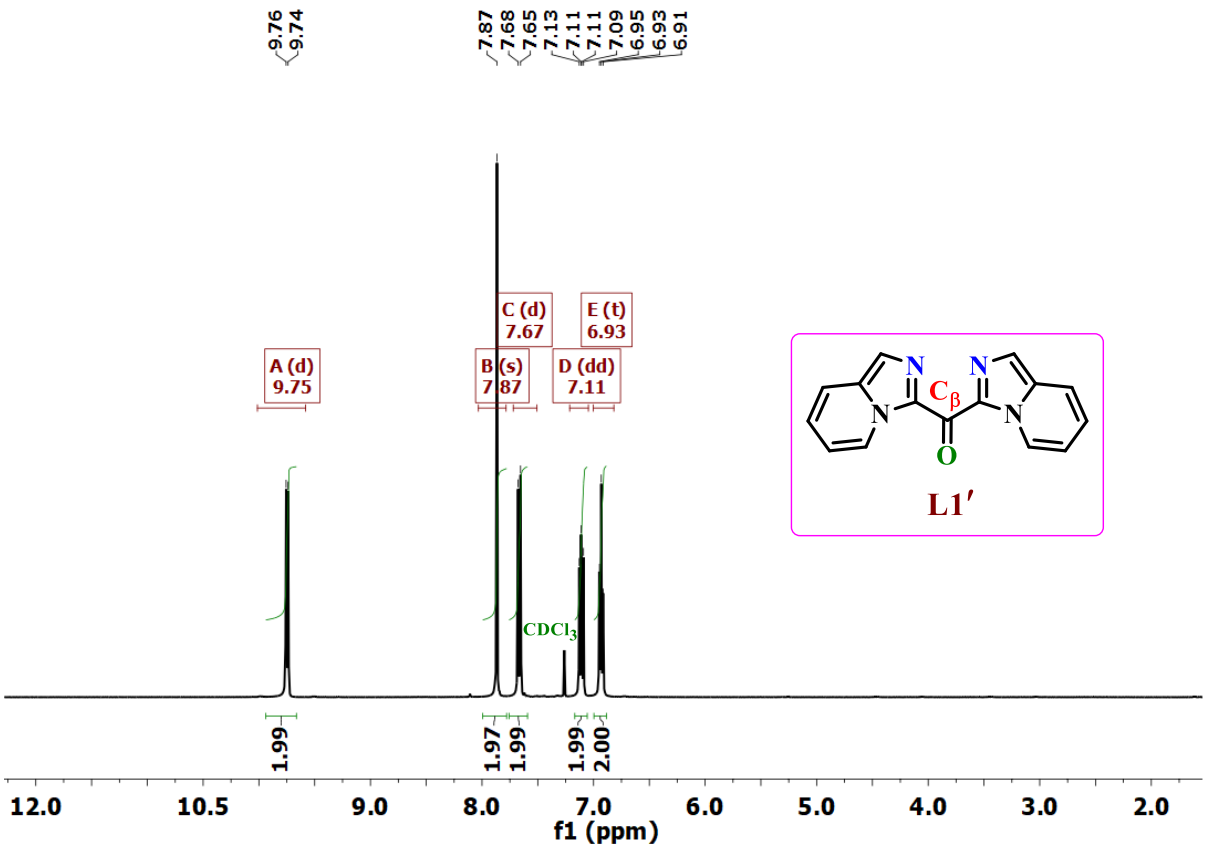


Fig. S2m ^{1}H NMR of **L1′** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

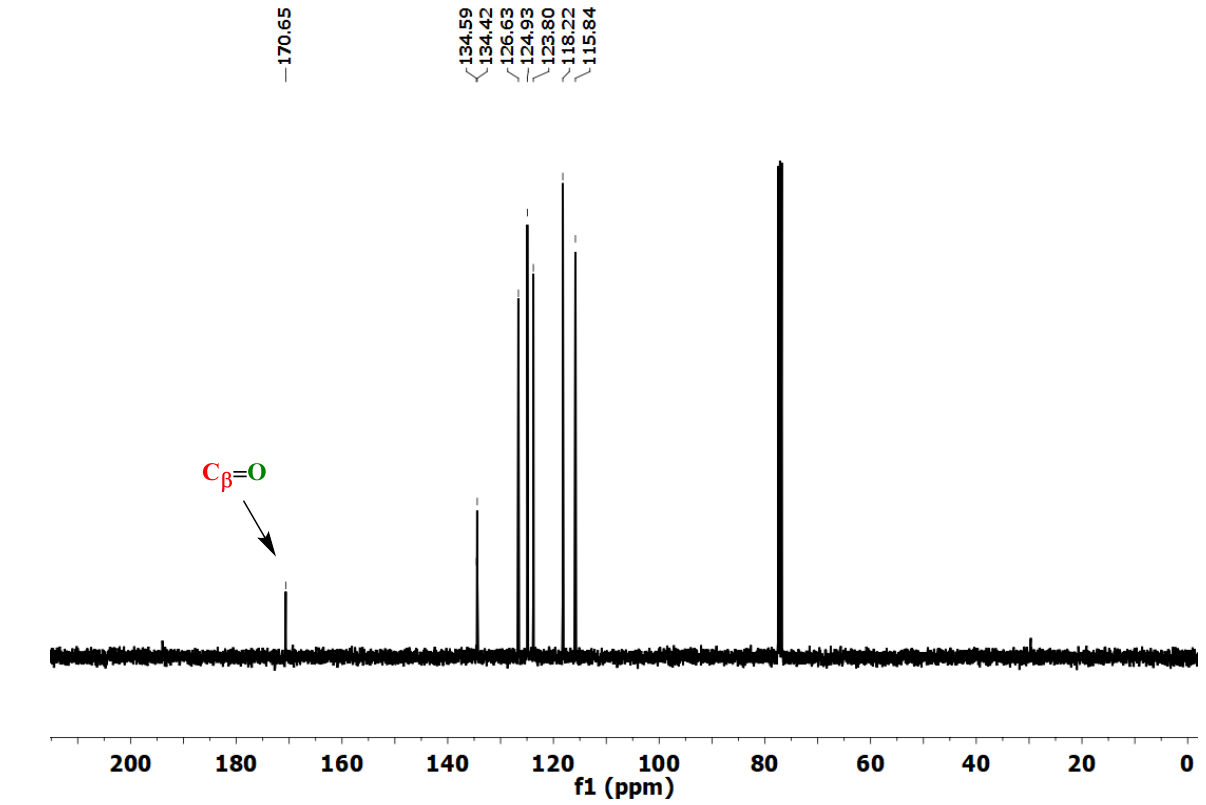


Fig. S2n ^{13}C NMR of **L1′** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

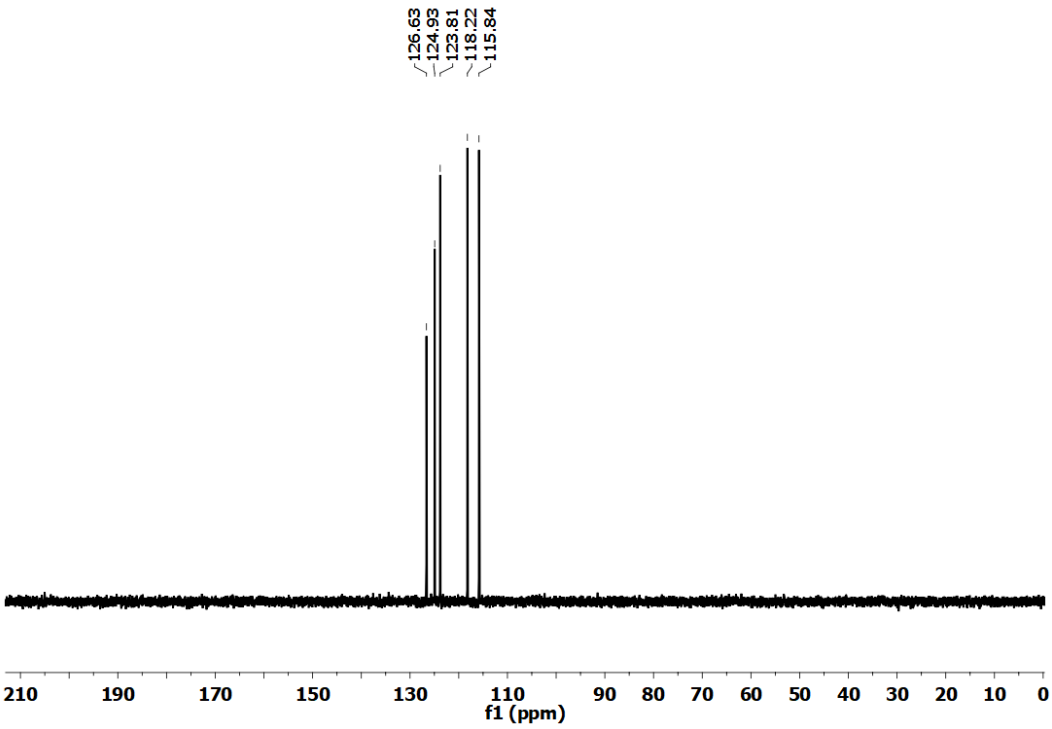


Fig. S2o DEPT-135 NMR of **L1′** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

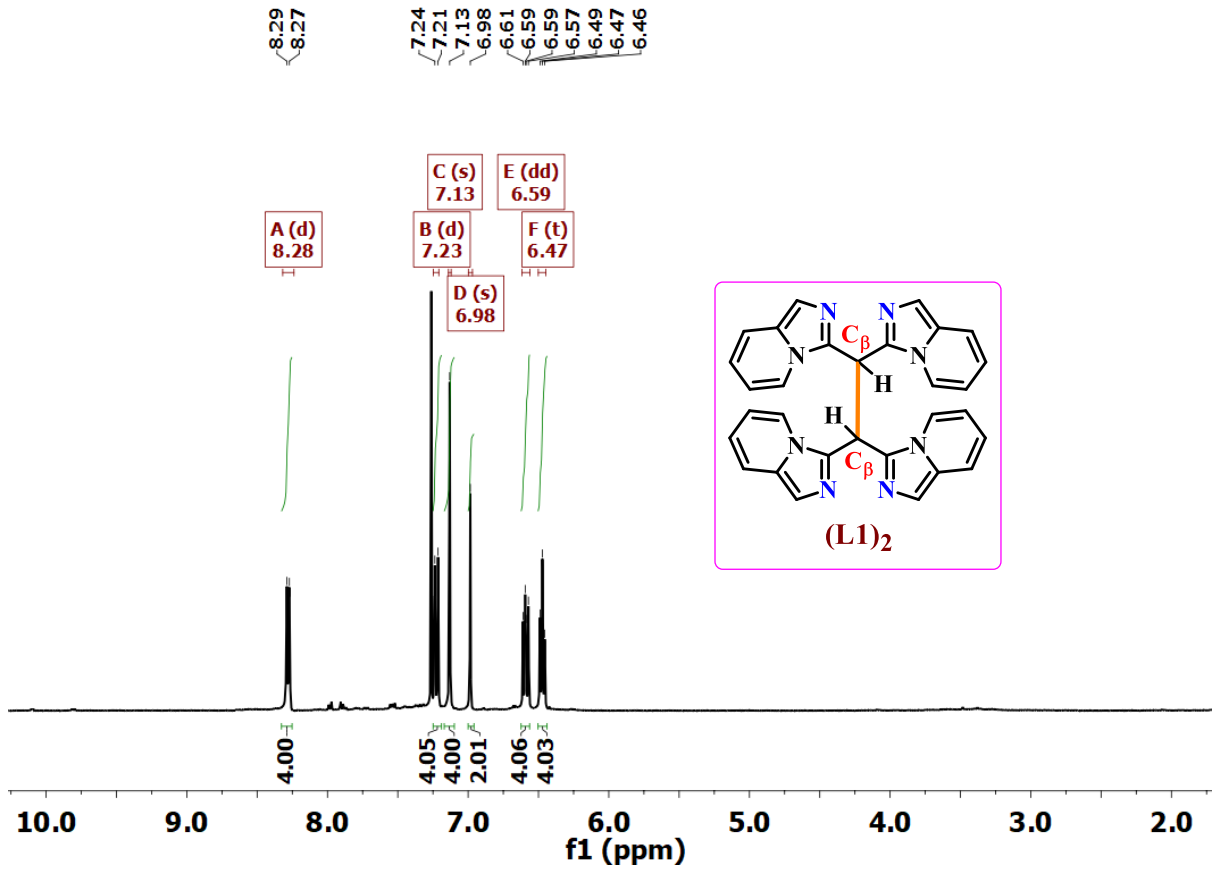


Fig. S2p ^{1}H NMR of **(L1)$_2$** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

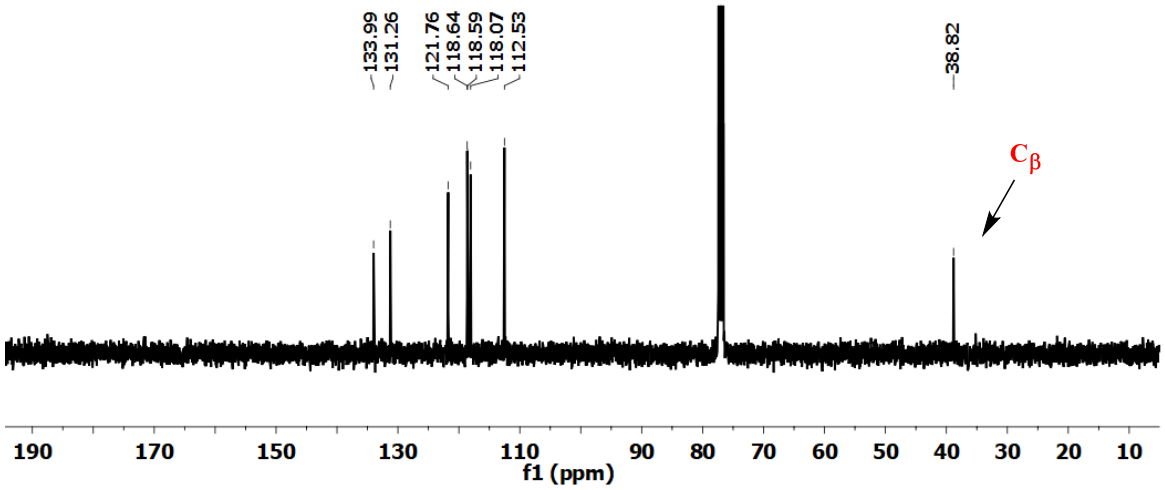


Fig. S2q ^{13}C NMR of **(L1)$_2$** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

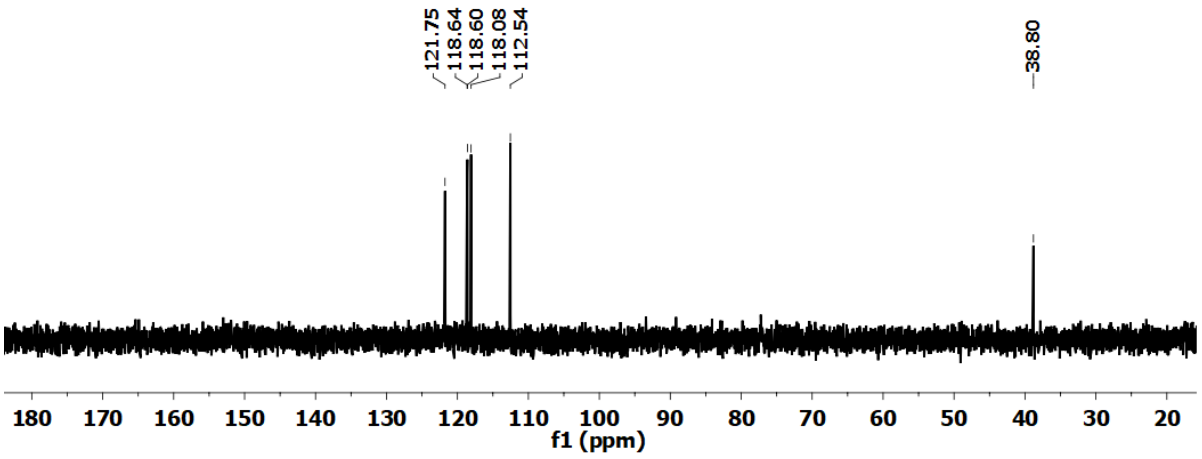


Fig. S2r DEPT-135 NMR of **(L1)$_2$** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

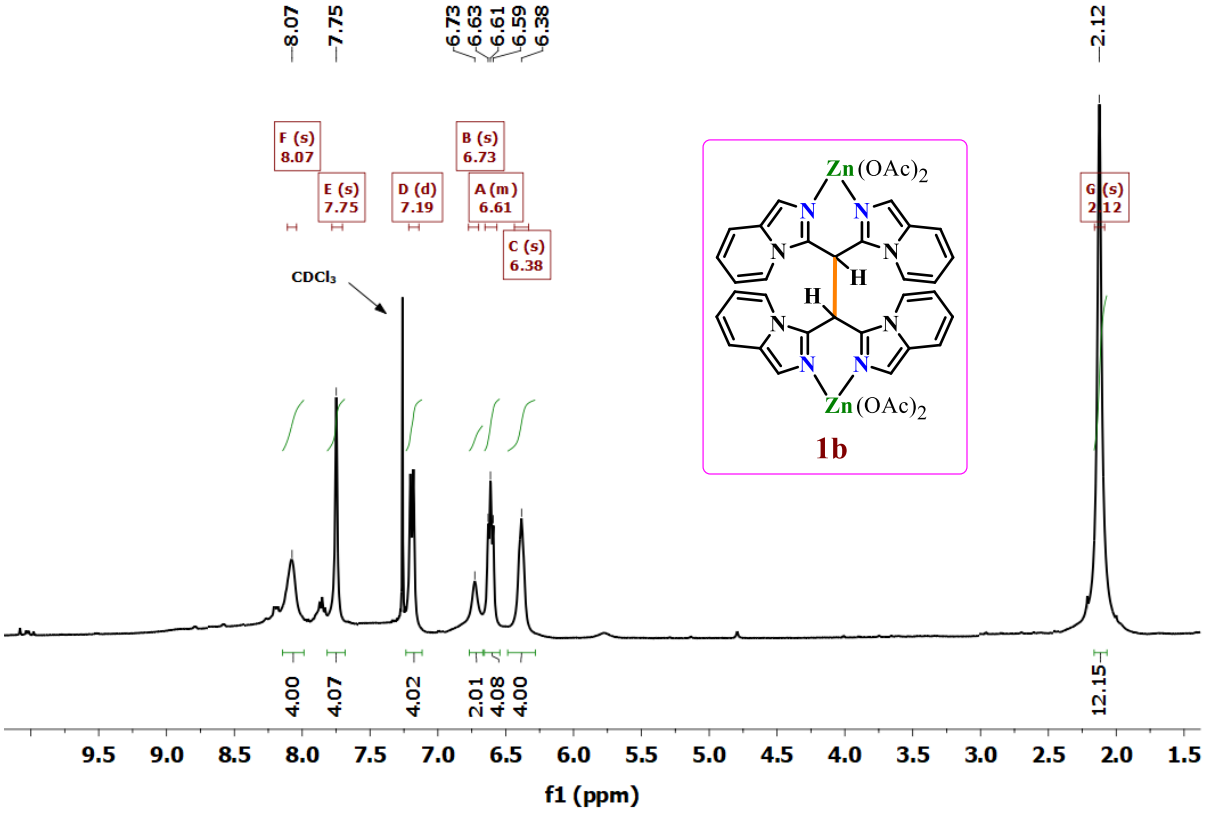


Fig. S2s ^{1}H NMR of **1b** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

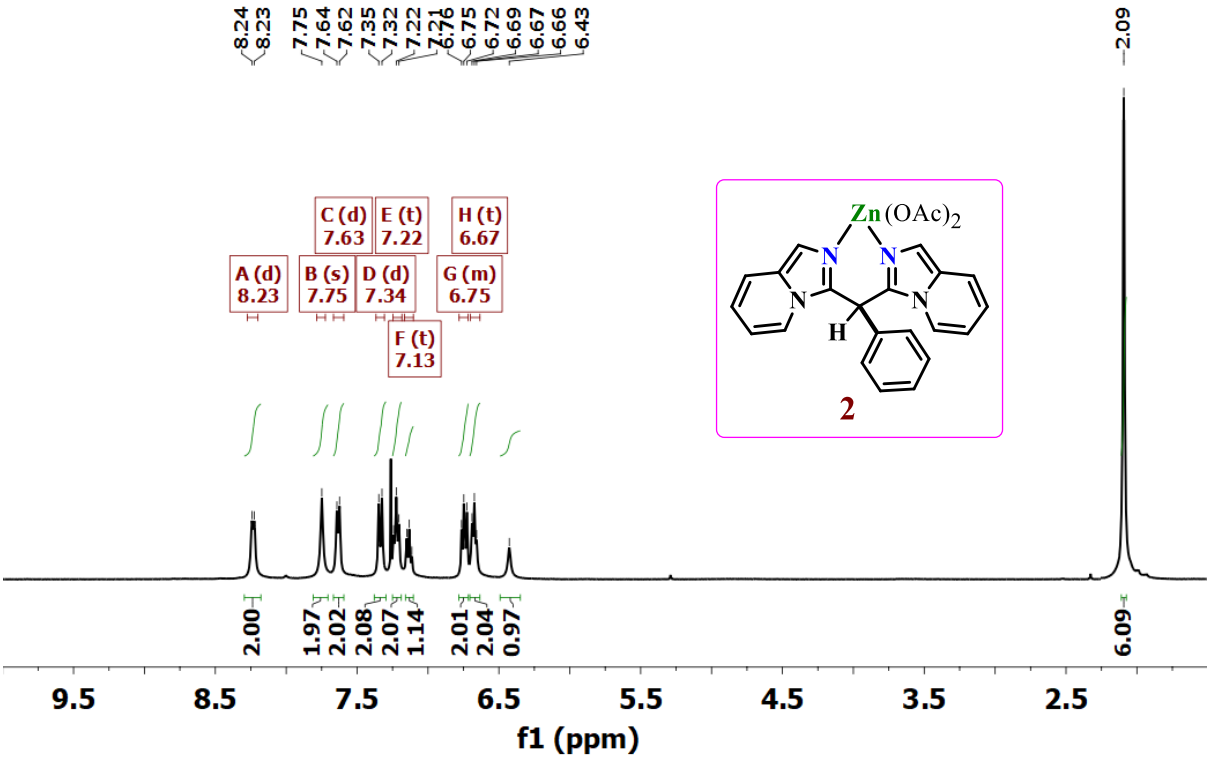


Fig. S2t ^{1}H NMR of **2** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

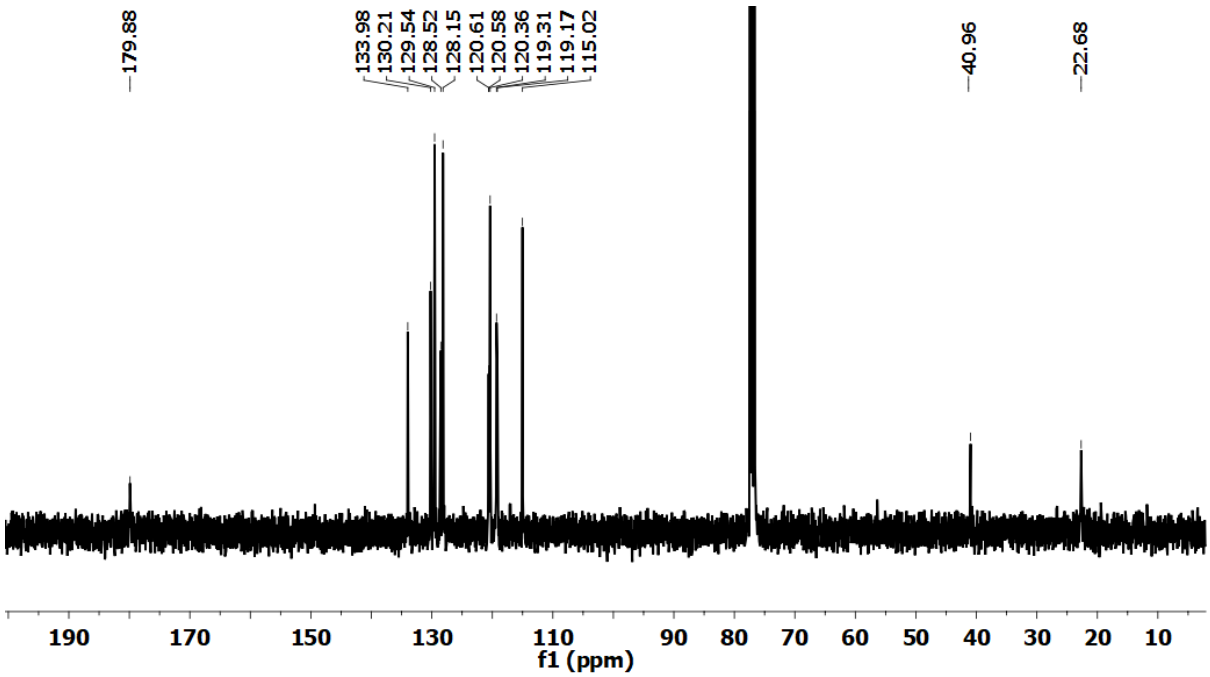


Fig. S2u ^{13}C NMR of **2** in $CDCl_3$ with TMS (δ = 0 ppm) as internal standard.

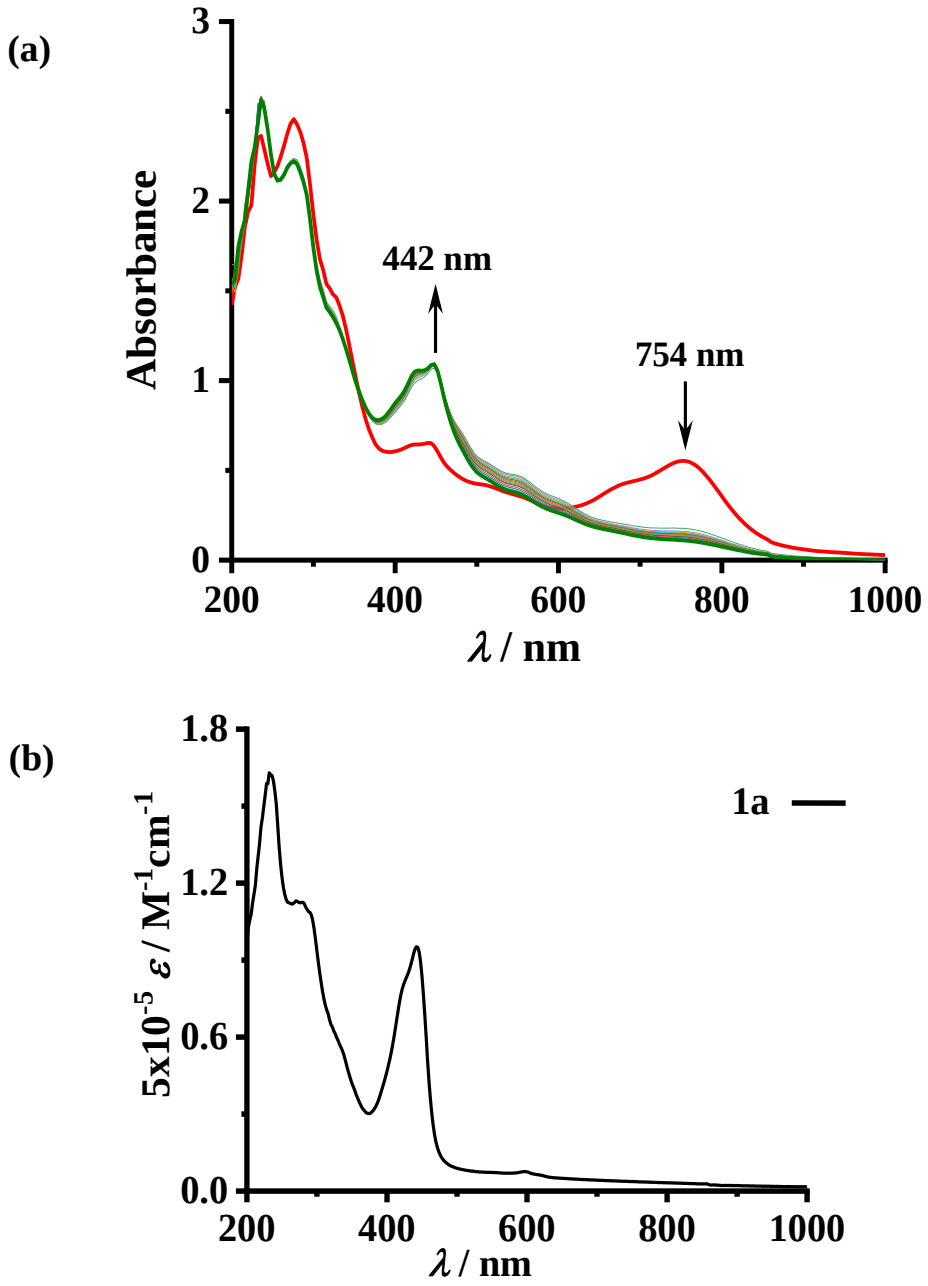


Fig. S3 (a) Immediate change in initial spectrum (red, under N_2) towards the formation of **1a** on exposure to air (green) at 298 K in CH_3OH. (b) UV-vis spectrum of pure **1a** in CH_3OH at 298 K.

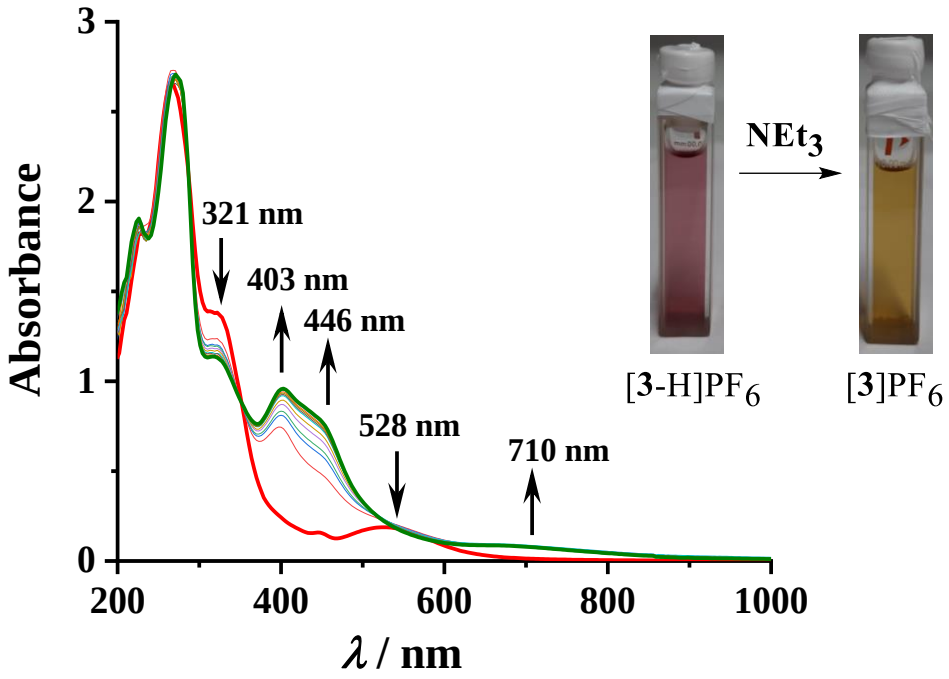


Fig. S4 Change in UV-vis. spectra for [**3**-H]PF_6→[**3**]PF_6 conversion (concentration ~6x10^{-5} M) in CH_3CN on addition of NEt_3 at 298 K. (Red line corresponds to [**3**-H]PF_6 and Green line corresponds to [**3**]PF_6). The change was followed over a period of 4 h.

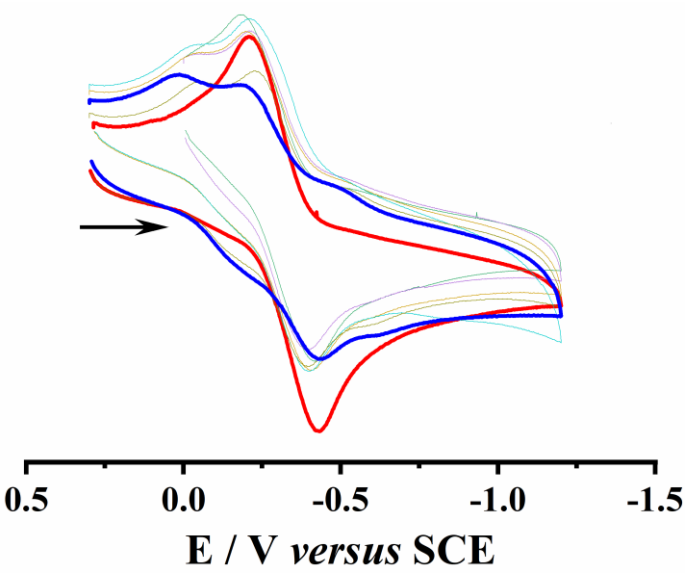


Fig. S5 Cyclic voltammograms of [**3**-H]PF_6 (Red) and after addition of NEt_3 (Blue) in CH_3CN/0.1 M $Et_4N^+ClO_4^-$/SCE, GC electrode, scan rate 100 mV s^{-1}. The change was followed over a period of 4 h.

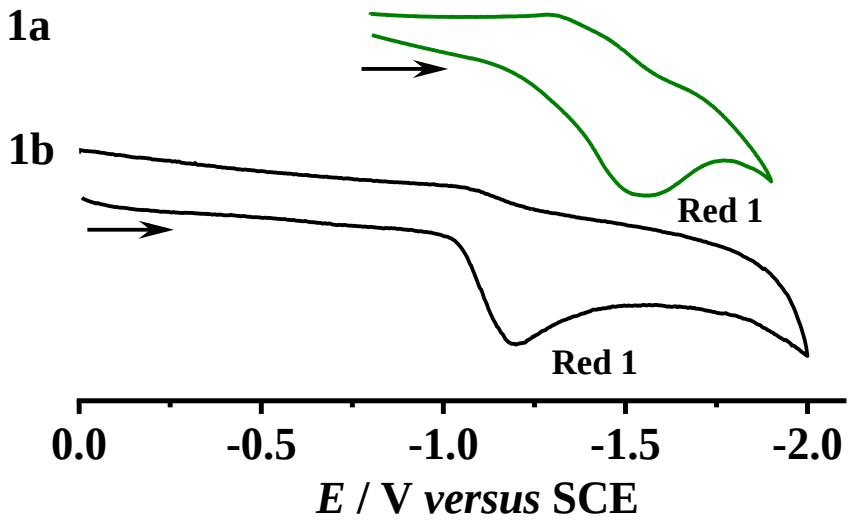
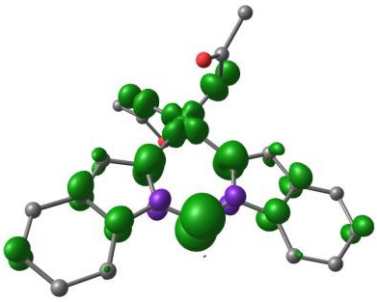
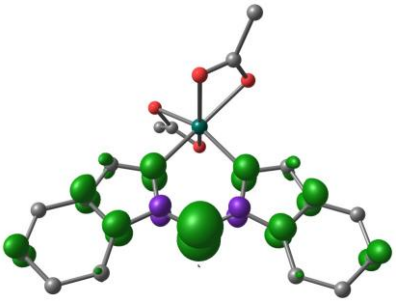


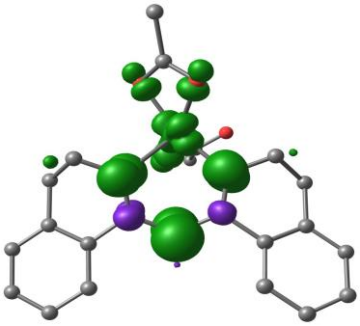
Fig. S6 Cyclic voltammograms in CH_3CN/0.1 M $Et_4N^+ClO_4^-$/SCE, GC electrode, scan rate 100 mV s^{-1}.



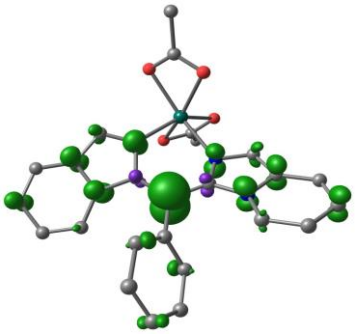
{Cu^{II}-L1$^{\bullet}$}
(*S* = 1)



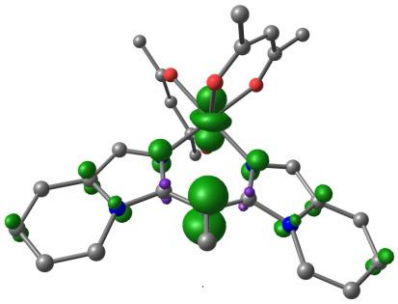
{Zn^{II}-L1$^{\bullet}$}
(*S* = 1/2)



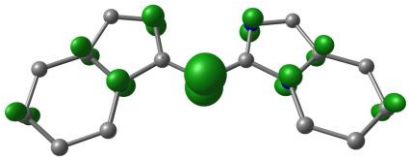
{Cu^{II}-L4$^{\bullet}$}
(*S* = 1)



{Zn^{II}-L2$^{\bullet}$}
(*S* = 1/2)

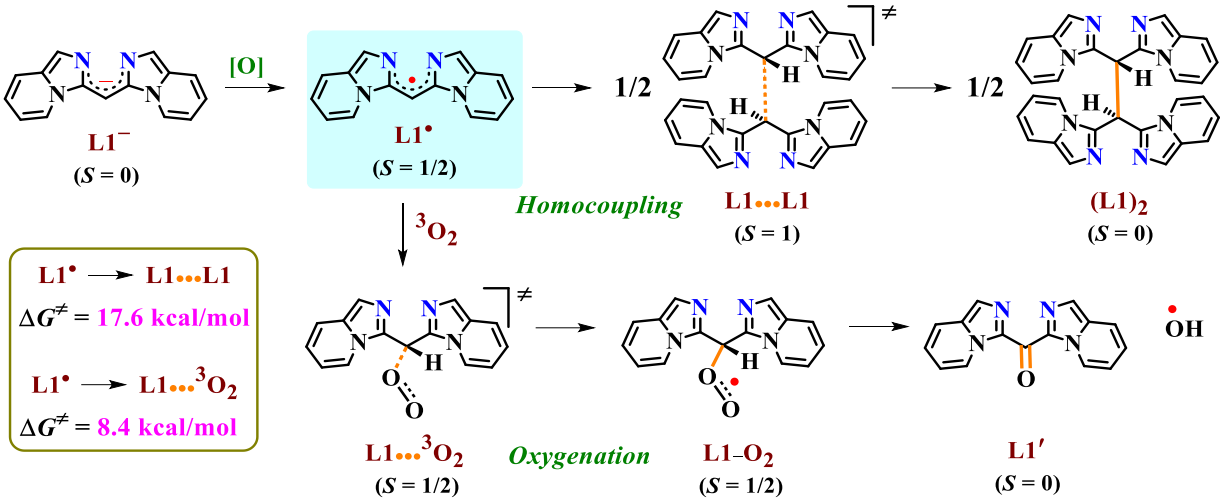


{Ru^{II}-L3$^{\bullet}$}
(*S* = 1/2)



{L1$^{\bullet}$}
(*S* = 1/2)

Fig. S7 Mulliken spin density plots of in-situ generated {M^{II}-L$^{\bullet}$} (Isosurface value 0.006).



Scheme S2 Mechanistic outline for homocoupling versus oxygenation of L1•.

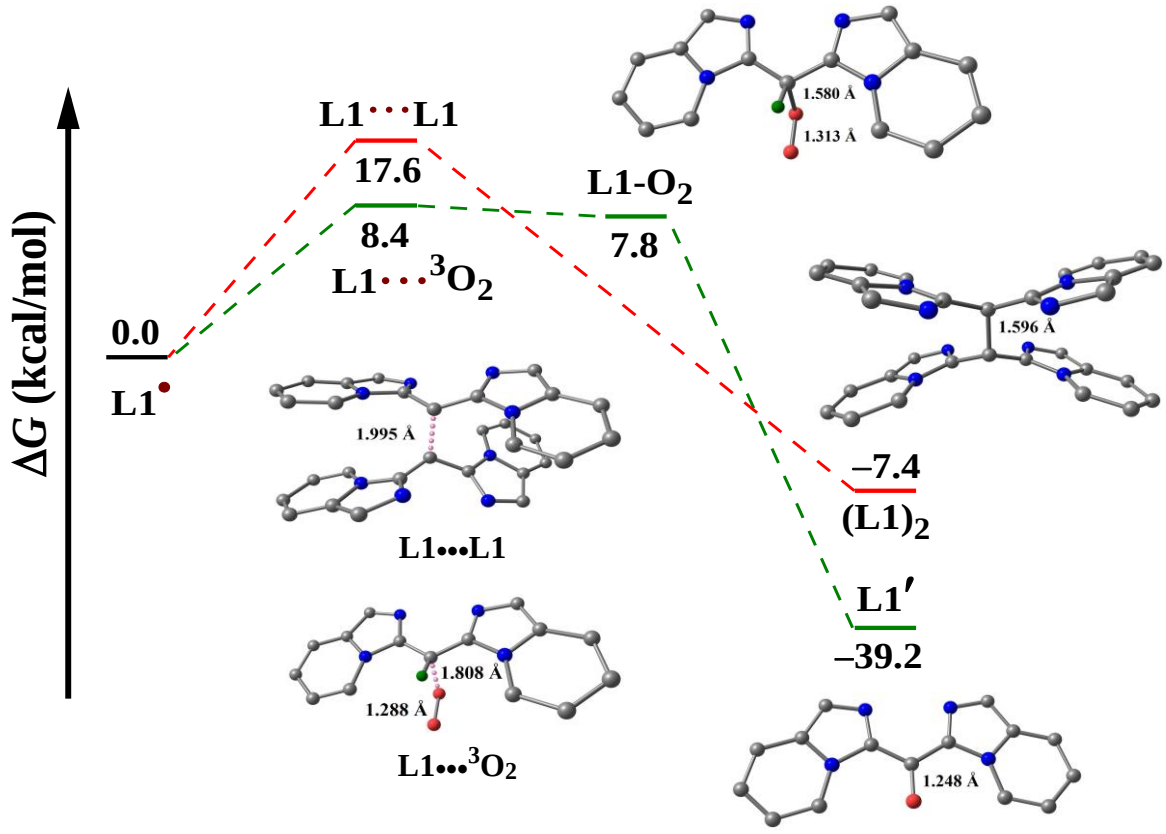


Fig. S8 Gibbs free energy (Δ*G*) profile (not to the scale) for oxygenation versus homocoupling of L1• at the M06-L level.

Imaginary Frequencies (ν_i) for the Transition State (TS)

TS	$[L1•••L1]^{\neq}$	$[L1•••{}^3O_2]^{\neq}$
ν_i, cm^{-1}	1179	223

Table S1 Selected crystallographic parameters

complex	**1a**	**1b.**$2H_2O$	**1c**	$(L1)_2.H_2O$
empirical formula	$C_{38}H_{36}N_8O_9Cu_2$	$C_{38}H_{38}N_8O_{10}Zn_2$	$C_{46}H_{44}N_4O_8Cu_2$	$C_{30}H_{24}N_8O$
formula weight	875.83	897.50	907.93	512.57
crystal system	Orthorhombic	Triclinic	Monoclinic	Monoclinic
space group	$P2_12_12_1$	P-1	I2/a	I 1 2/a 1
a (Å)	16.2048(5)	8.9786(4)	22.943(4)	25.4894(9)
b (Å)	22.1257(6)	10.6986(4)	8.4666(11)	7.8244(3)
c (Å)	22.3600(6)	11.1021(6)	23.193(4)	25.5780(14)
α (deg)	90	63.830(5)	90	90
β(deg)	90	87.600(4)	112.08(2)	92.559(4)
γ (deg)	90	75.968(4)	90	90
V ($Å^3$)	8017.0(4)	925.98(8)	4174.7(13)	5096.2(4)
Z	8	1	4	8
μ (mm^{-1})	1.124	1.360	1.078	0.086
ρ_{calcd} (g cm^{-3})	1.451	1.545	1.445	1.336
T (K)	150(2)	150(2)	150(2)	150(2)
F (000)	3600	442	1880	2144
θ range (deg)	1.886 to 29.229	2.197 to 31.050	1.944 to 26.442	2.199 to 24.110
data/restraints /parameters	14111/0/1037	3217/12/267	3648/30/273	4484/0/355
R_1,$wR_2[I> 2\sigma(I)]$	0.0675, 0.1450	0.0401, 0.0961	0.0996, 0.1849	0.0698, 0.1638
R_1, wR_2 (all data)	0.0921, 0.1653	0.0474, 0.1017	0.2161, 0.2541	0.1097, 0.1975
GOF on F^2	1.030	1.052	1.025	1.021
largest difference in peak and hole (e $Å^{-3}$)	0.668, -0.522	0.519, -0.411	0.591, -0.667	0.260, -0.293

Table S2 Selected crystallographic parameters

complex	**2**	[**3**-H]PF_6
empirical formula	$C_{25}H_{22}N_4O_4Zn$	$C_{26}H_{28}N_4O_4PF_6Ru$
formula weight	507.83	706.56
crystal system	Triclinic	Triclinic
space group	P-1	P-1
a (Å)	10.2232(4)	7.8784(3)
b (Å)	15.4947(8)	12.9044(5)
c (Å)	17.3250(9)	14.3059(6)
α (deg)	107.498(5)	72.540(4)
β(deg)	91.042(4)	85.511(3)
γ (deg)	102.343(4)	86.024(3)
V (Å^3)	2546.8(2)	1381.55(10)
Z	4	2
μ (mm^{-1})	1.000	0.707
ρ_{calcd} (g cm^{-3})	1.324	1.698
T (K)	150(2)	150(2)
F (000)	1048	714
θ range (deg)	2.400 to 30.599	2.539 to 24.999
data/restraints /parameters	8902/0/617	4827/153/448
R_1,wR_2[$I > 2\sigma(I)$]	0.1004, 0.2536	0.0540, 0.1003
R_1, wR_2 (all data)	0.1468, 0.3025	0.0782, 0.1141
GOF on F^2	1.029	1.049
largest difference in peak and hole (e Å^{-3})	2.641, -1.981	0.692, -0.709

Table S3 Selected experimental bond lengths (Å)[a]

bond lengths	**1a**	bond lengths	**1c**	bond lengths	**1b**.2H_2O	**2**	bond lengths	$(L1)_2.H_2O$	bond lengths	[**3**-H] PF_6
Cu1-N1	2.007(8)	Cu1-N1	1.999(8)	Zn1-N1	2.075(2)	2.042(6)	N1-C1	1.314(4)	Ru1-N1	2.062(4)
Cu1-N2	1.986(8)	Cu1-N2	2.006(8)	Zn1-N2	2.079(2)	2.021(6)	N2-C3	1.324(4)	Ru1-N2	2.045(4)
Cu1-O1	1.982(7)	Cu1-O1	1.930(7)	Zn1-O1	2.338(2)	1.972(5)	C2-C1	1.510(4)	Ru1-O1	1.999(3)
Cu1-O3	1.945(7)	Cu1-O3	2.015(7)	Zn1-O2	2.077(2)	–	C2-C3	1.509(4)	Ru1-O2	1.992(3)
Cu1-O5	2.304(8)	Cu1-O4	2.376(8)	Zn1-O3	2.293(2)	1.967(5)	C2-C16	1.550(4)	Ru1-O3	2.018(3)
Cu2-N5	1.979(8)	C2-C2′	1.313(18)	Zn1-O4	2.053(2)	–	C17-N5	1.319(4)	Ru1-O4	2.006(3)
Cu2-N6	1.993(8)	C4-C5	1.383(15)	N1-C1	1.330(3)	1.344(9)	C24-N6	1.321(4)	N1-C1	1.322(6)
Cu2-O5	1.968(7)	N1-C1	1.318(11)	N2-C3	1.331(3)	1.344(9)	C16-C17	1.509(4)	N2-C3	1.335(6)
Cu2-O7	1.971(7)	N2-C3	1.317(11)	C2-C1	1.502(4)	1.478(10)	C16-C24	1.505(4)	C2-C1	1.491(6)
Cu2-O8	1.998(9)	C1-C2	1.513(12)	C2-C3	1.494(3)	1.472(10)			C2-C3	1.502(6)
N1-C1	1.348(12)	C3-C2	1.496(14)	C2-C2′	1.585(6)	–			C2-C16	1.527(6)
N2-C3	1.327(12)	C12-C13	1.433(14)	C2-C16	–	1.551(10)				
C1-C2	1.486(14)	C21-O1	1.265(15)	C16-O1	1.247(4)	–				
C3-C2	1.491(13)	C23-O3	1.298(14)	C16-O2	1.262(4)	–				
C2-C16	1.606(15)	C23-O4	1.244(12)	C22-O1	–	1.280(11)				
C31-O1	1.259(13)			C22-O2	–	1.214(10)				
C31-O2	1.281(13)									

[a]Asymmetric units of **1a** and **2** are composed of two independent molecules (molecule A and molecule B). Bond lengths of molecule A are listed here.

Table S4 Selected experimental bond angles (deg)

bond angle	**1a** (Molecule A)	bond angle	**1b.**$2H_2O$	bond angle	$(L1)_2.H_2O$
N1-Cu1-N2	89.6(3)	N1-Zn1-N2	90.28(9)	C1-C2-C3	111.5(2)
N1-Cu1-O1	154.8(3)	N1-Zn1-O1	154.27(9)	C1-C2-C16	111.1(2)
N1-Cu1-O3	89.3(3)	N1-Zn1-O2	95.57(9)	C3-C2-C16	113.5(2)
N2-Cu1-O1	90.9(3)	N1-Zn1-O3	93.59(8)	C2-C1-N1	126.2(3)
N2-Cu1-O3	178.7(3)	N1-Zn1-O4	107.44(9)	C2-C3-N2	123.2(3)
O1-Cu1-O3	89.8(3)	N2-Zn1-O1	94.40(9)	C2-C1-N3	122.3(3)
N5-Cu2-N6	89.4(3)	N2-Zn1-O2	100.10(9)	N1-C1-N3	111.4(3)
N5-Cu2-O7	91.3(3)	N2-Zn1-O3	153.71(9)	C2-C3-N4	125.8(3)
N6-Cu2-O7	164.3(3)	N2-Zn1-O4	94.75(9)	N2-C3-N4	111.0(3)
N6-Cu2-O5	93.0(3)	O1-Zn1-O2	58.70(8)		
N5-Cu2-O5	167.8(3)	O1-Zn1-O3	93.30(8)		
O6-Cu2-O8	88.3(4)	O1-Zn1-O4	97.38(9)		
C1-C2-C3	112.1(8)	O2-Zn1-O3	105.37(8)		
C1-C2-C16	110.5(7)	O2-Zn1-O4	152.51(9)		
C3-C2-C16	108.6(8)	O3-Zn1-O4	59.32(8)		
		C1-C2-C3	112.2(2)		
		C1-C2-C2′	110.9(3)		
		C3-C2-C2′	109.5(3)		

Table S5 Selected experimental bond angles (deg)

bond angle	**1c**	bond angle	**2** (Molecule A)	bond angle	[**3**-H]PF_6
N1-Cu1-N2	90.1(3)	N1-Zn1-N2	90.9(2)	N1-Ru1-N2	86.85(15)
N1-Cu1-O1	168.3(3)	N1-Zn1-O1	118.3(2)	N1-Ru1-O1	178.59(15)
N1-Cu1-O3	94.7(3)	N1-Zn1-O3	104.2(2)	N1-Ru1-O2	87.73(13)
N1-Cu1-O4	98.5(3)	N2-Zn1-O1	107.4(3)	N1-Ru1-O3	93.11(14)
N2-Cu1-O1	91.4(3)	N2-Zn1-O3	112.2(2)	N1-Ru1-O4	94.24(14)
N2-Cu1-O3	163.2(4)	O1-Zn1-O3	120.2(2)	N2-Ru1-O1	91.75(14)
N2-Cu1-O4	103.7(3)	C1-C2-C3	114.8(6)	N2-Ru1-O2	91.54(14)
O1-Cu1-O3	87.2(3)	C1-C2-C16	110.4(6)	N2-Ru1-O3	179.69(14)
O1-Cu1-O4	92.4(3)	C3-C2-C16	110.2(6)	N2-Ru1-O4	88.96(14)
O3-Cu1-O4	59.7(3)			O1-Ru1-O2	92.12(12)
C1-C2-C3	115.0(8)			O1-Ru1-O3	88.29(13)
C1-C2-C2′	123.2(12)			O1-Ru1-O4	85.92(12)
C3-C2-C2′	121.8(11)			O2-Ru1-O3	88.15(13)
				O2-Ru1-O4	177.99(13)
				O3-Ru1-O4	91.35(13)
				C1-C2-C3	111.2(4)
				C1-C2-C16	113.3(4)
				C3-C2-C16	111.9(4)

Table S6 EPR data in CH_3CN-toluene (1:1) at 100 K[a]

Complex	$g_{1/2}$	g_1	g_2	g_3	$g_{\|\|}$	$A_{\|\|}$ (mT)	$g_\perp$	$\langle g \rangle$[b]	Δg[c]
1a (two S=1/2)	-	-	-	-	2.199	17.6	1.997	-	-
1c (S=1)	5.168	-	-	-	2.381	16.2	2.074	-	-
[**3**]PF_6 (S=1)	4.690	2.415	2.188	1.823				2.156	0.592
[**3**-H]PF_6 (S=1/2)	-	2.494	2.127	1.703				2.133	0.791

[a]EPR spectra in CH_3CN-toluene/ 0.1 M $Et_4N^+ClO_4^-$ at 100 K. [b]$\langle g \rangle = \{(1/3)(g_1^2 + g_2^2 + g_3^2)\}^{1/2}$, [c]$\Delta g = g_1 - g_3$.

Table S7 Electrochemical data[a]

complex	$E°$[V] (ΔEp[mV])[b]	
	Red1	Red2
[**3**]PF_6	−0.07(60)	−0.29(90)
[**3**-H]PF_6	−0.33(270)	-

[a]From cyclic voltammetry in CH_3CN/0.1 M Et_4NClO_4 at 100 mVs^{-1}. [b]Potentials in V versus SCE; peak potential differences ΔE/mV (in parentheses).

Table S8 DFT calculated (M06L/LanL2DZ/6-31G**) Mulliken spin densities

complex	Cu/Zn	Ru	L(C_β)	OAc	acac
{Cu^{II}-L1$^-$} for **1a** (*S*=1/2)	0.603	-	0.165(0.004)	0.232	-
{Cu^{II}-L1$^\bullet$} for **1a** (*S*=1)	0.603	-	1.109(0.459)	0.288	-
1a (*S*=1) **{Cu^{II}(μ-(L1)$_2$)Cu^{II}}**	1.211	-	0.190(0.001)	0.599	-
{Zn^{II}-L1$^\bullet$} for **1b** (*S*=1/2)	-0.003	-	1.001(0.466)	0.002	-
{Cu^{II}-L4$^-$} for **1c** (*S*=1/2)	0.552	-	0.229(0.011)	0.219	-
{Cu^{II}-L4$^\bullet$} for **1c** (*S*=1)	0.588	-	1.064(0.640)	0.348	-
1c (*S*=1) **{Cu^{II}(μ-(L4)$_2$)Cu^{II}}**	1.064	-	0.339(0.012)	0.597	-
3 (*S*=1/2) **{Ru^{II}-L3$^\bullet$}**	-	0.302	0.681(0.397)	-	0.017
3$^+$ (*S*=1) **{Ru^{III}-L3$^\bullet$}**	-	0.812	0.978(0.499)	-	0.210
[3-H]$^+$ (*S*=1/2) **{Ru^{III}-HL3$^-$}**	-	0.790	0.004(-0.001)	-	0.206

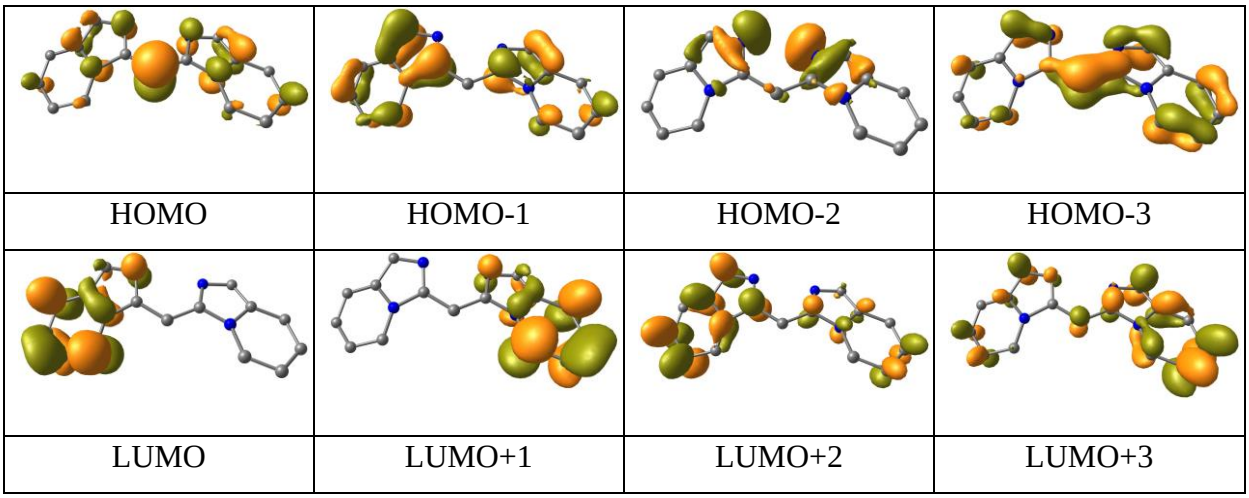
Table S9 DFT calculated selected MO compositions at (U)B3LYP level

complex[a]	MO	fragments	% contribution
{Cu^{II}-L1^{-}} for **1a**	SOMO	L1/Cu/ OAc	98/1/1
(*S*=1/2)	β-LUMO	L1/Cu/ OAc	23/57/21
{Cu^{II}-L1$^{\bullet}$} for **1a**	SOMO	L1/Cu/ OAc	98/1/1
(*S*=1)	β-LUMO	L1/Cu/ OAc	98/1/1
1a (*S*=1)	SOMO	L1/Cu/ OAc	100/0/0
{Cu^{II}(μ-(L1)$_2$)Cu^{II}}	β-LUMO	L1/Cu/ OAc	61/11/28
{Zn^{II}-L1^{-}} for **1b**	HOMO	L1/Zn/ OAc	99/0/0
(*S*=0)	LUMO	L1/Zn/ OAc	99/0/0
{Zn^{II}-L1$^{\bullet}$} for **1b**	SOMO	L1/Zn/ OAc	99/0/0
(*S*=1/2)	β-LUMO	L1/Zn/ OAc	99/0/0
1b (*S*=0)	SOMO	L1/Zn/ OAc	100/0/0
{Zn^{II}(μ-(L1)$_2$)Zn^{II}}	β-LUMO	L1/Zn/ OAc	98/1/2
{Cu^{II}-L4^{-}} for **1c**	HOMO	L4/Cu/ OAc	91/4/5
(*S*=1/2)	LUMO	L4/Cu/ OAc	36/48/16
{Cu^{II}-L4$^{\bullet}$} for **1c**	SOMO	L4/Cu/ OAc	9/14/76
(*S*=1)	β-LUMO	L4/Cu/ OAc	86/7/7
1c (*S*=1)	SOMO	L4/Cu/ OAc	7/13/80
{Cu^{II}(μ-(L4)$_2$)Cu^{II}}	β-LUMO	L4/Cu/ OAc	27/53/20
3^{-} (*S*=0)	HOMO	L3/Ru/ acac	80/16/3
{Ru^{II}-L3^{-}}	LUMO	L3/Ru/ acac	95/2/3
3 (*S*=1/2)	SOMO	L3/Ru/ acac	83/14/3
{Ru^{II}-L3$^{\bullet}$}	β-LUMO	L3/Ru/ acac	98/1/0
3^{+} (*S*=1)	SOMO	L3/Ru/ acac	94/5/1
{Ru^{III}-L3$^{\bullet}$}	β-LUMO	L3/Ru/ acac	98/1/1
[3-H]$^{+}$ (*S*=1/2)	SOMO	L3/Ru/ acac	12/48/41
{Ru^{III}-HL3^{-}}	β-LUMO	L3/Ru/ acac	9/70/21

[a]DFT optimized stable configuration are considered here.

Table S10 Composition and energies of selected molecular orbitals of $\mathbf{L}^{-}$ (*S*=0)

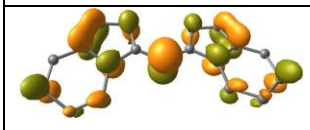
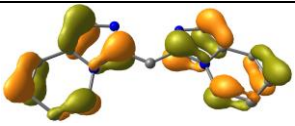
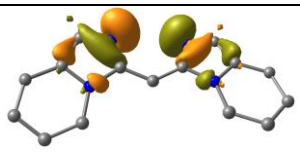
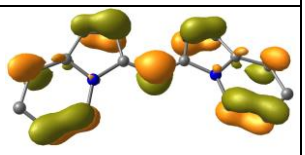
MO	energy (eV)	% composition	
		ring	C_β
HOMO-5	-2.354	0.98	0.02
HOMO-4	-2.185	0.99	0.01
HOMO-3	-1.606	0.85	0.15
HOMO-2	-1.481	0.99	0.01
HOMO-1	-0.614	1.00	0.00
HOMO	1.350	0.68	0.32
LUMO	2.015	1.00	0.00
LUMO+1	2.327	1.00	0.00
LUMO+2	3.725	1.00	0.00
LUMO+3	4.156	0.95	0.05
LUMO+4	5.560	0.98	0.02
LUMO+5	6.725	0.93	0.07



HOMO	HOMO-1	HOMO-2	HOMO-3
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S11 Composition and energies of selected molecular orbitals of **L1•** (*S*=1/2)

MO	energy (eV)	% composition	
		azo	ring
		α-spin	
HOMO-5	-6.572	1.00	0.00
HOMO-4	-6.417	0.98	0.02
HOMO-3	-6.167	0.86	0.14
HOMO-2	-6.003	0.99	0.01
HOMO-1	-4.893	1.00	0.00
SOMO	-3.499	0.77	0.23
LUMO	-1.663	1.00	0.00
LUMO+1	-1.654	1.00	0.00
LUMO+2	-0.632	1.00	0.00
LUMO+3	-0.051	0.95	0.05
LUMO+4	1.119	1.00	0.00
LUMO+5	1.564	0.86	0.14
		β-spin	
HOMO-5	-3.880	0.89	0.11
HOMO-4	-3.472	0.99	0.01
HOMO-3	-3.081	0.99	0.01
HOMO-2	-3.069	0.99	0.01
HOMO-1	-2.463	0.89	0.11
HOMO	-2.347	1.00	0.00
LUMO	1.223	0.74	0.26
LUMO+1	2.859	1.00	0.00
LUMO+2	2.959	1.00	0.00
LUMO+3	3.023	1.00	0.00
LUMO+4	3.760	0.94	0.06
LUMO+5	3.769	0.99	0.01

α-spin			
			
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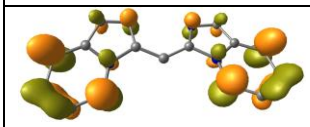
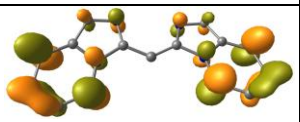
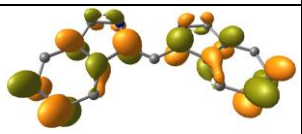
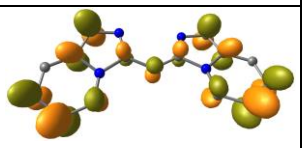
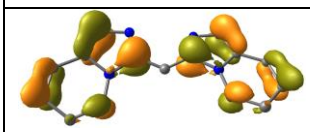
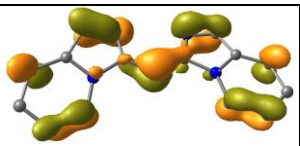
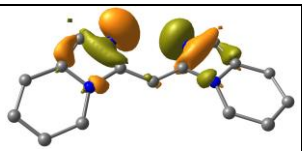
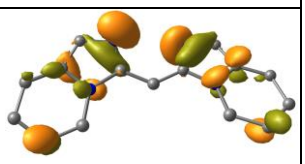
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
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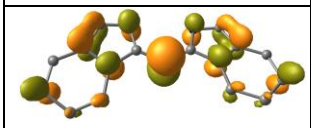
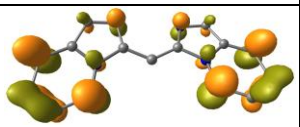
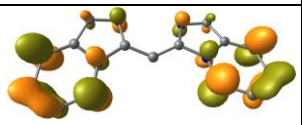
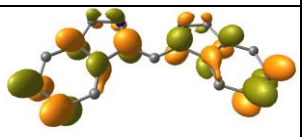
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S12 Composition and energies of selected molecular orbitals of **(L1)$_2$** (*S*=0)

MO	energy (eV)	% composition	
		azo	ring
HOMO-5	-5.635	1.00	0.00
HOMO-4	-5.603	0.99	0.01
HOMO-3	-4.822	0.99	0.01
HOMO-2	-4.753	0.92	0.08
HOMO-1	-4.600	0.90	0.10
HOMO	-4.424	1.00	0.00
LUMO	-1.528	0.96	0.04
LUMO+1	-1.463	1.00	0.00
LUMO+2	-1.372	1.00	0.00
LUMO+3	-1.340	1.00	0.00
LUMO+4	-0.829	0.85	0.15
LUMO+5	-0.338	0.99	0.01

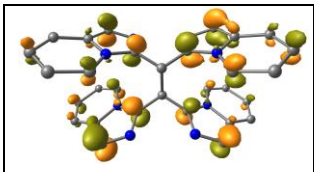
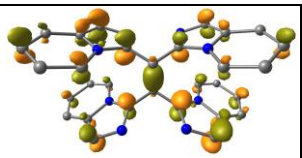
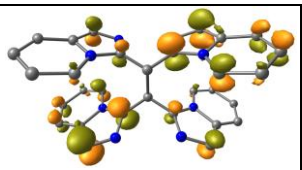
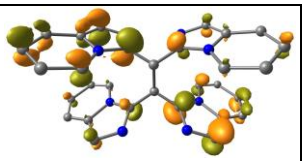
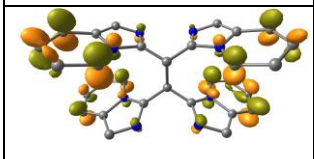
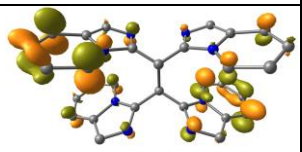
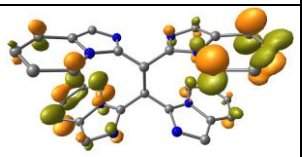
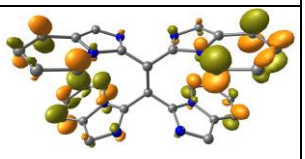
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S13 Composition and energies of selected molecular orbitals of {Cu^{II}-L1^{-}} (*S*=1/2)

MO	energy (eV)	% composition		
		Cu	L1	OAc
		α-spin		
HOMO-5	-3.328	0.01	0.07	0.92
HOMO-4	-2.903	0.04	0.03	0.92
HOMO-3	-2.728	0.10	0.01	0.89
HOMO-2	-2.711	0.22	0.22	0.56
HOMO-1	-2.425	0.00	1.00	0.00
SOMO	-0.662	0.01	0.98	0.01
LUMO	1.806	0.01	0.99	0.00
LUMO+1	1.870	0.00	1.00	0.00
LUMO+2	2.971	0.01	0.99	0.01
LUMO+3	3.587	0.07	0.91	0.02
LUMO+4	3.942	0.70	0.18	0.13
LUMO+5	3.964	0.62	0.23	0.15
		β-spin		
HOMO-5	-3.335	0.05	0.03	0.91
HOMO-4	-3.250	0.01	0.07	0.92
HOMO-3	-2.881	0.03	0.02	0.95
HOMO-2	-2.583	0.15	0.01	0.84
HOMO-1	-2.426	0.00	0.99	0.00
HOMO	-0.648	0.02	0.97	0.01
LUMO	1.143	0.57	0.23	0.21
LUMO+1	1.832	0.02	0.96	0.01
LUMO+2	1.881	0.00	1.00	0.00
LUMO+3	2.977	0.00	0.99	0.01
LUMO+4	3.590	0.07	0.91	0.02
LUMO+5	3.946	0.70	0.18	0.13

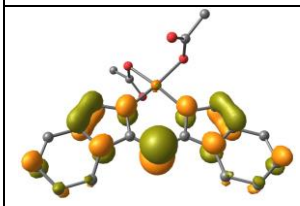
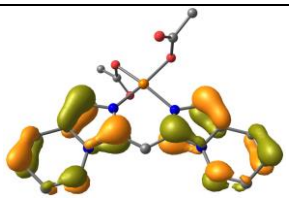
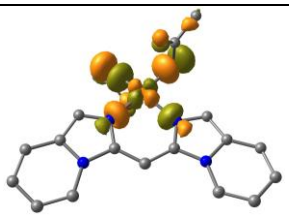
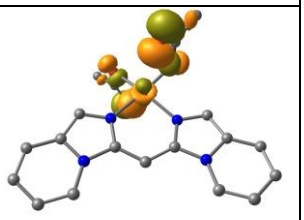
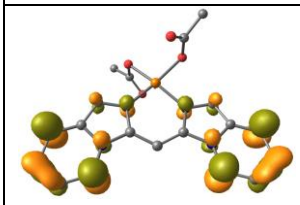
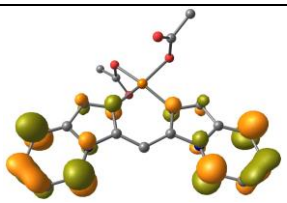
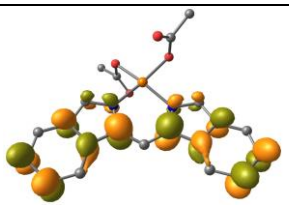
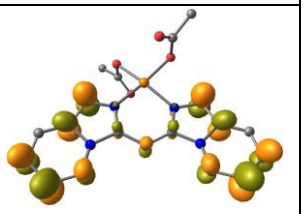
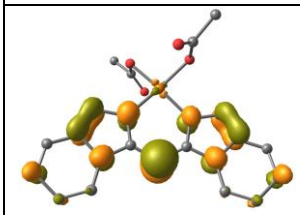
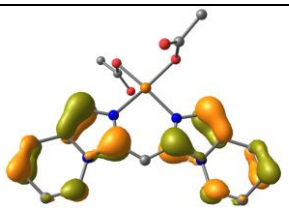
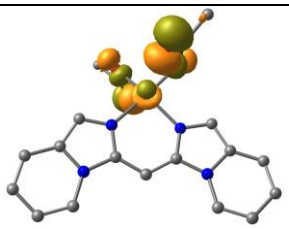
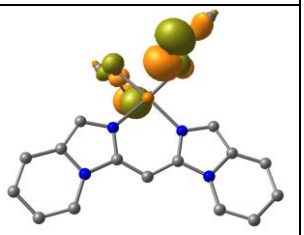
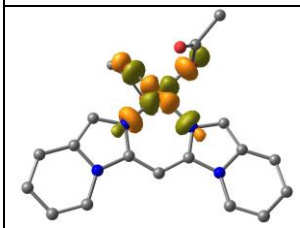
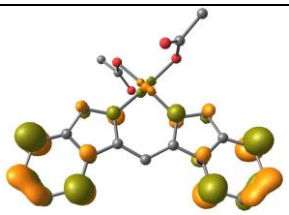
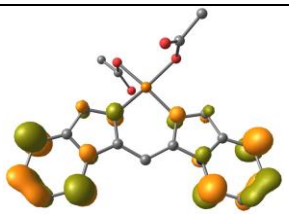
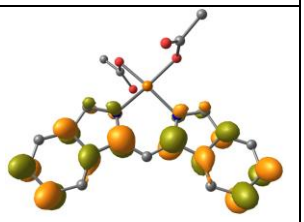
α-spin			
			
SOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S14 Composition and energies of selected molecular orbitals of {Cu^{II}-L1$^{\bullet}$} (*S*=1)

MO	energy (eV)	% composition		
		Cu	L1	OAc
		α-spin		
HOMO-5	-6.231	0.02	0.06	0.92
HOMO-4	-6.066	0.00	0.99	0.01
HOMO-3	-5.881	0.14	0.10	0.77
HOMO-2	-5.729	0.14	0.11	0.75
SOMO 2	-5.493	0.13	0.02	0.85
SOMO 1	-4.665	0.01	0.98	0.01
LUMO	-1.727	0.01	0.99	0.00
LUMO+1	-1.672	0.00	1.00	0.00
LUMO+2	-0.726	0.00	0.99	0.01
LUMO+3	-0.049	0.01	0.98	0.01
LUMO+4	0.912	0.00	0.99	0.01
LUMO+5	1.062	0.14	0.84	0.01
		β-spin		
HOMO-5	-6.782	0.13	0.10	0.77
HOMO-4	-6.203	0.05	0.04	0.91
HOMO-3	-6.142	0.01	0.06	0.93
HOMO-2	-5.837	0.00	1.00	0.00
HOMO-1	-5.783	0.05	0.02	0.93
HOMO	-5.281	0.17	0.02	0.81
LUMO	-3.141	0.01	0.98	0.01
LUMO+1	-1.991	0.57	0.19	0.23
LUMO+2	-1.589	0.02	0.98	0.01
LUMO+3	-1.544	0.00	1.00	0.00
LUMO+4	-0.547	0.00	0.99	0.01
LUMO+5	0.211	0.02	0.97	0.01

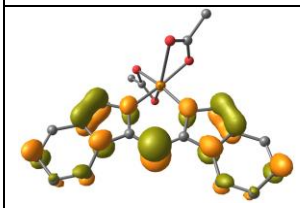
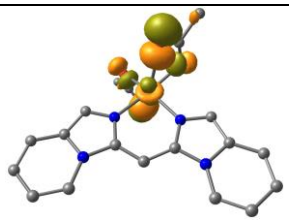
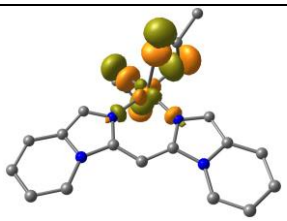
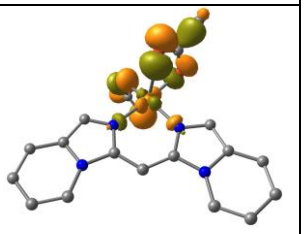
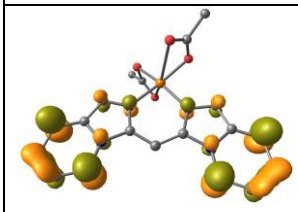
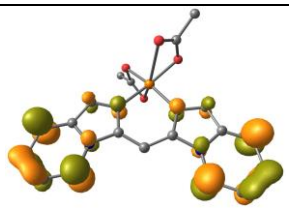
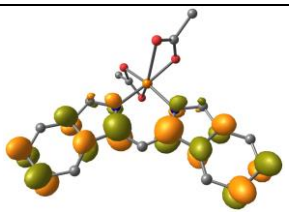
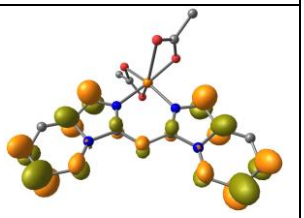
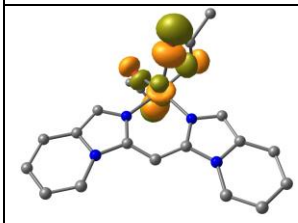
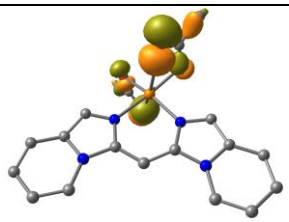
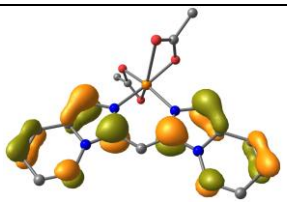
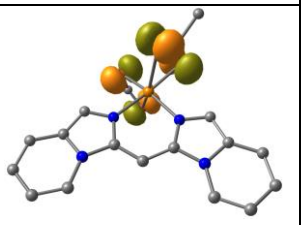
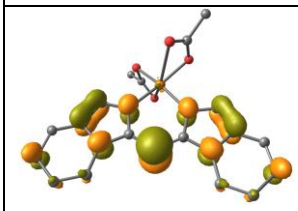
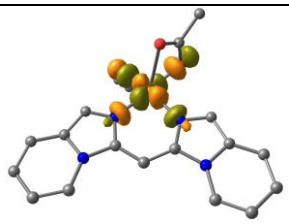
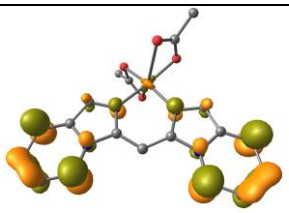
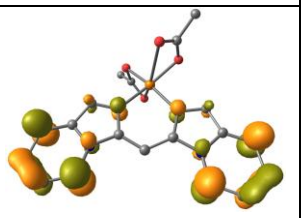
α-spin			
			
SOMO 1	SOMO 2	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S15 Composition and energies of selected molecular orbitals of **1a**, {Cu^{II}(μ-$(L1)_2$)Cu^{II}} (*S*=1)

MO	energy (eV)	% composition		
		Cu	$(L1)_2$	OAc
		α-spin		
HOMO-5	-6.223	0.10	0.07	0.83
HOMO-4	-6.121	0.14	0.05	0.82
HOMO-3	-5.969	0.00	0.97	0.02
HOMO-2	-5.879	0.00	0.98	0.01
SOMO 2	-5.715	0.00	0.98	0.02
SOMO 1	-5.520	0.00	1.00	0.00
LUMO	-1.466	0.01	0.98	0.01
LUMO+1	-1.392	0.00	0.99	0.00
LUMO+2	-1.248	0.02	0.97	0.01
LUMO+3	-1.185	0.01	0.99	0.01
LUMO+4	-1.016	0.02	0.97	0.01
LUMO+5	-0.437	0.00	0.99	0.01
		β-spin		
HOMO-5	-6.080	0.17	0.10	0.73
HOMO-4	-5.979	0.01	0.93	0.06
HOMO-3	-5.925	0.17	0.12	0.71
HOMO-2	-5.878	0.02	0.90	0.08
HOMO-1	-5.714	0.01	0.97	0.03
HOMO	-5.524	0.00	0.99	0.00
LUMO	-2.852	0.61	0.11	0.28
LUMO+1	-2.576	0.59	0.18	0.23
LUMO+2	-1.455	0.01	0.98	0.01
LUMO+3	-1.383	0.00	0.99	0.00
LUMO+4	-1.241	0.02	0.97	0.01
LUMO+5	-1.179	0.00	0.99	0.01

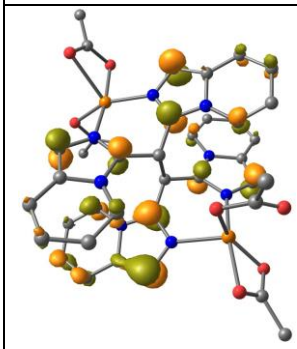
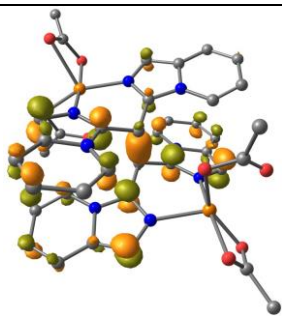
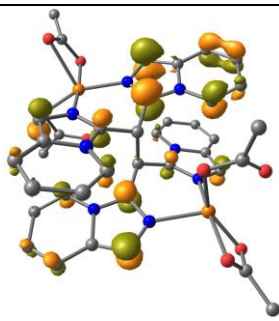
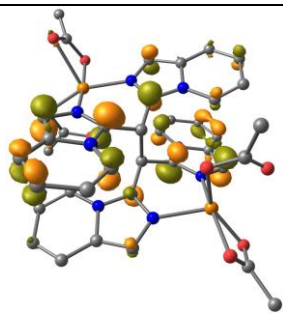
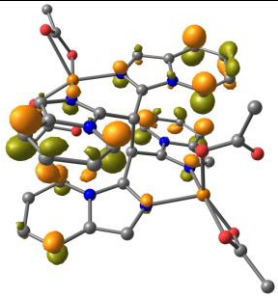
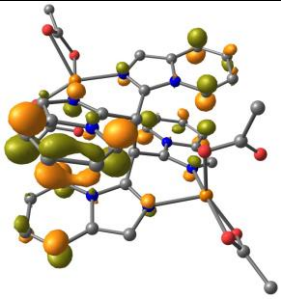
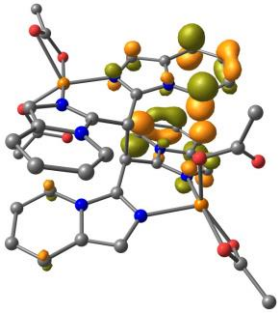
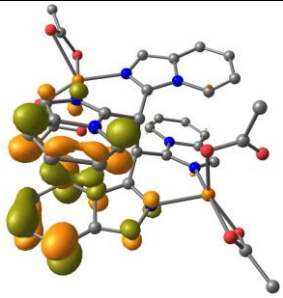
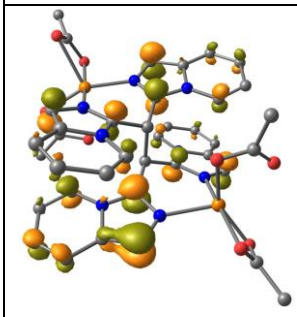
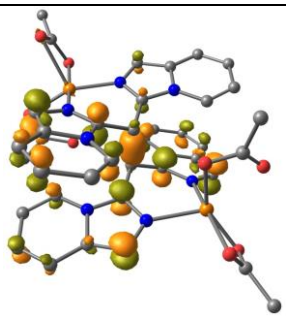
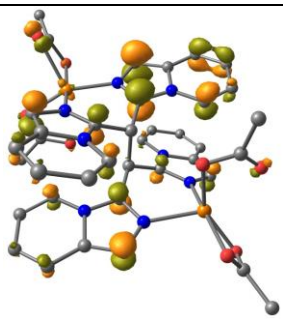
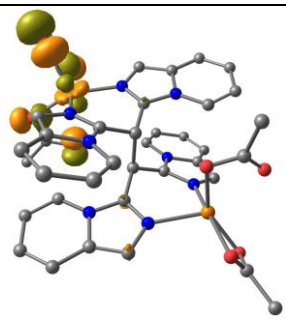
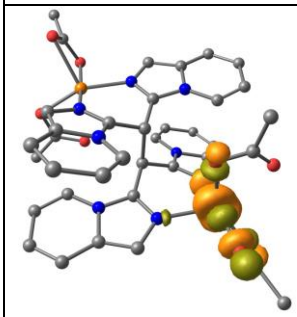
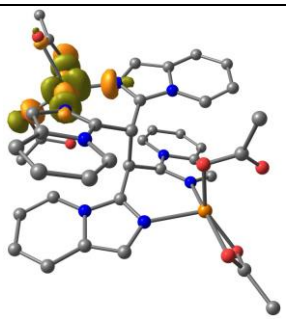
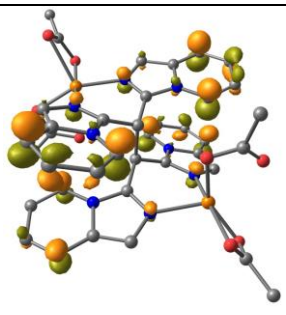
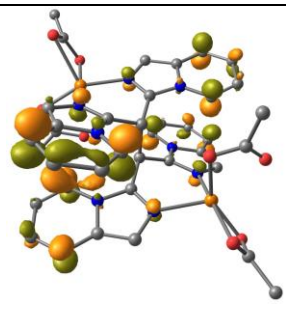
α-spin			
			
SOMO 1	SOMO 2	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S16 Composition and energies of selected molecular orbitals of {Zn^{II}-L1^{-}} (*S*=0)

MO	energy (eV)	% composition		
		Zn	L1	OAc
HOMO-5	-3.733	0.00	0.03	0.97
HOMO-4	-3.422	0.05	0.16	0.79
HOMO-3	-3.340	0.00	0.94	0.06
HOMO-2	-3.266	0.04	0.03	0.93
HOMO-1	-2.017	0.00	1.00	0.00
HOMO	-0.163	0.00	0.99	0.00
LUMO	2.105	0.00	0.99	0.00
LUMO+1	2.156	0.00	1.00	0.00
LUMO+2	3.296	0.00	0.99	0.01
LUMO+3	3.912	0.02	0.96	0.02
LUMO+4	4.144	0.20	0.07	0.73
LUMO+5	4.322	0.04	0.07	0.90

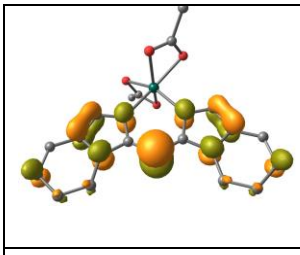
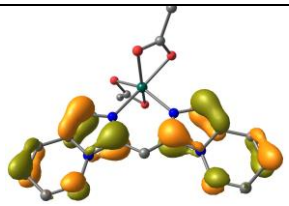
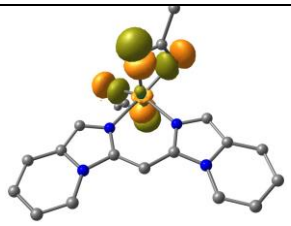
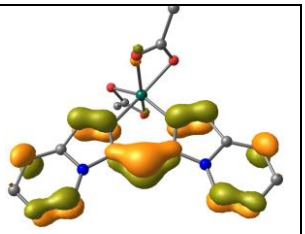
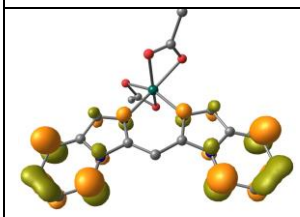
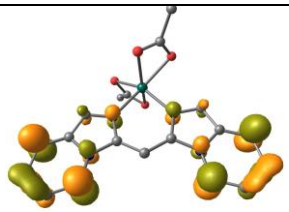
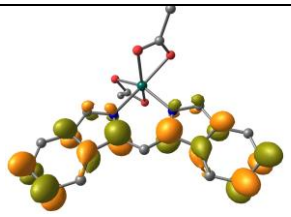
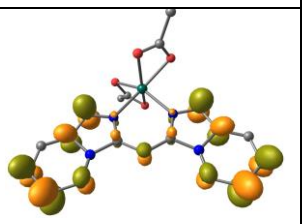
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S17 Composition and energies of selected molecular orbitals of {Zn^{II}-L1$^{\bullet}$} (*S*=1/2)

MO	energy (eV)	% composition		
		Zn	L1	OAc
		α-spin		
HOMO-5	-6.438	0.01	0.04	0.95
HOMO-4	-6.413	0.00	0.04	0.96
HOMO-3	-6.135	0.04	0.05	0.91
HOMO-2	-5.923	0.03	0.02	0.95
HOMO-1	-5.909	0.00	0.99	0.01
SOMO	-4.494	0.00	0.99	0.01
LUMO	-1.583	0.00	0.99	0.01
LUMO+1	-1.536	0.00	1.00	0.00
LUMO+2	-0.577	0.00	0.99	0.01
LUMO+3	0.094	0.01	0.99	0.00
LUMO+4	1.116	0.00	1.00	0.00
LUMO+5	1.343	0.01	0.99	0.00
		β-spin		
HOMO-5	-6.567	0.05	0.07	0.88
HOMO-4	-6.434	0.01	0.04	0.95
HOMO-3	-6.410	0.00	0.03	0.96
HOMO-2	-6.132	0.04	0.05	0.91
HOMO-1	-5.920	0.03	0.02	0.94
HOMO	-5.681	0.00	1.00	0.00
LUMO	-2.962	0.00	0.99	0.00
LUMO+1	-1.458	0.00	0.99	0.00
LUMO+2	-1.416	0.00	1.00	0.00
LUMO+3	-0.400	0.00	0.99	0.01
LUMO+4	0.359	0.01	0.99	0.01
LUMO+5	1.326	0.00	0.97	0.00

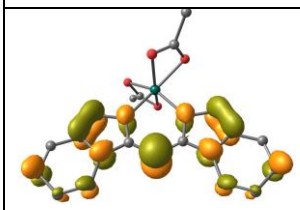
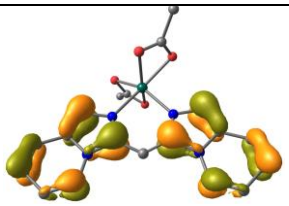
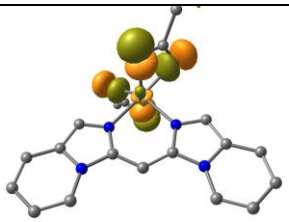
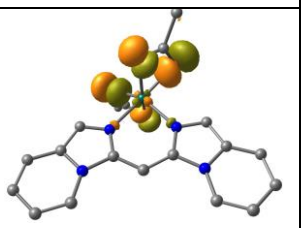
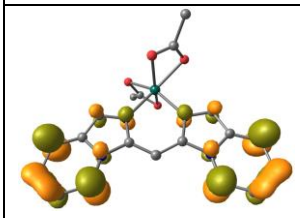
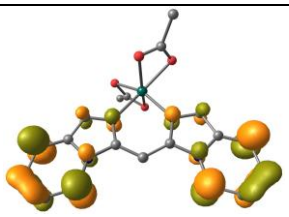
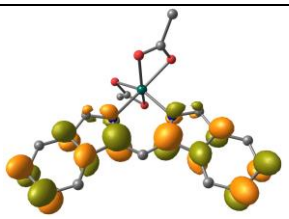
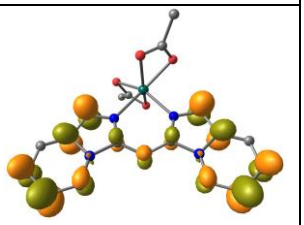
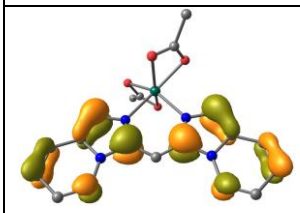
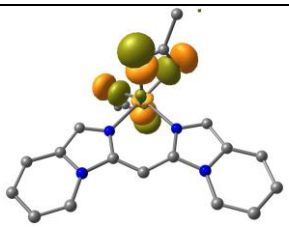
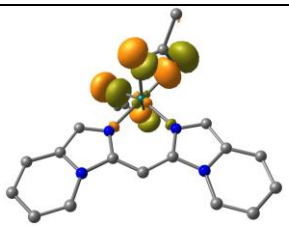
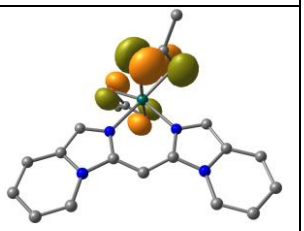
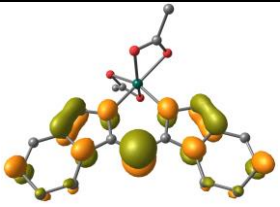
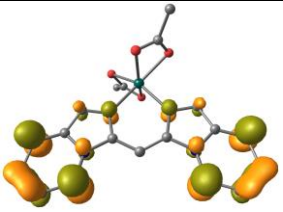
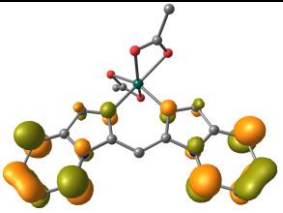
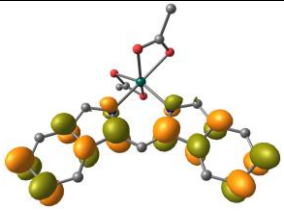
α-spin			
			
SOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S18 Composition and energies of selected molecular orbitals of **1b**, {Zn^{II}(μ-$(L1)_2$)Zn^{II}} (*S*=0)

MO	energy (eV)	% composition		
		Zn	L1	OAc
HOMO-5	-6.435	0.04	0.03	0.93
HOMO-4	-6.435	0.04	0.04	0.92
HOMO-3	-5.958	0.00	1.00	0.00
HOMO-2	-5.866	0.00	0.99	0.00
HOMO-1	-5.714	0.00	0.99	0.01
HOMO	-5.510	0.00	1.00	0.00
LUMO	-1.453	0.01	0.98	0.02
LUMO+1	-1.383	0.00	0.99	0.01
LUMO+2	-1.243	0.00	0.99	0.01
LUMO+3	-1.207	0.00	0.99	0.01
LUMO+4	-0.985	0.00	0.99	0.01
LUMO+5	-0.409	0.00	0.99	0.01

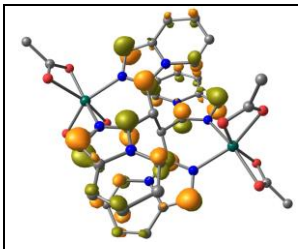
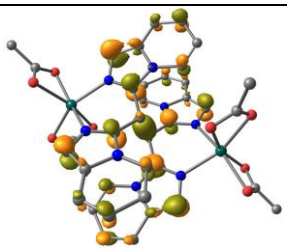
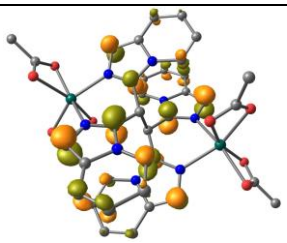
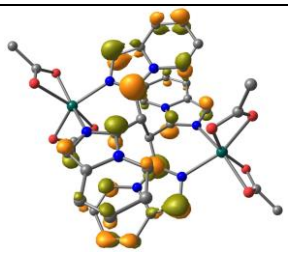
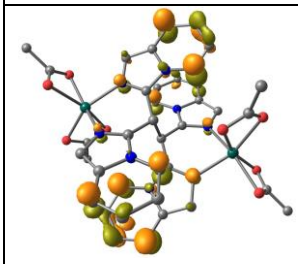
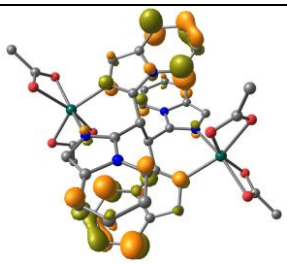
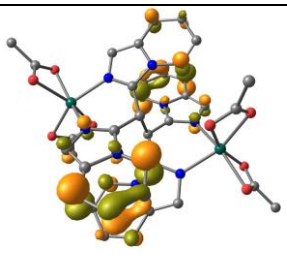
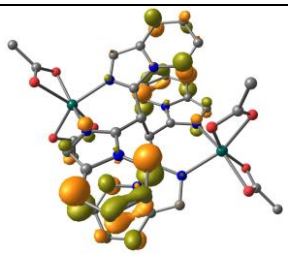
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S19 Composition and energies of selected molecular orbitals of {Cu^{II}-$L4^{-}$} (*S*=1/2)

MO	energy (eV)	% composition		
		Cu	L4	OAc
		α-spin		
HOMO-5	-3.189	0.05	0.88	0.07
HOMO-4	-3.099	0.10	0.41	0.49
HOMO-3	-2.971	0.03	0.06	0.91
HOMO-2	-2.411	0.21	0.37	0.42
HOMO-1	-2.237	0.20	0.24	0.56
SOMO	-1.128	0.04	0.91	0.05
LUMO	1.775	0.01	0.98	0.01
LUMO+1	2.412	0.01	0.97	0.02
LUMO+2	2.622	0.00	0.99	0.01
LUMO+3	2.781	0.01	0.98	0.01
LUMO+4	3.800	0.70	0.10	0.20
LUMO+5	3.867	0.56	0.10	0.34
		β-spin		
HOMO-5	-3.285	0.12	0.40	0.48
HOMO-4	-3.085	0.13	0.57	0.30
HOMO-3	-2.982	0.11	0.34	0.55
HOMO-2	-2.919	0.04	0.11	0.85
HOMO-1	-1.996	0.26	0.22	0.52
HOMO	-1.051	0.06	0.87	0.07
LUMO	1.239	0.48	0.36	0.16
LUMO+1	1.918	0.13	0.83	0.04
LUMO+2	2.415	0.01	0.97	0.02
LUMO+3	2.623	0.00	0.99	0.01
LUMO+4	2.781	0.01	0.98	0.01
LUMO+5	3.803	0.70	0.10	0.20

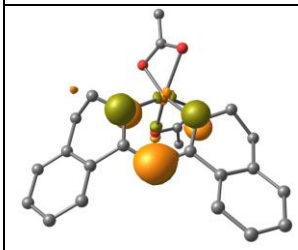
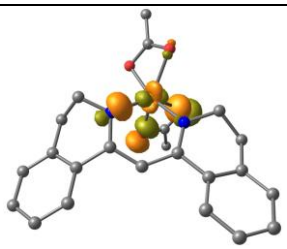
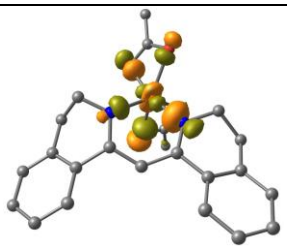
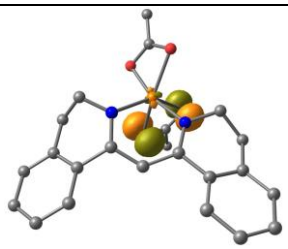
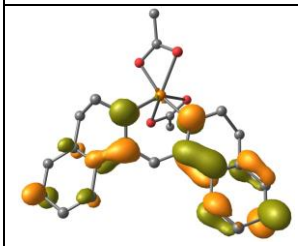
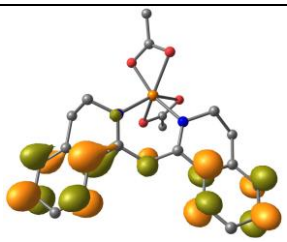
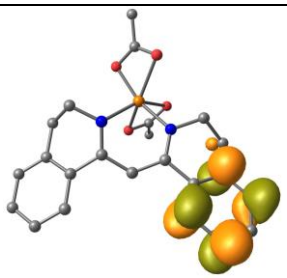
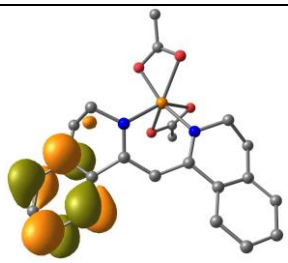
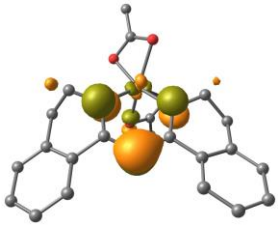
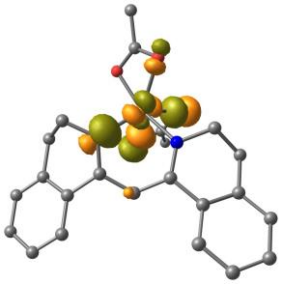
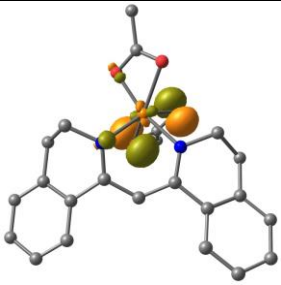
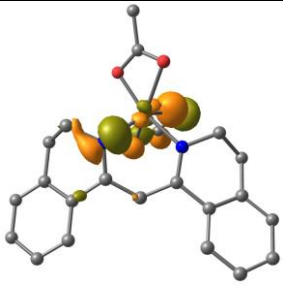
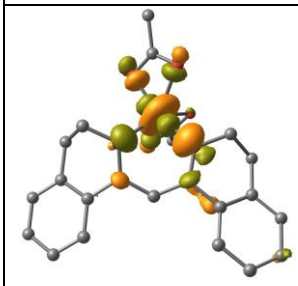
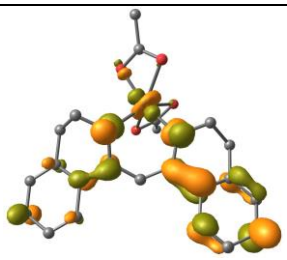
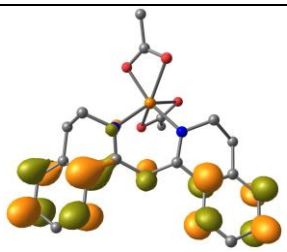
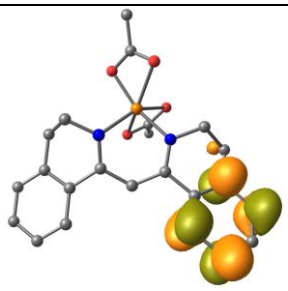
α-spin			
			
SOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S20 Composition and energies of selected molecular orbitals of {Cu^{II}-L4$^{\bullet}$} (*S*=1)

MO	energy (eV)	% composition		
		Cu	L4	OAc
		α-spin		
HOMO-5	-6.932	0.06	0.78	0.16
HOMO-4	-6.796	0.02	0.92	0.06
HOMO-3	-6.648	0.03	0.12	0.85
HOMO-2	-6.312	0.12	0.52	0.37
SOMO 2	-6.209	0.14	0.37	0.49
SOMO 1	-5.907	0.14	0.09	0.76
LUMO	-2.043	0.01	0.98	0.01
LUMO+1	-1.007	0.00	0.97	0.03
LUMO+2	-0.472	0.00	0.98	0.02
LUMO+3	-0.300	0.00	0.97	0.03
LUMO+4	0.595	0.03	0.95	0.02
LUMO+5	0.924	0.33	0.12	0.55
		β-spin		
HOMO-5	-6.936	0.03	0.87	0.10
HOMO-4	-6.715	0.11	0.49	0.40
HOMO-3	-6.656	0.05	0.57	0.48
HOMO-2	-6.521	0.03	0.09	0.88
HOMO-1	-6.483	0.12	0.34	0.54
HOMO	-5.603	0.20	0.16	0.64
LUMO	-3.729	0.07	0.86	0.07
LUMO+1	-2.727	0.53	0.22	0.25
LUMO+2	-1.661	0.06	0.91	0.03
LUMO+3	-0.832	0.01	0.97	0.02
LUMO+4	-0.478	0.00	0.98	0.02
LUMO+5	-0.311	0.00	0.98	0.02

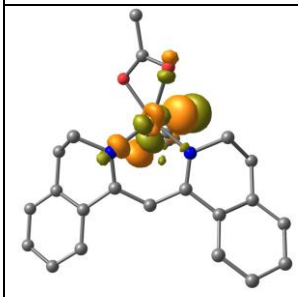
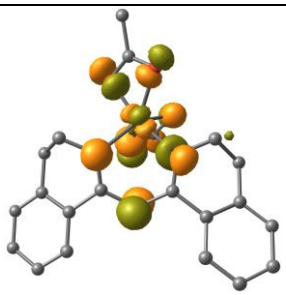
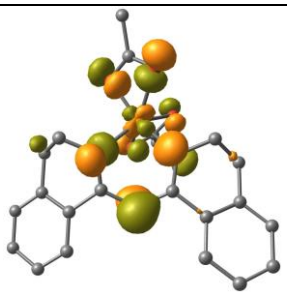
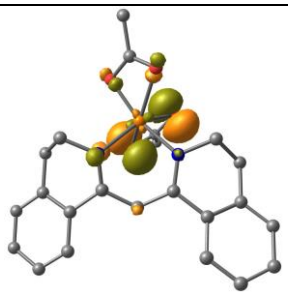
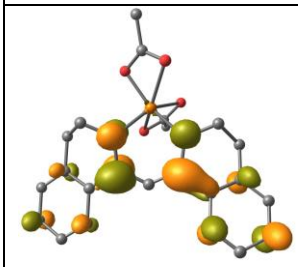
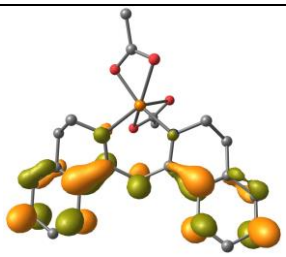
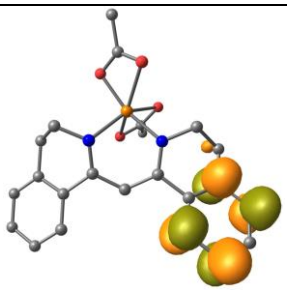
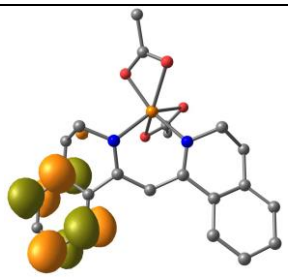
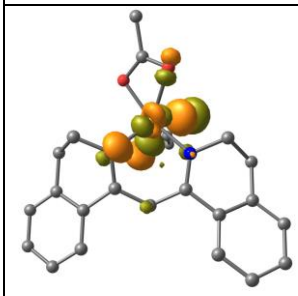
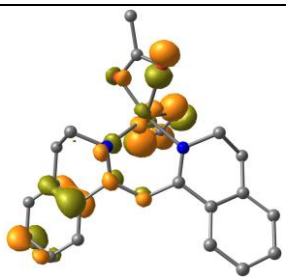
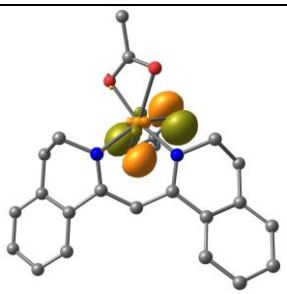
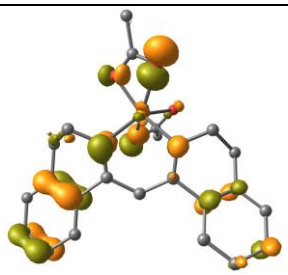
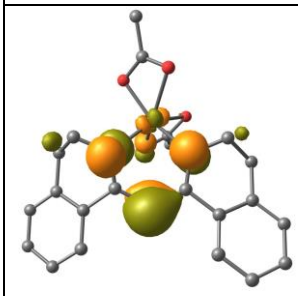
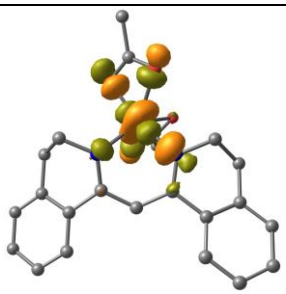
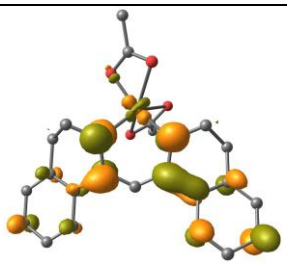
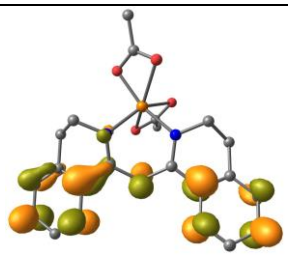
α-spin			
			
SOMO 1	SOMO 2	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S21 Composition and energies of selected molecular orbitals of **1c**, {Cu^{II}(μ-$(L4)_2$)Cu^{II}} (*S*=1)

MO	energy (eV)	% composition		
		Cu	$(L4)_2$	OAc
		α-spin		
HOMO-5	-6.537	0.08	0.07	0.85
HOMO-4	-6.420	0.07	0.07	0.86
HOMO-3	-6.250	0.18	0.20	0.62
HOMO-2	-6.227	0.18	0.22	0.60
SOMO 2	-6.137	0.15	0.12	0.73
SOMO 1	-6.068	0.13	0.07	0.80
LUMO	-2.338	0.03	0.96	0.01
LUMO+1	-2.216	0.01	0.98	0.01
LUMO+2	-2.166	0.02	0.97	0.01
LUMO+3	-1.494	0.00	0.99	0.01
LUMO+4	-0.558	0.01	0.98	0.01
LUMO+5	-0.529	0.01	0.99	0.00
		β-spin		
HOMO-5	-6.701	0.03	0.08	0.89
HOMO-4	-6.633	0.02	0.07	0.91
HOMO-3	-6.472	0.06	0.05	0.89
HOMO-2	-6.372	0.04	0.04	0.92
HOMO-1	-6.003	0.15	0.03	0.82
HOMO	-5.903	0.17	0.03	0.80
LUMO	-2.694	0.53	0.27	0.20
LUMO+1	-2.667	0.51	0.29	0.20
LUMO+2	-2.272	0.09	0.87	0.04
LUMO+3	-2.157	0.04	0.95	0.01
LUMO+4	-2.119	0.05	0.93	0.02
LUMO+5	-1.475	0.00	0.99	0.01

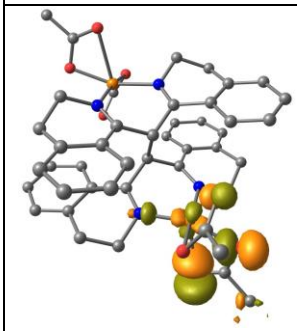
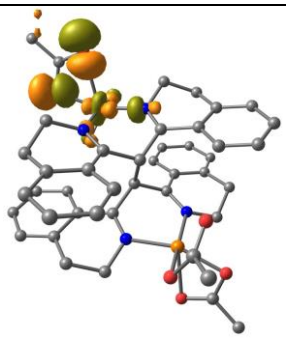
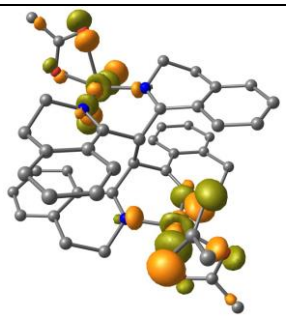
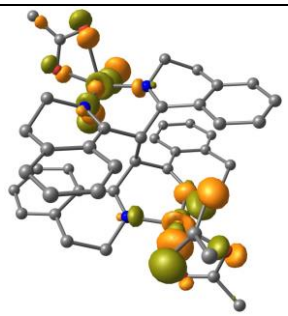
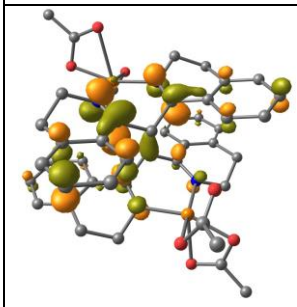
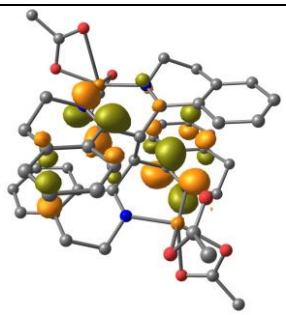
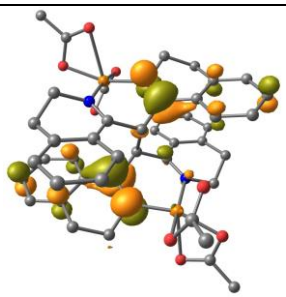
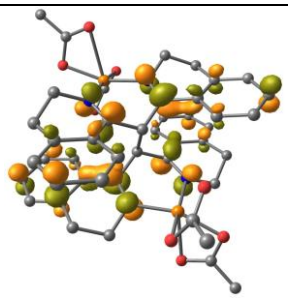
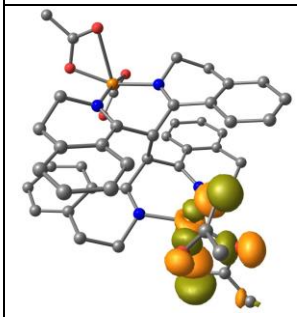
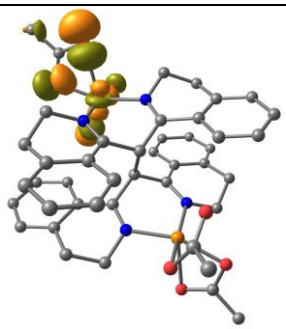
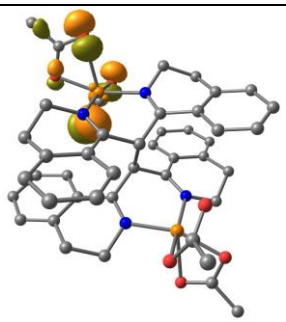
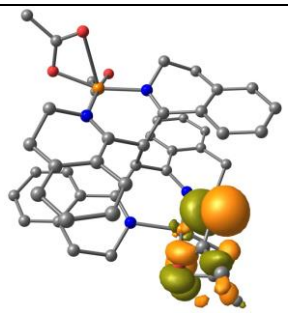
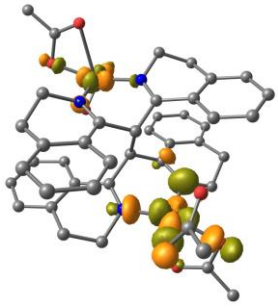
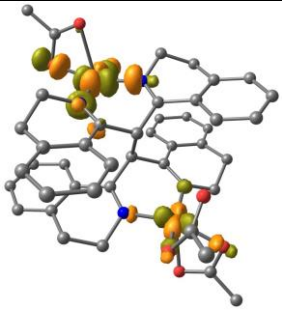
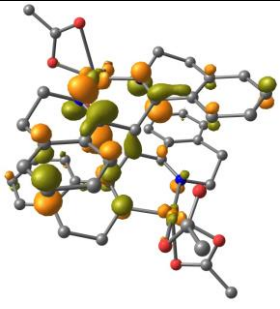
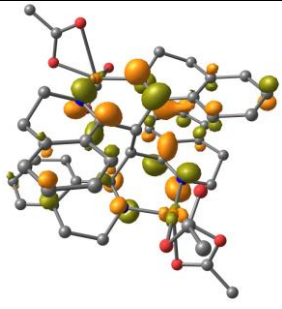
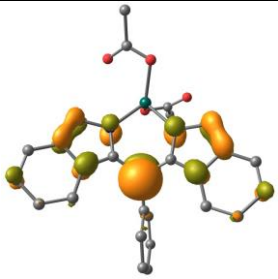
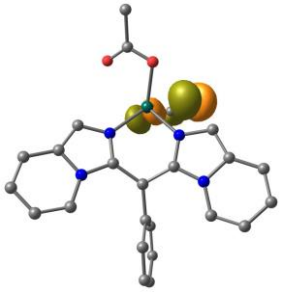
α-spin			
			
SOMO 1	SOMO 2	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S22 Composition and energies of selected molecular orbitals of {Zn^{II}-L2^{-}} (*S*=0)

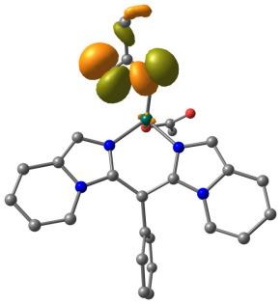
MO	energy (eV)	% composition		
		Zn	L2	OAc
HOMO-5	-2.282	0.04	0.04	0.92
HOMO-4	-2.174	0.03	0.05	0.92
HOMO-3	-1.844	0.00	0.97	0.03
HOMO-2	-1.740	0.02	0.03	0.95
HOMO-1	-1.431	0.01	0.02	0.97
HOMO	-0.193	0.00	0.99	0.01
LUMO	1.153	0.00	0.99	0.01
LUMO+1	1.222	0.00	1.00	0.00
LUMO+2	1.524	0.00	1.00	0.00
LUMO+3	1.718	0.00	1.00	0.00
LUMO+4	2.663	0.00	1.00	0.00
LUMO+5	3.040	0.00	0.99	0.01



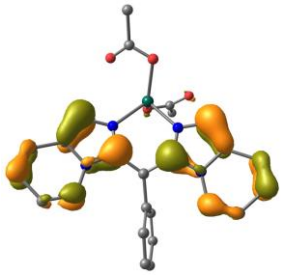
HOMO



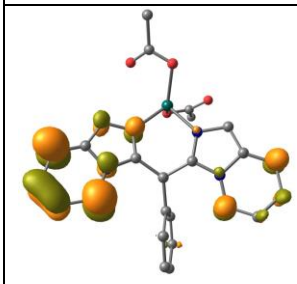
HOMO-1



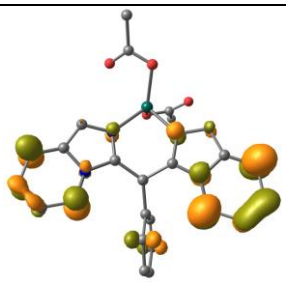
HOMO-2



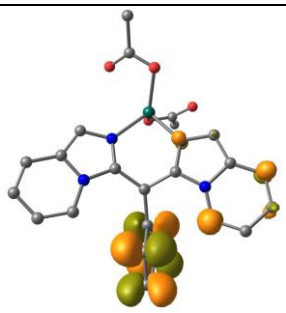
HOMO-3



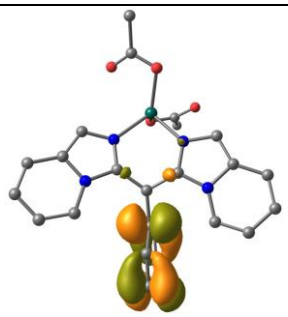
LUMO



LUMO+1



LUMO+2



LUMO+3

Table S23 Composition and energies of selected molecular orbitals of {Zn^{II}-L2$^{\bullet}$} (*S*=1/2)

MO	energy (eV)	% composition		
		Zn	L2	OAc
		α-spin		
HOMO-5	-5.481	0.01	0.04	0.95
HOMO-4	-5.452	0.00	0.03	0.97
HOMO-3	-5.437	0.04	0.03	0.93
HOMO-2	-4.991	0.04	0.04	0.92
HOMO-1	-4.806	0.03	0.02	0.95
SOMO	-4.283	0.00	0.99	0.01
LUMO	-2.219	0.00	1.00	0.00
LUMO+1	-2.184	0.00	0.99	0.01
LUMO+2	-1.602	0.00	1.00	0.00
LUMO+3	-1.403	0.00	0.99	0.01
LUMO+4	-1.268	0.00	0.99	0.01
LUMO+5	-0.389	0.00	0.99	0.01
		β-spin		
HOMO-5	-5.479	0.01	0.03	0.96
HOMO-4	-5.451	0.00	0.03	0.97
HOMO-3	-5.432	0.04	0.04	0.92
HOMO-2	-5.409	0.00	0.98	0.02
HOMO-1	-4.986	0.04	0.04	0.92
HOMO	-4.802	0.03	0.02	0.95
LUMO	-3.730	0.00	0.99	0.01
LUMO+1	-2.129	0.00	1.00	0.00
LUMO+2	-2.088	0.00	0.99	0.01
LUMO+3	-1.486	0.00	1.00	0.00
LUMO+4	-1.299	0.00	0.99	0.01
LUMO+5	-1.189	0.01	0.99	0.00

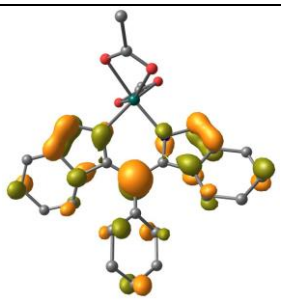
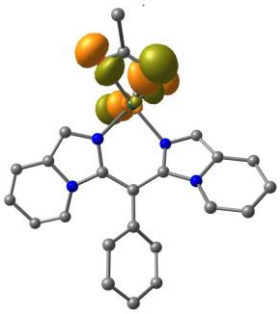
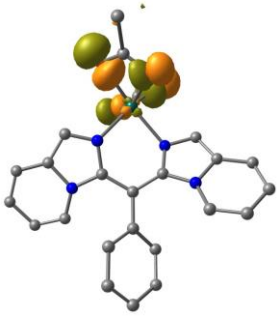
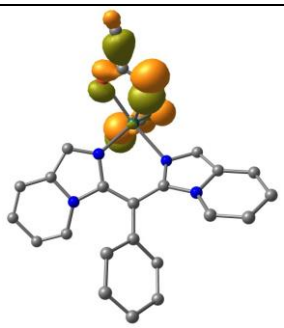
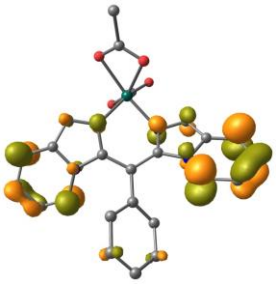
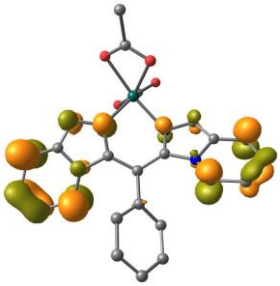
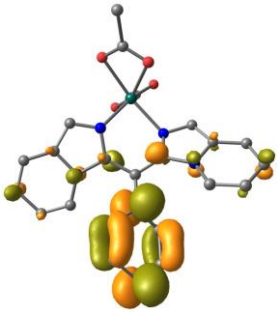
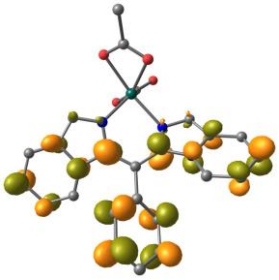
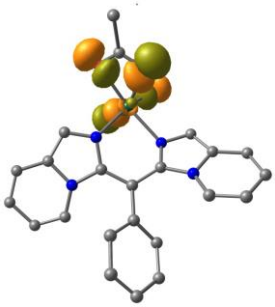
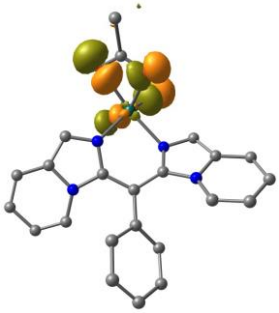
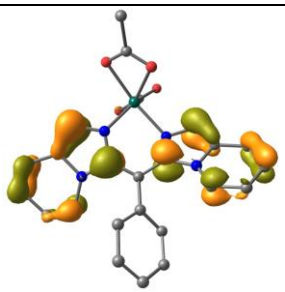
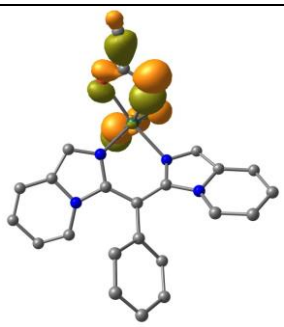
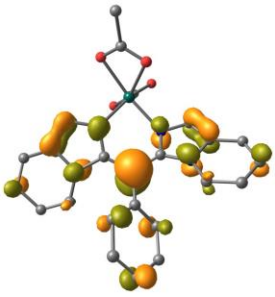
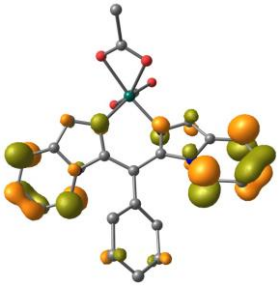
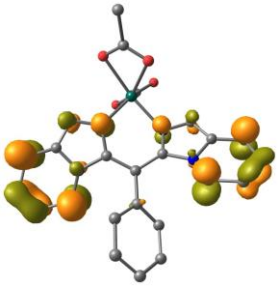
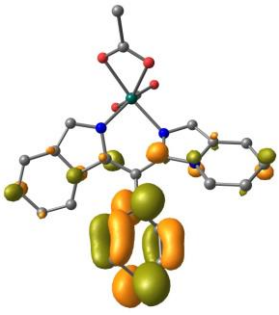
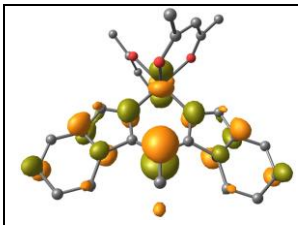
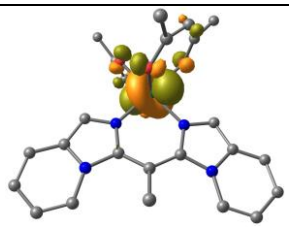
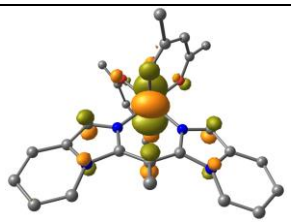
α-spin			
			
SOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

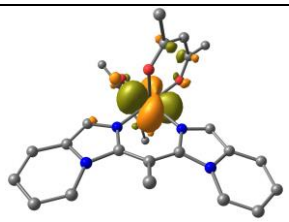
Table S24 Composition and energies of selected molecular orbitals of **3**$^{-}$, {Ru^{II}-L3^{-}} (*S*=0)

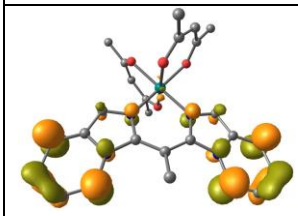
MO	energy (eV)	% composition		
		Ru	L3	acac
HOMO-5	-2.547	0.04	0.04	0.92
HOMO-4	-2.014	0.00	1.00	0.00
HOMO-3	-1.195	0.78	0.08	0.14
HOMO-2	-1.078	0.62	0.22	0.16
HOMO-1	-0.765	0.73	0.08	0.19
HOMO	0.019	0.16	0.80	0.04
LUMO	2.205	0.02	0.95	0.03
LUMO+1	2.255	0.01	0.97	0.02
LUMO+2	2.625	0.04	0.05	0.91
LUMO+3	2.721	0.06	0.06	0.88
LUMO+4	3.349	0.01	0.98	0.01
LUMO+5	3.882	0.47	0.31	0.22

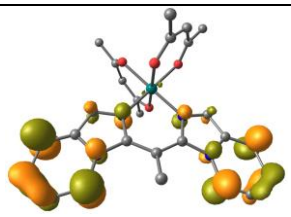

HOMO

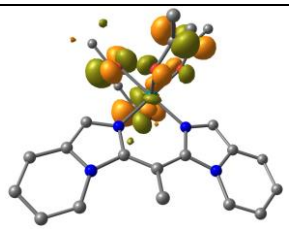

HOMO-1


HOMO-2


HOMO-3


LUMO


LUMO+1


LUMO+2

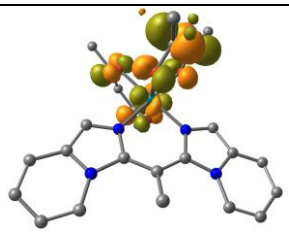

LUMO+3

Table S25 Composition and energies of selected molecular orbitals of **3**, {Ru^{II}-L3$^{\bullet}$} (*S*=1/2)

MO	energy (eV)	% composition		
		Ru	L3	acac
		α-spin		
HOMO-5	-5.432	0.13	0.05	0.82
HOMO-4	-5.360	0.00	1.00	0.00
HOMO-3	-4.665	0.76	0.08	0.16
HOMO-2	-4.632	0.56	0.18	0.26
HOMO-1	-4.109	0.64	0.06	0.30
SOMO	-3.584	0.14	0.83	0.03
LUMO	-1.082	0.01	0.98	0.01
LUMO+1	-1.037	0.01	0.98	0.01
LUMO+2	-0.189	0.03	0.04	0.93
LUMO+3	-0.133	0.01	0.94	0.05
LUMO+4	-0.102	0.05	0.11	0.84
LUMO+5	0.685	0.06	0.93	0.01
		β-spin		
HOMO-5	-5.711	0.27	0.06	0.68
HOMO-4	-5.380	0.05	0.04	0.91
HOMO-3	-5.240	0.00	1.00	0.00
HOMO-2	-4.555	0.76	0.08	0.16
HOMO-1	-4.015	0.65	0.07	0.28
HOMO	-4.005	0.54	0.30	0.16
LUMO	-2.171	0.21	0.74	0.05
LUMO+1	-0.992	0.02	0.98	0.00
LUMO+2	-0.932	0.03	0.96	0.01
LUMO+3	-0.162	0.04	0.05	0.91
LUMO+4	-0.091	0.05	0.07	0.88
LUMO+5	0.042	0.02	0.98	0.00

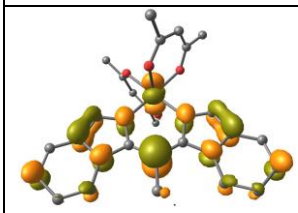
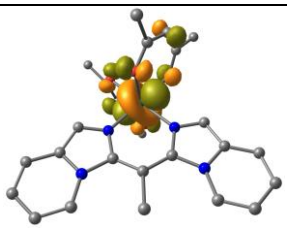
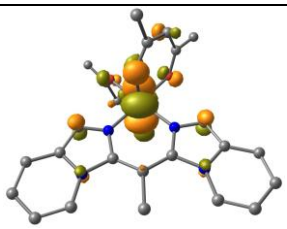
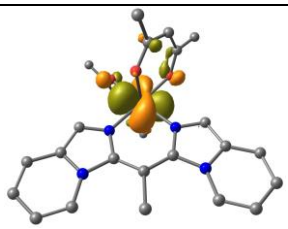
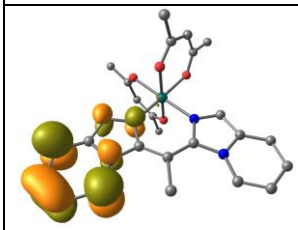
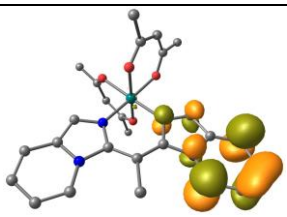
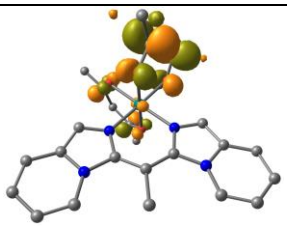
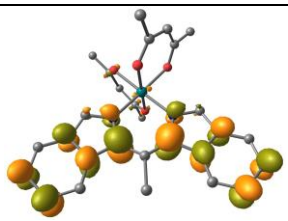
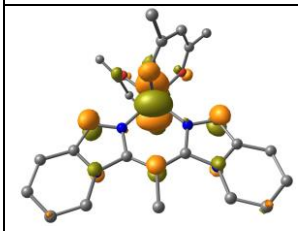
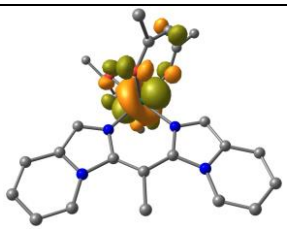
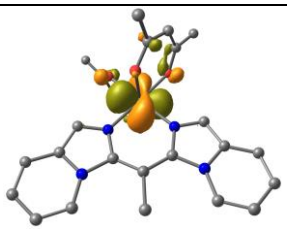
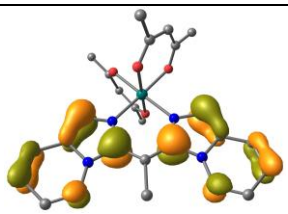
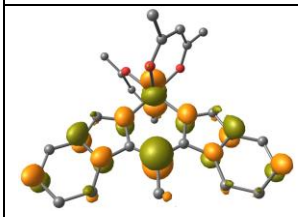
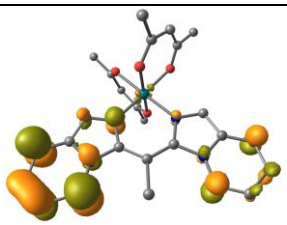
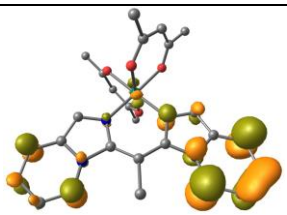
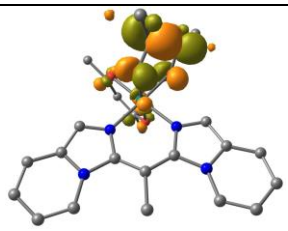
α-spin			
			
SOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S26 Composition and energies of selected molecular orbitals of $\mathbf{3}^{+}$, {Ru^{III}-L3$^{\bullet}$} (*S*=1)

MO	energy (eV)	% composition		
		Ru	L3	acac
		α-spin		
HOMO-5	-9.254	0.73	0.09	0.18
HOMO-4	-9.099	0.42	0.15	0.43
HOMO-3	-8.587	0.30	0.11	0.59
HOMO-2	-8.544	0.03	0.90	0.07
SOMO 2	-8.516	0.19	0.06	0.75
SOMO 1	-7.168	0.05	0.94	0.01
LUMO	-4.016	0.01	0.98	0.01
LUMO+1	-3.989	0.01	0.99	0.00
LUMO+2	-3.605	0.20	0.06	0.74
LUMO+3	-3.569	0.10	0.06	0.84
LUMO+4	-3.408	0.39	0.07	0.54
LUMO+5	-3.225	0.08	0.88	0.04
		β-spin		
HOMO-5	-9.605	0.07	0.87	0.06
HOMO-4	-9.197	0.59	0.07	0.35
HOMO-3	-8.804	0.26	0.10	0.63
HOMO-2	-8.639	0.44	0.07	0.49
HOMO-1	-8.351	0.02	0.96	0.02
HOMO	-8.283	0.48	0.12	0.41
LUMO	-6.091	0.70	0.09	0.21
LUMO+1	-5.603	0.06	0.93	0.01
LUMO+2	-3.886	0.02	0.97	0.01
LUMO+3	-3.837	0.02	0.97	0.01
LUMO+4	-3.549	0.04	0.04	0.92
LUMO+5	-3.511	0.07	0.06	0.87

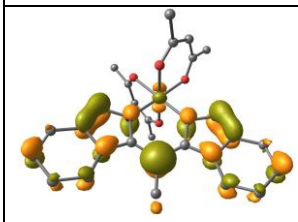
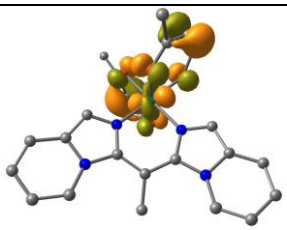
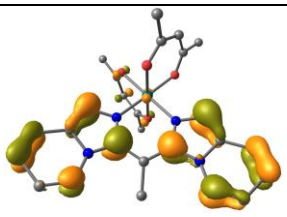
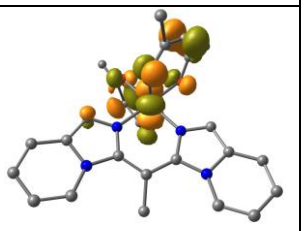
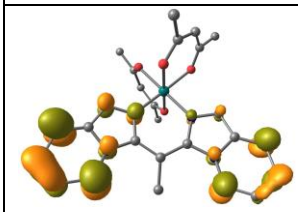
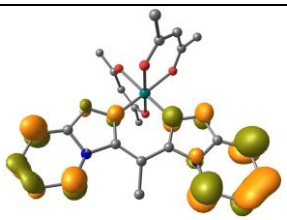
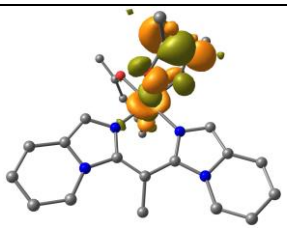
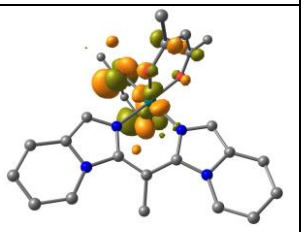
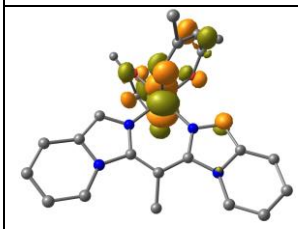
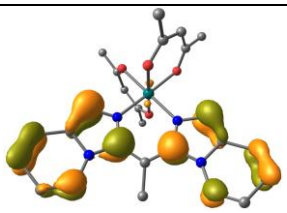
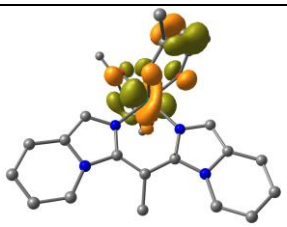
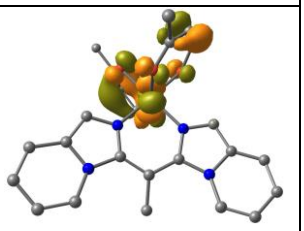
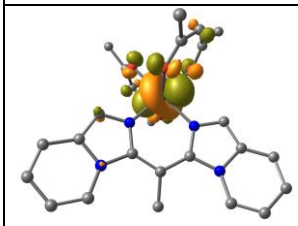
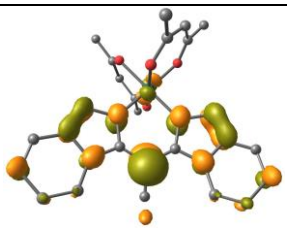
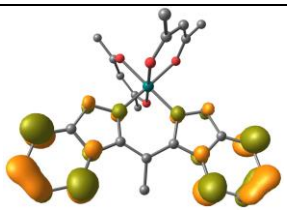
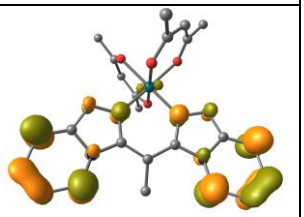
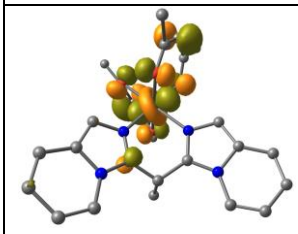
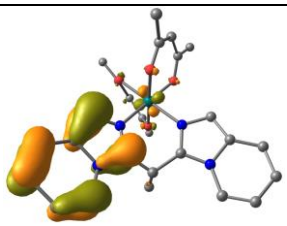
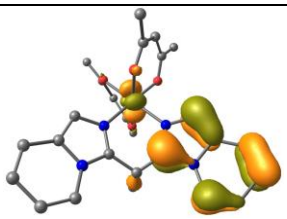
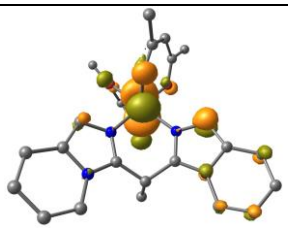
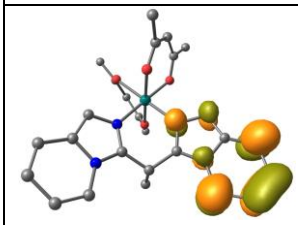
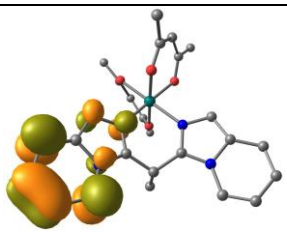
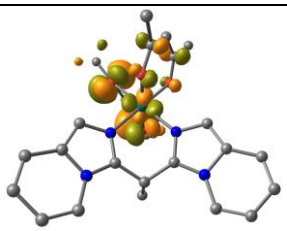
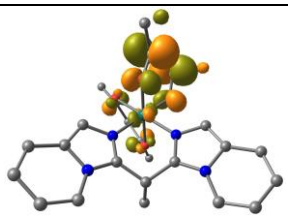
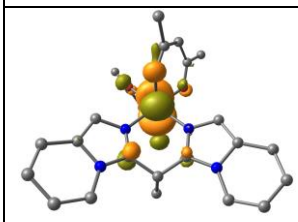
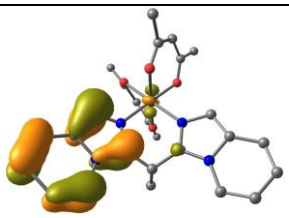
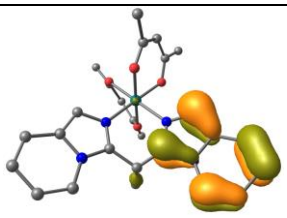
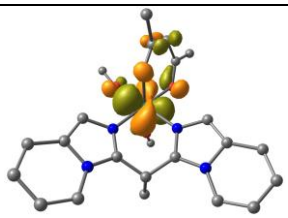
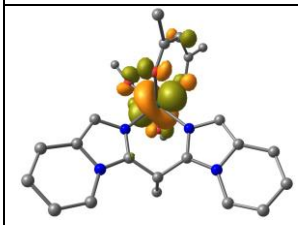
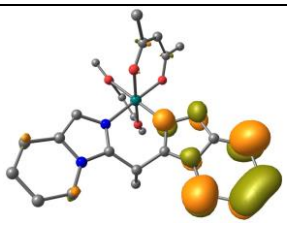
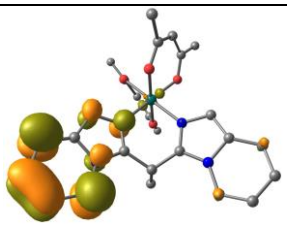
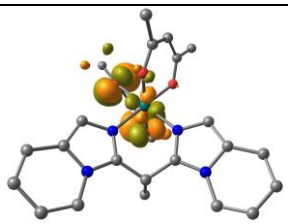
α-spin			
			
SOMO 1	SOMO 2	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

Table S27 Composition and energies of selected molecular orbitals of [**3**-H]$^{+}$, {Ru^{III}-HL3} (*S*=1/2)

MO	energy (eV)	% composition		
		Ru	HL3	acac
		α-spin		
HOMO-5	-9.073	0.10	0.04	0.86
HOMO-4	-8.858	0.72	0.08	0.20
HOMO-3	-8.504	0.59	0.21	0.20
HOMO-2	-8.406	0.14	0.82	0.04
HOMO-1	-8.311	0.06	0.86	0.08
SOMO	-8.227	0.31	0.11	0.58
LUMO	-3.849	0.01	0.96	0.03
LUMO+1	-3.768	0.01	0.97	0.02
LUMO+2	-3.673	0.08	0.05	0.87
LUMO+3	-3.585	0.04	0.07	0.89
LUMO+4	-2.950	0.04	0.95	0.01
LUMO+5	-2.630	0.08	0.88	0.04
		β-spin		
HOMO-5	-9.159	0.31	0.06	0.64
HOMO-4	-8.843	0.03	0.04	0.93
HOMO-3	-8.490	0.68	0.08	0.24
HOMO-2	-8.421	0.02	0.96	0.01
HOMO-1	-8.299	0.05	0.93	0.02
HOMO	-8.168	0.66	0.16	0.18
LUMO	-5.576	0.64	0.07	0.28
LUMO+1	-3.844	0.01	0.94	0.05
LUMO+2	-3.734	0.02	0.97	0.01
LUMO+3	-3.623	0.07	0.04	0.89
LUMO+4	-3.554	0.05	0.08	0.87
LUMO+5	-2.934	0.03	0.95	0.02

α-spin			
			
SOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3
β-spin			
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
LUMO	LUMO+1	LUMO+2	LUMO+3

A. Optimized cartesian coordinates using (U)B3LYP density functional (coordinates for the stable electronic states are only given).

{Cu^{II}-$L1^{-}$} for **1a** (*S*=1/2)

O	3.533218000	11.724164000	8.158772000
O	2.749348000	12.531886000	6.212988000
N	2.461383000	7.995143000	4.278515000
N	-0.872027000	7.866417000	7.934593000
O	-0.608544000	12.797867000	5.579849000
N	0.128565000	9.795212000	7.502806000
N	2.055950000	9.869950000	5.386934000
C	-1.311358000	6.558209000	7.949627000
H	-0.867618000	5.893181000	7.219771000
C	1.715509000	8.558377000	5.305464000
O	0.276509000	12.659583000	7.641502000
C	3.292905000	9.015746000	3.717061000
C	3.597850000	12.491271000	7.187167000
C	4.146280000	8.658502000	2.640768000
H	4.777180000	9.429868000	2.208976000
C	-1.394205000	8.836393000	8.848235000
C	0.785601000	7.862121000	6.095925000
H	0.623256000	6.809431000	5.910785000
C	0.061654000	8.494299000	7.120869000
C	-2.251099000	6.165203000	8.849110000
H	-2.583184000	5.132512000	8.846538000
C	3.003939000	10.148885000	4.438341000
H	3.403800000	11.147270000	4.354824000
C	2.490524000	6.701873000	3.797692000
H	1.830946000	5.993381000	4.282285000
C	-0.744931000	10.006458000	8.536591000
H	-0.837218000	10.989850000	8.970201000
C	3.315296000	6.376028000	2.768048000
H	3.323440000	5.354617000	2.402826000
C	4.167121000	7.374769000	2.168579000
H	4.819805000	7.098887000	1.346323000
C	-2.798978000	7.108157000	9.794146000
H	-3.547990000	6.778423000	10.507218000
C	-2.372427000	8.407881000	9.782986000
H	-2.768926000	9.138882000	10.481502000
C	4.745786000	13.498872000	7.068771000
H	4.343088000	14.517224000	7.083086000
H	5.263425000	13.370651000	6.112249000
H	5.452220000	13.372626000	7.891818000
C	-0.498688000	13.186718000	6.751815000
C	-1.315442000	14.382329000	7.252514000
H	-1.978999000	14.748415000	6.466380000
H	-0.638730000	15.184272000	7.565980000

H	-1.903736000	14.095717000	8.130707000
Cu	1.308713000	11.245469000	6.691866000

{Cu^{II}-L1$^{\bullet}$} for **1a** (*S*=1)

O	3.370821000	11.514934000	8.142975000
O	2.810046000	12.575739000	6.260318000
N	2.429115000	8.056901000	4.248014000
N	-0.824333000	7.900987000	7.985921000
O	-0.515627000	12.563188000	5.513724000
N	0.119606000	9.856526000	7.506684000
N	2.076471000	9.925427000	5.401034000
C	-1.222234000	6.581747000	8.035348000
H	-0.777524000	5.908584000	7.314751000
C	1.719069000	8.622406000	5.302617000
O	0.227680000	12.733647000	7.611818000
C	3.243539000	9.064047000	3.692124000
C	3.595992000	12.373276000	7.272046000
C	4.071609000	8.741848000	2.594707000
H	4.696457000	9.520065000	2.170416000
C	-1.339565000	8.857413000	8.883962000
C	0.798026000	7.933958000	6.111256000
H	0.636665000	6.880185000	5.926645000
C	0.076157000	8.551011000	7.147672000
C	-2.135131000	6.190424000	8.968400000
H	-2.440070000	5.150764000	8.997655000
C	2.984441000	10.207507000	4.448481000
H	3.400494000	11.200689000	4.367168000
C	2.424037000	6.775339000	3.739332000
H	1.767229000	6.061012000	4.217336000
C	-0.717942000	10.058441000	8.540559000
H	-0.831760000	11.044242000	8.966395000
C	3.225278000	6.470294000	2.680072000
H	3.212513000	5.459573000	2.288904000
C	4.067281000	7.464810000	2.091936000
H	4.697373000	7.203172000	1.249197000
C	-2.681171000	7.132556000	9.894776000
H	-3.405809000	6.802073000	10.630548000
C	-2.284874000	8.445748000	9.848713000
H	-2.678080000	9.184995000	10.537906000
C	4.821255000	13.272214000	7.345747000
H	4.503357000	14.291500000	7.588565000
H	5.326061000	13.313198000	6.376220000
H	5.508280000	12.916671000	8.115044000
C	-0.528299000	13.113375000	6.628815000
C	-1.434726000	14.301471000	6.914301000
H	-2.152800000	14.435735000	6.104007000
H	-0.822453000	15.204431000	7.007757000
H	-1.957524000	14.165519000	7.865471000

Cu	1.320281000	11.345348000	6.707664000

1a, {Cu^{II}-(μ-(L1)$_2$)-Cu^{II}} (*S*=1)

O	3.317755000	11.321927000	8.079984000
O	2.602093000	12.670604000	6.441311000
N	2.140088000	8.100995000	4.173811000
N	-0.637801000	7.802606000	7.978756000
O	-0.437433000	12.710932000	5.284489000
N	0.020430000	9.827838000	7.416900000
N	1.852931000	10.016774000	5.229751000
C	-0.768477000	6.435584000	8.172594000
H	0.017059000	5.811739000	7.776193000
C	1.823300000	8.690353000	5.369665000
O	-0.061491000	12.723257000	7.475780000
C	2.375050000	9.136935000	3.241153000
C	3.411419000	12.366087000	7.380985000
C	2.716009000	8.788564000	1.908075000
H	2.894450000	9.585335000	1.194269000
C	-1.591812000	8.711496000	8.487913000
C	1.552651000	7.968061000	6.656944000
H	1.380143000	6.909804000	6.443054000
C	0.327208000	8.531640000	7.329885000
C	-1.846719000	5.961017000	8.851385000
H	-1.925195000	4.888885000	8.989679000
C	2.185411000	10.316564000	3.944296000
H	2.247767000	11.337134000	3.600184000
C	2.231493000	6.760662000	3.816976000
H	2.029003000	6.024093000	4.588842000
C	-1.137873000	9.966595000	8.116128000
H	-1.553694000	10.942729000	8.307373000
C	2.557857000	6.450493000	2.533127000
H	2.626108000	5.403718000	2.259683000
C	2.807181000	7.469794000	1.558892000
H	3.065765000	7.187257000	0.544012000
C	-2.839883000	6.849797000	9.373542000
H	-3.690404000	6.445325000	9.911726000
C	-2.710627000	8.199928000	9.196696000
H	-3.442056000	8.901721000	9.582438000
C	4.531185000	13.360739000	7.651954000
H	4.124012000	14.196227000	8.231745000
H	4.916538000	13.771499000	6.715663000
H	5.333006000	12.896572000	8.229525000
C	-0.631457000	13.201758000	6.413575000
C	-1.529626000	14.407736000	6.614852000
H	-2.140660000	14.578055000	5.727352000
H	-0.905354000	15.289540000	6.794183000
H	-2.164516000	14.272444000	7.494572000
N	2.398432000	7.964827000	10.122715000

N	5.157176000	8.139030000	6.507221000
N	4.204544000	6.149078000	6.684889000
N	2.393558000	6.027611000	9.062703000
C	5.484659000	9.483591000	6.590274000
H	4.772908000	10.131238000	7.090863000
C	2.557643000	7.344968000	8.910889000
C	2.123771000	6.962058000	11.079584000
C	1.920331000	7.345975000	12.431077000
H	1.708851000	6.573860000	13.162733000
C	6.038581000	7.197919000	5.929188000
C	2.837163000	8.041481000	7.609479000
H	3.013741000	9.102942000	7.800023000
C	4.052461000	7.444898000	6.944296000
C	6.671452000	9.904832000	6.073704000
H	6.920094000	10.957536000	6.145717000
C	2.131870000	5.769403000	10.374221000
H	1.985021000	4.763736000	10.735374000
C	2.482776000	9.307618000	10.474443000
H	2.714821000	10.020729000	9.689979000
C	5.400761000	5.973020000	6.065343000
H	5.738409000	4.995119000	5.756280000
C	2.284912000	9.652315000	11.775425000
H	2.352477000	10.700395000	12.043531000
C	1.997033000	8.667135000	12.773927000
H	1.844414000	8.977504000	13.802037000
C	7.580238000	8.987776000	5.456474000
H	8.517340000	9.353790000	5.050681000
C	7.268771000	7.657393000	5.391686000
H	7.939632000	6.933536000	4.941544000
O	1.458850000	4.737751000	6.281220000
O	0.525270000	3.236691000	7.648990000
O	4.122109000	3.556396000	8.953798000
O	3.836305000	2.898532000	6.886086000
C	0.587579000	3.799442000	6.549813000
C	-0.354325000	3.443911000	5.410740000
H	0.217934000	2.964846000	4.609548000
H	-1.130456000	2.760737000	5.757263000
H	-0.807406000	4.347220000	4.991302000
C	4.373247000	2.718838000	8.024732000
C	5.258220000	1.528891000	8.283770000
H	5.986899000	1.757877000	9.063608000
H	4.634643000	0.696886000	8.628751000
H	5.759088000	1.220063000	7.364217000
Cu	1.090811000	11.379186000	6.579549000
Cu	2.881840000	4.556029000	7.671171000

{Zn^{II}-L1^{-}} for **1b** (*S*=0)

Zn	1.337904000	11.487124000	6.737186000

O	3.027483000	11.646140000	8.106124000
O	3.084901000	12.826266000	6.224410000
N	2.361636000	8.132656000	4.199539000
N	-0.745598000	7.923471000	8.040241000
O	-0.153222000	12.587591000	5.588224000
N	0.165460000	9.899445000	7.604175000
N	2.042099000	10.018770000	5.324459000
C	-1.130227000	6.598052000	8.054096000
H	-0.694100000	5.962377000	7.294150000
C	1.685485000	8.710293000	5.269761000
O	0.030143000	13.018198000	7.760279000
C	3.169330000	9.141585000	3.583489000
C	3.598475000	12.462537000	7.322859000
C	3.956057000	8.770946000	2.463312000
H	4.570663000	9.533612000	1.993697000
C	-1.257074000	8.853115000	9.001533000
C	0.805932000	8.010029000	6.117179000
H	0.646104000	6.956750000	5.930292000
C	0.124087000	8.605879000	7.195231000
C	-2.009882000	6.151447000	8.989112000
H	-2.298357000	5.105588000	8.983333000
C	2.932548000	10.279655000	4.318422000
H	3.351559000	11.268691000	4.207494000
C	2.343842000	6.839639000	3.717274000
H	1.702253000	6.140391000	4.238020000
C	-0.662694000	10.051719000	8.683046000
H	-0.782709000	11.021739000	9.142047000
C	3.103008000	6.500757000	2.641962000
H	3.073773000	5.479096000	2.278053000
C	3.934184000	7.485688000	1.992805000
H	4.535024000	7.199863000	1.135094000
C	-2.551040000	7.054798000	9.975755000
H	-3.252424000	6.683346000	10.716335000
C	-2.174289000	8.370751000	9.969574000
H	-2.564458000	9.073025000	10.700692000
C	4.964379000	13.022003000	7.706879000
H	4.939225000	14.115381000	7.665685000
H	5.710862000	12.687517000	6.978400000
H	5.258434000	12.693846000	8.705462000
C	-0.503336000	13.218933000	6.629717000
C	-1.613436000	14.259506000	6.524841000
H	-1.979861000	14.343665000	5.500187000
H	-1.237537000	15.230124000	6.864165000
H	-2.438042000	13.981820000	7.189682000

{Zn^{II}-L1$^{\bullet}$} for **1b** (*S*=1/2)

Zn	1.357764000	11.614479000	6.755332000
O	2.986320000	11.589568000	8.148521000

O	3.167185000	12.746222000	6.268265000
N	2.349273000	8.164426000	4.186615000
N	-0.724662000	7.947751000	8.060740000
O	-0.127967000	12.548738000	5.524258000
N	0.171885000	9.934713000	7.598483000
N	2.041774000	10.050633000	5.332660000
C	-1.097708000	6.620708000	8.091540000
H	-0.667059000	5.972894000	7.339848000
C	1.684320000	8.746527000	5.264732000
O	-0.062423000	12.990627000	7.693675000
C	3.143219000	9.162614000	3.587303000
C	3.642337000	12.362590000	7.382922000
C	3.927225000	8.826395000	2.462448000
H	4.536097000	9.598733000	2.005241000
C	-1.225431000	8.871222000	9.000095000
C	0.811371000	8.051629000	6.122614000
H	0.651525000	6.997570000	5.936589000
C	0.133583000	8.639182000	7.207179000
C	-1.969515000	6.188911000	9.046006000
H	-2.253818000	5.143035000	9.059803000
C	2.914447000	10.314303000	4.342626000
H	3.345077000	11.299269000	4.234341000
C	2.323939000	6.877122000	3.693322000
H	1.685755000	6.168726000	4.204204000
C	-0.636141000	10.091303000	8.663225000
H	-0.768303000	11.062840000	9.117090000
C	3.082484000	6.557824000	2.606986000
H	3.052781000	5.542462000	2.228786000
C	3.902114000	7.543634000	1.974295000
H	4.498322000	7.271187000	1.110541000
C	-2.499447000	7.097307000	10.014471000
H	-3.191214000	6.735397000	10.766962000
C	-2.128257000	8.418616000	9.986484000
H	-2.509891000	9.133571000	10.707228000
C	5.005103000	12.863435000	7.821207000
H	4.889754000	13.864071000	8.251895000
H	5.674234000	12.948810000	6.961963000
H	5.434824000	12.207638000	8.580084000
C	-0.567535000	13.170443000	6.541197000
C	-1.695675000	14.169885000	6.372788000
H	-2.248455000	13.981200000	5.451176000
H	-1.268242000	15.177254000	6.322422000
H	-2.364403000	14.138362000	7.236108000

1b, {Zn^{II}-(μ-(L1)$_2$)-Zn^{II}} (*S*=0)

Zn	1.370680000	11.601105000	6.713304000
O	3.019794000	11.324637000	8.166261000
O	3.087695000	12.966563000	6.689254000

N	2.053624000	8.141715000	4.166700000
N	-0.706027000	7.952128000	7.880877000
O	0.090045000	12.666616000	5.387582000
N	0.169604000	9.953670000	7.559732000
N	1.997828000	10.072046000	5.246529000
C	-0.978575000	6.592666000	7.905455000
H	-0.251299000	5.946331000	7.432698000
C	1.854778000	8.751353000	5.381237000
O	-0.054687000	13.017756000	7.568895000
C	2.334669000	9.158588000	3.226871000
C	3.563255000	12.391447000	7.701524000
C	2.575191000	8.795325000	1.876148000
H	2.790838000	9.580638000	1.159862000
C	-1.588579000	8.893929000	8.456780000
C	1.545158000	8.038155000	6.670572000
H	1.329550000	6.991169000	6.447313000
C	0.347848000	8.650063000	7.347180000
C	-2.120637000	6.159279000	8.503726000
H	-2.323146000	5.094531000	8.520575000
C	2.288131000	10.343273000	3.944595000
H	2.423345000	11.354428000	3.592597000
C	1.998258000	6.803796000	3.794452000
H	1.761673000	6.075397000	4.563362000
C	-1.001007000	10.129315000	8.232482000
H	-1.342299000	11.118494000	8.496563000
C	2.230050000	6.477736000	2.493854000
H	2.184933000	5.431861000	2.212359000
C	2.526112000	7.477984000	1.513777000
H	2.706706000	7.183079000	0.485636000
C	-3.038219000	7.080886000	9.103304000
H	-3.940394000	6.706110000	9.574497000
C	-2.774967000	8.422660000	9.077255000
H	-3.449991000	9.147475000	9.519215000
C	4.781170000	12.953775000	8.406356000
H	4.466771000	13.388623000	9.360992000
H	5.255702000	13.729077000	7.804099000
H	5.493906000	12.156090000	8.634175000
C	-0.414198000	13.284497000	6.378970000
C	-1.432486000	14.377863000	6.130095000
H	-2.015158000	14.163780000	5.232049000
H	-0.898838000	15.321133000	5.969569000
H	-2.087091000	14.500841000	6.994774000
N	2.303970000	7.934567000	10.150564000
N	5.063551000	8.124029000	6.436326000
N	4.187934000	6.122504000	6.757605000
N	2.359690000	6.004208000	9.070781000
C	5.336093000	9.483491000	6.411664000
H	4.608816000	10.129851000	6.884386000
C	2.502770000	7.324895000	8.936037000

C	2.022916000	6.917723000	11.090423000
C	1.782435000	7.281025000	12.441144000
H	1.566779000	6.495735000	13.157453000
C	5.946104000	7.182198000	5.860478000
C	2.812386000	8.038060000	7.646683000
H	3.028011000	9.085047000	7.869917000
C	4.009687000	7.426122000	6.970082000
C	6.478147000	9.916847000	5.813356000
H	6.680655000	10.981595000	5.796445000
C	2.069398000	5.733021000	10.372727000
H	1.934161000	4.721879000	10.724750000
C	2.359389000	9.272491000	10.522782000
H	2.595984000	10.000868000	9.753855000
C	5.358549000	5.946820000	6.084873000
H	5.699855000	4.957624000	5.820872000
C	2.127634000	9.598589000	11.823377000
H	2.172790000	10.644468000	12.104847000
C	1.831561000	8.598372000	12.803484000
H	1.650996000	8.893306000	13.831622000
C	7.395726000	8.995208000	5.213823000
H	8.297894000	9.369960000	4.742595000
C	7.132481000	7.653435000	5.239957000
H	7.807503000	6.928594000	4.798035000
Zn	2.986813000	4.475114000	7.604060000
O	1.337798000	4.751617000	6.150960000
O	1.269839000	3.109624000	7.627888000
O	4.267263000	3.409557000	8.929923000
O	4.412248000	3.058418000	6.748626000
C	0.794347000	3.684759000	6.615595000
C	-0.423475000	3.122402000	5.910626000
H	-0.108959000	2.687576000	4.956019000
H	-0.898045000	2.347076000	6.512822000
H	-1.136213000	3.920067000	5.682743000
C	4.771600000	2.791658000	7.938594000
C	5.789795000	1.698231000	8.187587000
H	6.372269000	1.912194000	9.085789000
H	5.256078000	0.754960000	8.347875000
H	6.444593000	1.575329000	7.323042000

{Cu^{II}-L4^{-}} for **1c** (*S*=1/2)

Cu	3.944204000	3.442572000	9.178226000
O	1.414912000	5.539560000	9.229478000
O	3.127681000	2.946376000	7.429486000
N	5.564929000	2.205698000	9.022691000
O	1.905105000	1.756867000	8.886513000
N	4.184475000	3.629473000	11.141013000
C	6.479700000	2.059999000	9.975697000
C	6.244607000	3.145915000	14.170575000

H	6.802541000	2.267280000	13.865073000
C	4.619357000	4.872705000	13.680937000
C	5.397789000	3.777535000	13.247419000
C	7.718217000	1.256385000	9.679772000
C	8.116606000	1.088857000	8.336229000
C	6.360477000	3.611464000	15.479946000
H	7.023162000	3.104863000	16.177103000
C	9.291333000	0.393182000	8.039536000
H	9.585381000	0.274291000	6.998640000
C	5.758706000	1.493131000	7.760389000
H	5.525827000	0.421638000	7.883337000
H	5.046171000	1.900080000	7.042445000
C	5.285634000	3.335193000	11.814066000
C	6.384834000	2.637370000	11.260789000
C	3.091704000	4.321208000	11.830832000
H	2.391158000	4.693477000	11.080201000
H	2.547170000	3.602619000	12.465032000
C	8.496337000	0.664512000	10.687016000
H	8.170013000	0.733147000	11.718937000
C	9.665598000	-0.031277000	10.382258000
H	10.250420000	-0.480048000	11.181220000
C	10.073957000	-0.159740000	9.053743000
H	10.982618000	-0.703604000	8.807613000
C	1.231716000	1.785618000	6.572987000
H	0.664744000	2.668345000	6.258100000
H	0.534825000	1.000139000	6.872880000
H	1.825719000	1.455735000	5.714725000
C	4.745977000	5.334950000	14.993484000
H	4.141583000	6.180731000	15.314703000
C	2.141668000	2.169292000	7.740717000
C	3.635369000	5.456341000	12.699312000
H	2.824576000	5.974672000	13.224827000
H	4.124518000	6.190124000	12.043143000
C	7.201311000	1.636896000	7.271738000
H	7.409310000	2.702032000	7.091814000
H	7.352365000	1.109708000	6.321778000
C	5.617024000	4.718258000	15.892601000
H	5.699221000	5.086335000	16.912393000
O	3.638988000	5.386431000	8.845950000
C	2.498742000	7.248681000	7.931792000
H	2.654808000	7.007886000	6.874140000
H	3.332673000	7.885348000	8.243993000
H	1.553370000	7.785402000	8.041851000
C	2.479990000	5.944689000	8.746381000
H	7.272522000	2.585634000	11.872851000

{Cu^{II}-L4$^{•}$} for **1c** (*S*=1)

Cu	3.514597000	3.164273000	9.101336000

O	3.054150000	5.783140000	9.260940000
O	2.683447000	2.632176000	7.307232000
N	5.246991000	1.703595000	9.160777000
O	1.700007000	2.150656000	9.207136000
N	3.789004000	3.424094000	11.084752000
C	6.277556000	1.997745000	9.923596000
C	5.977146000	3.226419000	14.053565000
H	6.650853000	2.437251000	13.735332000
C	4.095902000	4.702427000	13.620133000
C	5.009496000	3.726133000	13.168210000
C	7.665667000	1.589028000	9.542831000
C	7.930309000	1.379514000	8.173219000
C	6.066345000	3.711424000	15.356573000
H	6.816438000	3.311780000	16.032170000
C	9.218588000	1.027908000	7.767568000
H	9.418367000	0.873786000	6.710299000
C	5.504332000	1.023263000	7.891902000
H	5.590137000	-0.055921000	8.100091000
H	4.626674000	1.170614000	7.259404000
C	4.912132000	3.274274000	11.746768000
C	6.100552000	2.736104000	11.138294000
C	2.619037000	3.970954000	11.783010000
H	1.894042000	4.269308000	11.028196000
H	2.179680000	3.166092000	12.390686000
C	8.694717000	1.399904000	10.477367000
H	8.498615000	1.509457000	11.539360000
C	9.975151000	1.039078000	10.061893000
H	10.760520000	0.892047000	10.797129000
C	10.240856000	0.862748000	8.703012000
H	11.237555000	0.583732000	8.373712000
C	0.527644000	1.548654000	7.178251000
H	-0.130420000	2.366129000	6.864400000
H	-0.040096000	0.865790000	7.812107000
H	0.878278000	1.038801000	6.278192000
C	4.203393000	5.188772000	14.923928000
H	3.502381000	5.945327000	15.266667000
C	1.693675000	2.128755000	7.935864000
C	3.021165000	5.151551000	12.663112000
H	2.149234000	5.530420000	13.205632000
H	3.376881000	5.959866000	12.010416000
C	6.777313000	1.532547000	7.214183000
H	6.633262000	2.589517000	6.951072000
H	6.963220000	0.984865000	6.284740000
C	5.185569000	4.704249000	15.788963000
H	5.251843000	5.088169000	16.802812000
O	4.779230000	4.569389000	8.508192000
C	4.897653000	6.928693000	8.206002000
H	4.862627000	6.942410000	7.111530000
H	5.951111000	6.897589000	8.497388000

H	4.424058000	7.833691000	8.589269000
C	4.165527000	5.692301000	8.711638000
H	7.009231000	2.943487000	11.687520000

1c, {Cu^{II}-(μ-(L4)$_2$)-Cu^{II}} (*S*=1)

Cu	4.141345000	3.772433000	9.145541000
O	2.875594000	5.305596000	9.099433000
O	3.343749000	3.138802000	7.425243000
N	5.824616000	2.565569000	9.040280000
O	2.354068000	2.112413000	9.134277000
N	4.462244000	3.926538000	11.164609000
C	6.761059000	2.479170000	9.925214000
C	6.640089000	3.194239000	14.061507000
H	7.532199000	2.792092000	13.600143000
C	4.451754000	4.255152000	13.995655000
C	5.569003000	3.713157000	13.313650000
C	7.773348000	1.388942000	9.868600000
C	7.989937000	0.747479000	8.625086000
C	6.602174000	3.204139000	15.455243000
H	7.444819000	2.798401000	16.005359000
C	8.920823000	-0.285276000	8.532192000
H	9.083663000	-0.767227000	7.571722000
C	5.780844000	1.579086000	7.941904000
H	5.255134000	0.690871000	8.320435000
H	5.164756000	2.009670000	7.154411000
C	5.551166000	3.731359000	11.826543000
C	6.859264000	3.540806000	11.041344000
C	3.178381000	4.069654000	11.877367000
H	2.485577000	4.561414000	11.195580000
H	2.800964000	3.055759000	12.064595000
C	8.481416000	0.945611000	10.996675000
H	8.353782000	1.401502000	11.969467000
C	9.392709000	-0.104475000	10.892710000
H	9.922540000	-0.435364000	11.779725000
C	9.622401000	-0.715143000	9.660777000
H	10.336647000	-1.529332000	9.577753000
C	1.415161000	1.811758000	6.928162000
H	0.748062000	2.618375000	6.606193000
H	0.823351000	1.022041000	7.392996000
H	1.921645000	1.432968000	6.036180000
C	4.432415000	4.262415000	15.389207000
H	3.571587000	4.681431000	15.903916000
C	2.423342000	2.370509000	7.915720000
C	3.335661000	4.847880000	13.175153000
H	2.393018000	4.838444000	13.731643000
H	3.560731000	5.899898000	12.947333000
C	7.173798000	1.215290000	7.451522000
H	7.638537000	2.092315000	6.980828000

H	7.107636000	0.436884000	6.684806000
C	5.499347000	3.736289000	16.122099000
H	5.466596000	3.744246000	17.207923000
O	4.610028000	6.111380000	7.944265000
C	2.502987000	7.276210000	7.815201000
H	1.823040000	6.858765000	7.065042000
H	3.083031000	8.078912000	7.356341000
H	1.888096000	7.664468000	8.631421000
C	3.417385000	6.167643000	8.313406000
N	8.400682000	5.903487000	12.454133000
N	9.762058000	4.541567000	10.329711000
C	7.463631000	5.989514000	11.569807000
C	7.583798000	5.275463000	7.433536000
H	6.691910000	5.677728000	7.895224000
C	9.771851000	4.213930000	7.498548000
C	8.654901000	4.755992000	8.180984000
C	6.450776000	7.079187000	11.627254000
C	6.234613000	7.720287000	12.871035000
C	7.621390000	5.266023000	6.039792000
H	6.778719000	5.672165000	5.490016000
C	5.303117000	8.752414000	12.964750000
H	5.140615000	9.234079000	13.925421000
C	8.444677000	6.889957000	13.552518000
H	8.969461000	7.778560000	13.173601000
H	9.061683000	6.459788000	14.339514000
C	8.673056000	4.737307000	9.668081000
C	7.365181000	4.927969000	10.453605000
C	11.045733000	4.398140000	9.616682000
H	11.738392000	3.905759000	10.298177000
H	11.423642000	5.411928000	9.429900000
C	5.741644000	7.522261000	10.499752000
H	5.868890000	7.066684000	9.526757000
C	4.829732000	8.571731000	10.604527000
H	4.299095000	8.902417000	9.717919000
C	4.600482000	9.182029000	11.836722000
H	3.885765000	9.995741000	11.920385000
C	9.790885000	4.207153000	6.104987000
H	10.651490000	3.788088000	5.589945000
C	10.887935000	3.620536000	8.318588000
H	11.830469000	3.629926000	7.761912000
H	10.662604000	2.568482000	8.545994000
C	7.051844000	7.252786000	14.043959000
H	6.587986000	6.375376000	14.514803000
H	7.118046000	8.031096000	14.810769000
C	8.723929000	4.733809000	5.372510000
H	8.756434000	4.726208000	4.286677000
Cu	10.083868000	4.696430000	12.348500000
O	11.349056000	3.162697000	12.395174000
O	10.882632000	5.331267000	14.067814000

O	11.871788000	6.355758000	12.357337000
C	12.811902000	6.658107000	14.562716000
H	13.477613000	5.851172000	14.886728000
H	13.405004000	7.445933000	14.096332000
H	12.305732000	7.039666000	15.453709000
C	11.803057000	6.098786000	13.576163000
O	9.613878000	2.358963000	13.550578000
C	11.719784000	1.192060000	13.679928000
H	12.400741000	1.609186000	14.429344000
H	11.139017000	0.390405000	14.139697000
H	12.333677000	0.802447000	12.863599000
C	10.806483000	2.301392000	13.181434000
H	7.632576000	3.222885000	11.734337000
H	6.591782000	5.246006000	9.760772000

3^{-}, {Ru^{II}-L3^{-}} (*S*=0)

Ru	0.242596000	18.290121000	6.794500000
O	-0.781906000	18.370118000	4.972294000
O	1.266754000	18.173884000	8.618037000
O	1.521556000	16.763326000	6.063570000
O	-1.073169000	16.738943000	7.393680000
N	2.444195000	21.735127000	5.657574000
N	1.555274000	19.776404000	6.186721000
N	-1.008174000	19.786169000	7.520869000
N	-1.960147000	21.753512000	7.892335000
C	2.781288000	23.074912000	5.574178000
H	2.023447000	23.779754000	5.881176000
C	-2.103213000	19.573805000	8.308698000
H	-2.377484000	18.575113000	8.609576000
C	3.443250000	20.734296000	5.434261000
C	4.712098000	21.137136000	4.949951000
H	5.447219000	20.365213000	4.737071000
C	5.000871000	22.465730000	4.778464000
H	5.971279000	22.780907000	4.406001000
C	2.845007000	19.550969000	5.798446000
H	3.241877000	18.547624000	5.786705000
C	4.012734000	23.450840000	5.132766000
H	4.244808000	24.509927000	5.074523000
C	-4.186101000	22.508304000	9.415985000
H	-5.061384000	22.833274000	9.970960000
C	-2.211665000	23.096212000	8.116600000
H	-1.502454000	23.793676000	7.697140000
C	0.065486000	21.771655000	6.430674000
C	1.284003000	21.107857000	6.110519000
C	-2.746999000	20.762045000	8.560388000
C	-0.905499000	21.115232000	7.239348000
C	-3.297229000	23.483908000	8.839917000
H	-3.468528000	24.544822000	8.994974000

C	-3.892020000	21.176493000	9.284507000
H	-4.511234000	20.410807000	9.744846000
C	-0.554257000	17.584448000	4.004818000
C	-0.926222000	16.080410000	8.470212000
C	-1.467279000	17.789205000	2.801492000
H	-2.511571000	17.661238000	3.110846000
H	-1.251718000	17.096867000	1.981506000
H	-1.365183000	18.817572000	2.434703000
C	1.020759000	17.308529000	9.511197000
C	1.935396000	17.383483000	10.728157000
H	2.977324000	17.259321000	10.409148000
H	1.701612000	16.625328000	11.482351000
H	1.856712000	18.376823000	11.185982000
C	0.427338000	16.569608000	3.933359000
H	0.459063000	15.994227000	3.013319000
C	0.019447000	16.311636000	9.489278000
H	-0.022233000	15.649993000	10.348972000
C	1.370514000	16.226889000	4.920908000
C	-1.906887000	14.925686000	8.644949000
H	-2.934317000	15.295460000	8.542774000
H	-1.803199000	14.421927000	9.611301000
H	-1.752194000	14.190733000	7.845177000
C	2.346316000	15.093975000	4.621979000
H	3.376103000	15.465962000	4.692028000
H	2.196552000	14.653354000	3.631221000
H	2.238560000	14.308988000	5.380413000
C	-0.334364000	23.010197000	5.644527000
H	-1.415519000	23.012610000	5.455261000
H	-0.101127000	23.995349000	6.094185000
H	0.145297000	23.007878000	4.657275000

3, {Ru^{II}-L3$^{•}$} (*S*=1/2)

Ru	0.264320000	18.320494000	6.868466000
O	-0.757031000	18.451409000	5.068167000
O	1.281851000	18.121939000	8.676740000
O	1.507173000	16.810405000	6.117136000
O	-1.069715000	16.800496000	7.429576000
N	2.433942000	21.718367000	5.625812000
N	1.565422000	19.776748000	6.281297000
N	-0.957143000	19.803516000	7.592441000
N	-1.986416000	21.759333000	7.859501000
C	2.745263000	23.049490000	5.409753000
H	1.970519000	23.771838000	5.609007000
C	-2.019822000	19.600794000	8.413975000
H	-2.255204000	18.617832000	8.788001000
C	3.442616000	20.729064000	5.513649000
C	4.728377000	21.101391000	5.048264000
H	5.478999000	20.325381000	4.937603000

C	5.000337000	22.413193000	4.767463000
H	5.980890000	22.711462000	4.411164000
C	2.862852000	19.551858000	5.942406000
H	3.283091000	18.560646000	6.003144000
C	3.987333000	23.402857000	4.976390000
H	4.199700000	24.453073000	4.808990000
C	-4.206418000	22.499353000	9.388205000
H	-5.075665000	22.815211000	9.955623000
C	-2.327047000	23.096757000	7.968258000
H	-1.690337000	23.806900000	7.466599000
C	0.031158000	21.735277000	6.363208000
C	1.274886000	21.096622000	6.101250000
C	-2.697976000	20.788052000	8.605489000
C	-0.917716000	21.116239000	7.227416000
C	-3.414551000	23.471598000	8.697622000
H	-3.658900000	24.526363000	8.760012000
C	-3.838204000	21.181619000	9.348671000
H	-4.389042000	20.417217000	9.887352000
C	-0.537390000	17.688961000	4.070868000
C	-0.923308000	16.068607000	8.462693000
C	-1.463212000	17.925813000	2.890638000
H	-2.497637000	17.729690000	3.196466000
H	-1.221501000	17.294031000	2.031926000
H	-1.411146000	18.977741000	2.587534000
C	1.052528000	17.207010000	9.531522000
C	1.993670000	17.214760000	10.723475000
H	3.021651000	17.060731000	10.374916000
H	1.748500000	16.443566000	11.458428000
H	1.962709000	18.196668000	11.209252000
C	0.440778000	16.680271000	3.971743000
H	0.470560000	16.127970000	3.039242000
C	0.043347000	16.224362000	9.473729000
H	0.009770000	15.515330000	10.293230000
C	1.372446000	16.300972000	4.956385000
C	-1.922452000	14.930010000	8.577415000
H	-2.942271000	15.322553000	8.494248000
H	-1.824944000	14.376346000	9.515083000
H	-1.778653000	14.236745000	7.740024000
C	2.338220000	15.169651000	4.648574000
H	3.369471000	15.519240000	4.776146000
H	2.218669000	14.776302000	3.635634000
H	2.185858000	14.355732000	5.367017000
C	-0.350514000	22.984979000	5.592012000
H	-1.427912000	22.997087000	5.399145000
H	-0.099019000	23.941438000	6.077163000
H	0.135693000	22.986448000	4.611433000

3^{+}, {Ru^{III}-L3$^{\bullet}$} (*S*=1)

Ru	0.247381000	18.367705000	6.807282000
O	-0.733644000	18.451922000	5.031352000
O	1.234640000	18.261193000	8.581310000
O	1.478108000	16.899109000	6.070858000
O	-1.032989000	16.893612000	7.439711000
N	2.518253000	21.817561000	5.778713000
N	1.573347000	19.869483000	6.252060000
N	-1.015884000	19.887019000	7.478953000
N	-2.031391000	21.837657000	7.782702000
C	2.877356000	23.152241000	5.671802000
H	2.129641000	23.886239000	5.922415000
C	-2.157741000	19.646509000	8.160834000
H	-2.450774000	18.645168000	8.432560000
C	3.487673000	20.812196000	5.587664000
C	4.795256000	21.163628000	5.177856000
H	5.517737000	20.370832000	5.015973000
C	5.119150000	22.483968000	5.012062000
H	6.115923000	22.774509000	4.698920000
C	2.855240000	19.618566000	5.901465000
H	3.244523000	18.612777000	5.881647000
C	4.140367000	23.487019000	5.285454000
H	4.394587000	24.537977000	5.205745000
C	-4.379317000	22.517570000	9.133109000
H	-5.293233000	22.812520000	9.636880000
C	-2.363046000	23.173580000	7.945469000
H	-1.670572000	23.904830000	7.563584000
C	0.090693000	21.865326000	6.436115000
C	1.329148000	21.205072000	6.177428000
C	-2.829707000	20.840713000	8.376457000
C	-0.918064000	21.218800000	7.207285000
C	-3.513232000	23.514963000	8.591696000
H	-3.750089000	24.567054000	8.703337000
C	-4.028276000	21.196951000	9.037048000
H	-4.637206000	20.408513000	9.466297000
C	-0.743067000	17.493590000	4.173671000
C	-0.735839000	16.036976000	8.349146000
C	-1.753802000	17.660218000	3.064433000
H	-2.756834000	17.746142000	3.497178000
H	-1.737924000	16.827912000	2.357755000
H	-1.554907000	18.592299000	2.523403000
C	1.231667000	17.224336000	9.341105000
C	2.250883000	17.262805000	10.454263000
H	3.251876000	17.389511000	10.027126000
H	2.233065000	16.359177000	11.067046000
H	2.061445000	18.132322000	11.093917000
C	0.109280000	16.377982000	4.181490000
H	-0.008435000	15.668459000	3.371646000
C	0.355038000	16.132246000	9.230610000
H	0.465992000	15.339133000	9.959937000

C	1.181817000	16.160501000	5.064262000
C	-1.700921000	14.880998000	8.468215000
H	-2.702277000	15.258806000	8.705471000
H	-1.400766000	14.166133000	9.237068000
H	-1.774234000	14.366021000	7.503945000
C	2.125284000	15.004053000	4.830955000
H	3.128439000	15.387232000	4.609347000
H	1.803778000	14.364006000	4.006745000
H	2.204852000	14.405949000	5.745123000
C	-0.216161000	23.174649000	5.733955000
H	-1.279152000	23.231110000	5.482470000
H	0.032846000	24.079719000	6.306447000
H	0.325655000	23.230744000	4.785816000

[3-H**]$^{+}$, {Ru^{III}-HL3}$^{+}$** (*S*=1/2)

Ru	4.352226000	12.112250000	3.568661000
O	6.160941000	12.311959000	2.653638000
O	2.543796000	11.931525000	4.475187000
O	4.681146000	13.862125000	4.571323000
O	3.455423000	13.181077000	2.070124000
N	6.296007000	9.324542000	6.128165000
N	3.962255000	8.173437000	2.039869000
N	3.953452000	10.299644000	2.598258000
N	5.290698000	10.972249000	5.071348000
C	6.180461000	10.394514000	7.041281000
C	6.905416000	8.131567000	6.492363000
H	6.972795000	7.364016000	5.733669000
C	4.557319000	9.127856000	2.818748000
C	7.384390000	7.987811000	7.756695000
H	7.857246000	7.051843000	8.030685000
C	5.548998000	11.406001000	6.339974000
H	5.279970000	12.396827000	6.665381000
C	5.745837000	8.868502000	3.701254000
H	5.662554000	7.826424000	4.035542000
C	2.924430000	8.793083000	1.307770000
C	7.892390000	13.384108000	1.470817000
H	8.458764000	13.553735000	2.391994000
H	8.083278000	14.202077000	0.774878000
H	8.261220000	12.451303000	1.031024000
C	0.459473000	12.603132000	5.336454000
H	-0.067142000	12.215528000	4.458684000
H	-0.074218000	13.472748000	5.722254000
H	0.448774000	11.811761000	6.093185000
C	6.427213000	13.243247000	1.803862000
C	2.952193000	10.122669000	1.686884000
H	2.327381000	10.942711000	1.372510000
C	7.082798000	9.021061000	2.920840000
H	7.095927000	8.362137000	2.047394000

H	7.931965000	8.760326000	3.559591000
H	7.194696000	10.055688000	2.591284000
C	4.233858000	6.819286000	1.895218000
H	5.054661000	6.419752000	2.474953000
C	5.485969000	14.067071000	1.170395000
H	5.869705000	14.786195000	0.457791000
C	5.733804000	9.717839000	4.943106000
C	6.684554000	10.229550000	8.357912000
H	6.589413000	11.052958000	9.056935000
C	7.275074000	9.048240000	8.711838000
H	7.666448000	8.906526000	9.712807000
C	2.143011000	8.002876000	0.424164000
H	1.345390000	8.482503000	-0.132149000
C	3.476742000	6.076162000	1.045227000
H	3.697153000	5.020144000	0.940481000
C	3.202763000	14.807161000	0.387138000
H	2.611519000	14.150941000	-0.260445000
H	3.774618000	15.496126000	-0.235867000
H	2.495942000	15.373596000	1.001335000
C	3.742886000	14.599665000	5.045410000
C	2.411013000	6.668689000	0.294855000
H	1.824220000	6.051575000	-0.375974000
C	2.401840000	14.207425000	5.200970000
H	1.726834000	14.932525000	5.637935000
C	4.186463000	15.968954000	5.500203000
H	4.971499000	15.868202000	6.256739000
H	3.365539000	16.557123000	5.912466000
H	4.626917000	16.506903000	4.654476000
C	4.085956000	13.968784000	1.279493000
C	1.886287000	12.922635000	4.963533000

B. *Optimized Cartesian coordinates using M06-L density functional for the transition state analysis and free energy calculation.*

L1• (*S*=1/2)

Zero-point correction= 0.230748 (Hartree/Particle)
Thermal correction to Energy= 0.244613
Thermal correction to Enthalpy= 0.245557
Thermal correction to Gibbs Free Energy= 0.187974
Sum of electronic and zero-point Energies= -796.882866
Sum of electronic and thermal Energies= -796.869001
Sum of electronic and thermal Enthalpies= -796.868057
Sum of electronic and thermal Free Energies= -796.925640

Cartesian Coordinates

N	1.520908000	-1.821421000	0.160784000
N	2.450321000	0.215941000	-0.003473000
N	-2.450320000	0.215939000	0.003483000
C	-2.853076000	-1.952646000	-0.183573000
H	-3.326821000	-2.921520000	-0.274519000
C	-4.822226000	-0.251242000	-0.054093000
H	-5.627976000	-0.974815000	-0.124999000
C	2.702345000	1.559658000	-0.132663000
H	1.840246000	2.210336000	-0.212104000
C	-5.074689000	1.093744000	0.066261000
H	-6.094221000	1.462887000	0.091799000
C	1.252024000	-0.507032000	0.047346000
C	-3.498903000	-0.717384000	-0.084975000
C	4.822225000	-0.251245000	0.054090000
H	5.627974000	-0.974820000	0.124998000
C	-3.988837000	2.007446000	0.162598000
H	-4.168186000	3.071582000	0.265344000
C	3.988841000	2.007444000	-0.162599000
H	4.168192000	3.071580000	-0.265340000
C	0.000000000	0.129111000	-0.000010000
C	3.498901000	-0.717383000	0.084989000
C	-2.702342000	1.559656000	0.132676000
H	-1.840242000	2.210329000	0.212148000
C	5.074692000	1.093739000	-0.066275000
H	6.094224000	1.462878000	-0.091831000
C	2.853072000	-1.952645000	0.183578000
H	3.326816000	-2.921519000	0.274528000
N	-1.520911000	-1.821423000	-0.160789000
C	-1.252025000	-0.507036000	-0.047353000
H	-0.000002000	1.214721000	-0.000042000

[L1$^{\bullet}$. . . L1$^{\bullet}$]$^{\neq}$ (*S*=1)

Zero-point correction= 0.462788 (Hartree/Particle)
Thermal correction to Energy= 0.490921
Thermal correction to Enthalpy= 0.491865
Thermal correction to Gibbs Free Energy= 0.403431
Sum of electronic and zero-point Energies= -1593.735621
Sum of electronic and thermal Energies= -1593.707488
Sum of electronic and thermal Enthalpies= -1593.706544
Sum of electronic and thermal Free Energies= -1593.794978

Cartesian Coordinates

N	2.377617000	9.101924000	4.570909000
N	-0.446067000	7.245667000	8.084274000
N	-0.691327000	9.435499000	7.697995000
N	1.712683000	10.616145000	6.097804000
C	-0.025776000	5.934235000	8.089213000
H	0.870540000	5.696290000	7.520832000
C	1.642948000	9.328618000	5.734544000
C	2.902161000	10.319236000	4.154373000
C	3.666004000	10.401445000	3.001354000
H	4.054678000	11.358513000	2.676148000
C	-1.542353000	7.680431000	8.848425000
C	1.197038000	8.238751000	6.551906000
H	1.237255000	7.272603000	6.047786000
C	0.032276000	8.356204000	7.403562000
C	-0.702064000	5.028898000	8.849681000
H	-0.354836000	4.002379000	8.859038000
C	2.455878000	11.224067000	5.153411000
H	2.662870000	12.286470000	5.193684000
C	2.559438000	7.918959000	3.839350000
H	2.123522000	7.013392000	4.237159000
C	-1.644909000	9.041375000	8.566133000
H	-2.377261000	9.733870000	8.958543000
C	3.367520000	7.993712000	2.694683000
H	3.548382000	7.073427000	2.147333000
C	3.914789000	9.181797000	2.263053000
H	4.527862000	9.209133000	1.368884000
C	-1.814185000	5.427079000	9.640090000
H	-2.333105000	4.691459000	10.246196000
C	-2.223862000	6.735638000	9.639516000
H	-3.068196000	7.067469000	10.234930000
N	1.934316000	8.654084000	9.801608000
N	4.672179000	7.218442000	6.095742000

N	3.175846000	5.670840000	6.680654000
N	2.532435000	6.500511000	9.661965000
C	5.387412000	8.381830000	5.925520000
H	5.041162000	9.250477000	6.472909000
C	2.473139000	7.657487000	8.998875000
C	1.652702000	8.065871000	11.044112000
C	1.103839000	8.872412000	12.057022000
H	0.879343000	8.421716000	13.018246000
C	5.017168000	6.034930000	5.418554000
C	2.846919000	7.935437000	7.631940000
H	3.260796000	8.939388000	7.522449000
C	3.564744000	6.932211000	6.872850000
C	6.455043000	8.391534000	5.080223000
H	6.997698000	9.319477000	4.940315000
C	2.044476000	6.733220000	10.894392000
H	1.992449000	5.953678000	11.642779000
C	1.679808000	9.980807000	9.542910000
H	1.847469000	10.330508000	8.526644000
C	4.052236000	5.113545000	5.817664000
H	3.967107000	4.082053000	5.504273000
C	1.163533000	10.756365000	10.537825000
H	0.950182000	11.796646000	10.322755000
C	0.868882000	10.202450000	11.812352000
H	0.445381000	10.834073000	12.586464000
C	6.847200000	7.211806000	4.392634000
H	7.705908000	7.236342000	3.730613000
C	6.134697000	6.051872000	4.563524000
H	6.408952000	5.136210000	4.049722000

(L1)$_2$ (*S*=0)

Zero-point correction= 0.470093 (Hartree/Particle)
Thermal correction to Energy= 0.496396
Thermal correction to Enthalpy= 0.497340
Thermal correction to Gibbs Free Energy= 0.414554
Sum of electronic and zero-point Energies= -1593.819259
Sum of electronic and thermal Energies= -1593.792957
Sum of electronic and thermal Enthalpies= -1593.792012
Sum of electronic and thermal Free Energies= -1593.874798

Cartesian Coordinates

N	-2.390345000	1.562911000	0.258194000
N	2.390524000	1.562850000	0.256023000
N	1.498703000	1.590344000	-1.785118000
N	-1.500652000	1.589990000	-1.783878000
C	2.639667000	1.407047000	1.602857000

H	1.819767000	1.041277000	2.209175000
C	-1.253685000	1.366163000	-0.500998000
C	-3.409652000	1.959931000	-0.633655000
C	-4.698327000	2.205777000	-0.116342000
H	-5.481816000	2.506124000	-0.804766000
C	3.408857000	1.960155000	-0.636812000
C	-0.000049000	0.794379000	0.075480000
H	0.000366000	0.971321000	1.158931000
C	1.253078000	1.366198000	-0.502033000
C	3.888060000	1.649730000	2.085560000
H	4.068332000	1.508103000	3.145142000
C	-2.797834000	1.966433000	-1.878397000
H	-3.249505000	2.217901000	-2.828526000
C	-2.637969000	1.407623000	1.605355000
H	-1.817379000	1.042119000	2.210883000
C	2.795765000	1.966821000	-1.880930000
H	3.246419000	2.218530000	-2.831477000
C	-3.885812000	1.650486000	2.089375000
H	-4.064889000	1.509299000	3.149217000
C	-4.938966000	2.055411000	1.222523000
H	-5.929091000	2.235470000	1.627706000
C	4.940211000	2.055123000	1.217704000
H	5.930777000	2.235082000	1.621854000
C	4.698058000	2.205981000	-0.120833000
H	5.480741000	2.506670000	-0.810025000
N	2.390527000	-1.562880000	-0.256031000
N	-2.390358000	-1.562922000	-0.258193000
N	-1.500607000	-1.590140000	1.783846000
N	1.498752000	-1.590236000	1.785135000
C	-2.638011000	-1.407564000	-1.605346000
H	-1.817441000	-1.041997000	-2.210873000
C	1.253092000	-1.366220000	0.502030000
C	3.408892000	-1.960101000	0.636811000
C	4.698094000	-2.205913000	0.120824000
H	5.480803000	-2.506525000	0.810019000
C	-3.409640000	-1.959996000	0.633659000
C	-0.000046000	-0.794420000	-0.075490000
H	0.000344000	-0.971360000	-1.158941000
C	-1.253675000	-1.366215000	0.500979000
C	-3.885876000	-1.650370000	-2.089340000
H	-4.064981000	-1.509116000	-3.149167000
C	2.795804000	-1.966759000	1.880931000
H	3.246493000	-2.218389000	2.831483000
C	2.639655000	-1.407117000	-1.602868000
H	1.819726000	-1.041452000	-2.209199000
C	-2.797809000	-1.966506000	1.878394000
H	-3.249448000	-2.218023000	2.828525000
C	3.888046000	-1.649784000	-2.085581000
H	4.068301000	-1.508191000	-3.145172000

C	4.940221000	-2.055110000	-1.217725000
H	5.930778000	-2.235089000	-1.621886000
C	-4.939011000	-2.055327000	-1.222479000
H	-5.929159000	-2.235311000	-1.627640000
C	-4.698329000	-2.205803000	0.116365000
H	-5.481802000	-2.506185000	0.804792000

[L1$^{\bullet}$. . . ^{3}O$_2$]$^{\neq}$ (*S*=1/2)

Zero-point correction= 0.238781 (Hartree/Particle)
Thermal correction to Energy= 0.254413
Thermal correction to Enthalpy= 0.255357
Thermal correction to Gibbs Free Energy= 0.194074
Sum of electronic and zero-point Energies= -947.191260
Sum of electronic and thermal Energies= -947.175628
Sum of electronic and thermal Enthalpies= -947.174684
Sum of electronic and thermal Free Energies= -947.235967

Cartesian Coordinates

N	2.240654000	21.701507000	5.326315000
N	1.289960000	19.676094000	5.367873000
N	-1.218959000	19.512835000	7.067690000
N	-1.741276000	21.411793000	8.131136000
C	2.606851000	23.000878000	5.578465000
H	2.055831000	23.517034000	6.356648000
C	-2.387373000	19.339858000	7.705427000
H	-2.928605000	18.404552000	7.659229000
C	2.935127000	20.900586000	4.410724000
C	4.009735000	21.467540000	3.701806000
H	4.547433000	20.849495000	2.990335000
C	4.358618000	22.775299000	3.926159000
H	5.188083000	23.221756000	3.388133000
C	2.299267000	19.658378000	4.482854000
H	2.545841000	18.769521000	3.918308000
C	3.645021000	23.545026000	4.882172000
H	3.927295000	24.570969000	5.087761000
C	-3.857130000	22.170657000	9.726881000
H	-4.678651000	22.494064000	10.357224000
C	-1.734518000	22.671090000	8.679993000
H	-0.861567000	23.281623000	8.476772000
C	0.344035000	21.465278000	6.853311000
C	1.237498000	20.909508000	5.872179000
C	-2.769028000	20.496060000	8.390714000
C	-0.827052000	20.764562000	7.308197000
C	-2.782727000	23.059611000	9.461238000

H	-2.769643000	24.054978000	9.890120000
C	-3.843527000	20.903206000	9.201918000
H	-4.642714000	20.196797000	9.399876000
H	0.194030000	22.544190000	6.748151000
O	1.355469000	21.734596000	8.327037000
O	1.449019000	22.994054000	8.577429000

L1-O_2 (*S*=1/2)

Zero-point correction= 0.239436 (Hartree/Particle)
Thermal correction to Energy= 0.255390
Thermal correction to Enthalpy= 0.256335
Thermal correction to Gibbs Free Energy= 0.194189
Sum of electronic and zero-point Energies= -947.191741
Sum of electronic and thermal Energies= -947.175786
Sum of electronic and thermal Enthalpies= -947.174842
Sum of electronic and thermal Free Energies= -947.236988

Cartesian Coordinates

N	-2.447291000	-0.028100000	-0.138120000
N	-1.494766000	1.965223000	0.195799000
N	1.495340000	1.963921000	0.204078000
N	2.447090000	-0.028267000	-0.138962000
C	-2.698257000	-1.371808000	-0.291369000
H	-1.841315000	-2.033161000	-0.224519000
C	2.825772000	2.138217000	0.089075000
H	3.278219000	3.117762000	0.159678000
C	-3.477249000	0.924793000	-0.129817000
C	-4.800151000	0.481744000	-0.318880000
H	-5.599262000	1.215744000	-0.317719000
C	-5.052790000	-0.854379000	-0.495612000
H	-6.068970000	-1.205973000	-0.639403000
C	-2.825168000	2.139501000	0.080126000
H	-3.277221000	3.119563000	0.146219000
C	-3.982800000	-1.788448000	-0.475968000
H	-4.173142000	-2.849059000	-0.593173000
C	5.052526000	-0.853940000	-0.498813000
H	6.068639000	-1.205247000	-0.643772000
C	2.697754000	-1.371383000	-0.297505000
H	1.840682000	-2.032774000	-0.233457000
C	-0.000141000	-0.070931000	0.099114000
C	-1.264061000	0.665797000	0.052552000
C	3.477420000	0.924177000	-0.126043000
C	1.264057000	0.665311000	0.054342000
C	3.982230000	-1.787713000	-0.483325000
H	4.172243000	-2.847903000	-0.604761000

C	4.800239000	0.481519000	-0.316585000
H	5.599567000	1.215268000	-0.312028000
H	0.000117000	-0.909478000	-0.611689000
O	-0.001024000	-0.892462000	1.448237000
O	0.001218000	-2.186154000	1.222676000

L1′ (*S*=0)

Zero-point correction= 0.226640 (Hartree/Particle)
Thermal correction to Energy= 0.240741
Thermal correction to Enthalpy= 0.241686
Thermal correction to Gibbs Free Energy= 0.183857
Sum of electronic and zero-point Energies= -871.540930
Sum of electronic and thermal Energies= -871.526828
Sum of electronic and thermal Enthalpies= -871.525884
Sum of electronic and thermal Free Energies= -871.583713

Cartesian Coordinates

N	1.442213000	1.809591000	-0.000568000
N	2.489070000	-0.174120000	0.000009000
N	-2.489070000	-0.174119000	-0.000013000
C	-2.760575000	2.027461000	0.000617000
H	-3.176719000	3.026453000	0.000905000
C	-4.827160000	0.454163000	0.000157000
H	-5.578167000	1.237386000	0.000364000
C	2.829431000	-1.507645000	0.000372000
H	1.996492000	-2.194392000	0.000544000
C	-5.168679000	-0.874994000	-0.000204000
H	-6.211166000	-1.175269000	-0.000272000
C	1.257053000	0.486277000	-0.000190000
C	-3.472149000	0.823519000	0.000258000
C	4.827160000	0.454164000	-0.000135000
H	5.578166000	1.237388000	-0.000332000
C	-4.149272000	-1.858688000	-0.000474000
H	-4.400623000	-2.913143000	-0.000754000
C	4.149273000	-1.858688000	0.000488000
H	4.400625000	-2.913142000	0.000767000
C	0.000000000	-0.248168000	-0.000031000
C	3.472149000	0.823519000	-0.000250000
C	-2.829429000	-1.507644000	-0.000373000
H	-1.996488000	-2.194389000	-0.000557000
C	5.168680000	-0.874992000	0.000229000
H	6.211167000	-1.175267000	0.000309000
C	2.760574000	2.027460000	-0.000608000
H	3.176717000	3.026453000	-0.000885000
N	-1.442214000	1.809592000	0.000561000

C -1.257053000 0.486278000 0.000159000
O -0.000001000 -1.496354000 -0.000013000

$^3O_2$ (*S*=1)

Zero-point correction= 0.003770 (Hartree/Particle)
Thermal correction to Energy= 0.006133
Thermal correction to Enthalpy= 0.007078
Thermal correction to Gibbs Free Energy= -0.016213
Sum of electronic and zero-point Energies= -150.303834
Sum of electronic and thermal Energies= -150.301471
Sum of electronic and thermal Enthalpies= -150.300527
Sum of electronic and thermal Free Energies= -150.323818

Cartesian Coordinates

O 0.000000000 0.000000000 0.608736000
O 0.000000000 0.000000000 -0.608736000

OH• (*S*=1/2)

Zero-point correction= 0.008603 (Hartree/Particle)
Thermal correction to Energy= 0.010964
Thermal correction to Enthalpy= 0.011908
Thermal correction to Gibbs Free Energy= -0.008320
Sum of electronic and zero-point Energies= -75.711202
Sum of electronic and thermal Energies= -75.708842
Sum of electronic and thermal Enthalpies= -75.707897
Sum of electronic and thermal Free Energies= -75.728125

Cartesian Coordinates

O 0.000000000 0.000000000 0.108133000
H 0.000000000 0.000000000 -0.865061000

{Cu^{II}-L1•} for **1a** (*S*=1)

Zero-point correction= 0.337264 (Hartree/Particle)
Thermal correction to Energy= 0.363813
Thermal correction to Enthalpy= 0.364757
Thermal correction to Gibbs Free Energy= 0.275634
Sum of electronic and zero-point Energies= -1449.946287
Sum of electronic and thermal Energies= -1449.919739
Sum of electronic and thermal Enthalpies= -1449.918794
Sum of electronic and thermal Free Energies= -1450.007918

Cartesian Coordinates

O	3.388453000	11.551618000	8.024152000
O	2.764517000	12.630332000	6.177532000
N	2.451918000	8.061795000	4.286445000
N	-0.839377000	7.927878000	7.959013000
O	-0.505424000	12.491582000	5.647898000
N	0.151584000	9.868748000	7.531909000
N	2.101120000	9.935531000	5.425667000
C	-1.261787000	6.621813000	7.968116000
H	-0.815276000	5.961900000	7.231899000
C	1.737097000	8.637318000	5.326854000
O	0.293828000	12.730225000	7.713788000
C	3.281746000	9.056802000	3.735486000
C	3.585835000	12.417199000	7.153115000
C	4.111102000	8.715555000	2.653608000
H	4.752870000	9.483138000	2.229371000
C	-1.347594000	8.874828000	8.868677000
C	0.803196000	7.957858000	6.118605000
H	0.627979000	6.904266000	5.922887000
C	0.083692000	8.574116000	7.149570000
C	-2.196069000	6.225465000	8.875841000
H	-2.521097000	5.189638000	8.872981000
C	3.021106000	10.201906000	4.483541000
H	3.437577000	11.197602000	4.395813000
C	2.432782000	6.783098000	3.787402000
H	1.757478000	6.083982000	4.269159000
C	-0.695539000	10.064669000	8.556067000
H	-0.791107000	11.046540000	9.002307000
C	3.238245000	6.460461000	2.737962000
H	3.213205000	5.445728000	2.352438000
C	4.094684000	7.436574000	2.157132000
H	4.730432000	7.164318000	1.319274000
C	-2.733941000	7.152176000	9.811238000
H	-3.477788000	6.820021000	10.530098000
C	-2.310874000	8.457508000	9.802935000
H	-2.702833000	9.187768000	10.505662000
C	4.808882000	13.302331000	7.182456000
H	4.514748000	14.320065000	7.463145000
H	5.267761000	13.369569000	6.190110000
H	5.538534000	12.933534000	7.907374000
C	-0.506037000	13.061079000	6.753924000
C	-1.445152000	14.206273000	7.048991000
H	-2.215986000	14.285463000	6.278495000
H	-0.877118000	15.143155000	7.077088000
H	-1.909662000	14.089411000	8.033917000
Cu	1.341499000	11.342153000	6.723064000

1a (*S*=1)

Zero-point correction= 0.681328 (Hartree/Particle)
Thermal correction to Energy= 0.731573
Thermal correction to Enthalpy= 0.732517
Thermal correction to Gibbs Free Energy= 0.595045
Sum of electronic and zero-point Energies= -2899.980869
Sum of electronic and thermal Energies= -2899.930624
Sum of electronic and thermal Enthalpies= -2899.929680
Sum of electronic and thermal Free Energies= -2900.067152

Cartesian Coordinates

O	3.180389000	11.248547000	8.096785000
O	2.764417000	12.651260000	6.408830000
N	2.437937000	8.160612000	4.301111000
N	-0.458492000	7.838929000	8.133596000
O	-0.299854000	12.793502000	5.418880000
N	0.085035000	9.863760000	7.463679000
N	1.887521000	10.063420000	5.264252000
C	-0.523251000	6.479441000	8.356150000
H	0.237524000	5.877245000	7.872568000
C	1.905370000	8.739689000	5.419851000
O	0.105244000	12.766507000	7.598637000
C	2.760558000	9.196443000	3.399288000
C	3.471713000	12.250850000	7.389958000
C	3.351052000	8.848647000	2.165374000
H	3.600778000	9.643939000	1.467837000
C	-1.370325000	8.734094000	8.729289000
C	1.594676000	8.005313000	6.671905000
H	1.407453000	6.945208000	6.441285000
C	0.408487000	8.573858000	7.370149000
C	-1.492733000	5.985244000	9.170753000
H	-1.516887000	4.911694000	9.338140000
C	2.391684000	10.366924000	4.042998000
H	2.458861000	11.393248000	3.707554000
C	2.671967000	6.829351000	4.009128000
H	2.366215000	6.095004000	4.755346000
C	-0.990535000	9.987905000	8.278273000
H	-1.407727000	10.961522000	8.496157000
C	3.249146000	6.520009000	2.816782000
H	3.435292000	5.473389000	2.594444000
C	3.599070000	7.533794000	1.880332000
H	4.059356000	7.256225000	0.935434000
C	-2.432763000	6.854489000	9.792443000
H	-3.198374000	6.440843000	10.443784000
C	-2.370375000	8.204135000	9.573372000

H	-3.075010000	8.891146000	10.034578000
C	4.735165000	13.019619000	7.697729000
H	4.628197000	13.516323000	8.668517000
H	4.949551000	13.774790000	6.937687000
H	5.582016000	12.329789000	7.790380000
C	-0.474993000	13.270278000	6.558501000
C	-1.348659000	14.473198000	6.787731000
H	-2.070009000	14.586257000	5.974569000
H	-0.721757000	15.371902000	6.815902000
H	-1.867823000	14.409652000	7.748873000
N	2.050887000	7.918618000	10.005648000
N	4.943381000	8.176087000	6.177225000
N	4.378849000	6.145500000	6.837041000
N	2.555122000	5.982035000	9.087658000
C	5.026857000	9.537570000	5.976921000
H	4.299056000	10.142744000	6.509802000
C	2.569803000	7.302809000	8.899329000
C	1.704411000	6.912484000	10.931209000
C	1.113566000	7.300268000	12.153098000
H	0.844897000	6.526365000	12.867439000
C	5.841109000	7.276732000	5.567804000
C	2.888801000	8.013955000	7.634885000
H	3.081501000	9.074614000	7.856035000
C	4.072700000	7.436286000	6.937129000
C	5.992675000	10.026936000	5.153713000
H	6.039907000	11.102020000	5.000371000
C	2.047497000	5.719204000	10.317180000
H	1.949309000	4.702865000	10.674603000
C	1.840704000	9.260707000	10.265781000
H	2.162503000	9.972348000	9.506592000
C	5.448912000	6.024297000	6.016202000
H	5.871719000	5.054853000	5.786374000
C	1.261506000	9.609598000	11.445990000
H	1.093615000	10.664812000	11.640202000
C	0.887459000	8.625664000	12.404598000
H	0.426546000	8.935002000	13.339186000
C	6.911593000	9.153082000	4.507364000
H	7.673200000	9.564318000	3.849788000
C	6.837747000	7.802554000	4.717671000
H	7.530665000	7.112532000	4.243062000
O	1.652422000	4.811474000	6.321279000
O	0.960671000	3.382351000	7.886732000
O	4.147031000	3.265913000	9.095969000
O	4.050097000	3.001902000	6.923540000
C	0.828183000	3.923871000	6.775293000
C	-0.351724000	3.603001000	5.886235000
H	-0.002476000	3.226282000	4.918688000
H	-1.005270000	2.860464000	6.349922000
H	-0.926613000	4.514036000	5.678592000

C	4.411361000	2.570280000	8.072510000
C	5.101335000	1.249504000	8.189252000
H	5.766798000	1.235694000	9.056350000
H	4.348150000	0.466167000	8.332503000
H	5.657476000	1.014433000	7.277803000
Cu	1.151748000	11.406422000	6.604392000
Cu	3.164485000	4.578773000	7.772977000
