Electronic Supplementary Information

Polyaromatic hydrocarbon derivatized azo-oximes of Cobalt(III): ligand-redox controlled electro-catalytic oxygen reduction reaction

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Table S1. Crystallographic Details of **2a**, **2b** and **2c**

	2a.$2C_6H_6$	**2b.** $2CH_2Cl_2$	**2c**
Empirical formula	$C_{81}H_{54}N_9O_3Co$	$C_{65}H_{46}Cl_4N_9O_3Co$	$C_{39}H_{30}CoN_9O_3$
fw	1260.26	1201.84	731.65
T /K	298K	138K	151K
Crystal system	orthorhombic	monoclinic	triclinic
Space group	*Pbca*	*P*21/c	$P\bar{1}$
a / Å	20.9681(18)	14.0861(5)	13.410(13)
b / Å	24.686(2)	16.1493(5)	14.787(14)
c / Å º	24.862(2)	25.2610(8)	20.20(2)
α/deg	90	90	110.18(4)
β/ deg	90	105.5320(10)	103.35(4)
γ/ deg	90	90	92.43(5)
V /Å^3	12869(2)	5536.5(3)	3625(6)
Z	8	4	4
D_c /Mgm^{-3}	1.301	1.442	1.341
μ/mm^{-1}	0.326	0.562	0.524
F(000)	5232	2472	1576
cryst size/mm^3	0.43×0.34×0.22	0.46×0.35×0.25	0.40×0.30×0.20
θ/deg	1.84–27.62	2.85–27.54	2.226–26.455
measured reflns	212552	80825	40582
unique reflns/R_{int}	14820/0.1961	12722/0.0499	14839/0.1536
[a]GOF on F^2	0.961	1.032	0.960
R1,[b] wR2[c] [$I > 2\sigma(I)$]	0.0717, 0.2001	0.0591, 0.1521	0.0798, 0.1694
R1, wR2	0.1753, 0.2632	0.0809, 0.1714	0.1747, 0.2170

[a]GOF = $\{\Sigma[w(F_o^2-F_c^2)^2]/(n-p)\}^{1/2}$. [b]R1 = $\Sigma||F_o|-|F_c||/\Sigma|F_o|$.
[c]wR2 = $[\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$ where $w = 1/[\sigma^2(F_o^2)+(aP)^2+bP]$, $P = (F_o^2+2F_c^2)/3$.

Table S2. Selected Experimental and Theoretical Bond Parameters of **2a, 2b** and **2c**

2a			**2b**			**2c**		
	Expt.	**Theo.**		**Expt.**	**Theo.**		**Expt.**	**Theo.**
Co1–N1	1.901(3)	1.930	Co1–N1	1.897(2)	1.963	Co1–N1	1.918(4)	1.928
Co1–N3	1.917(3)	1.966	Co1–N3	1.919(2)	2.016	Co1–N3	1.937(5)	1.955
Co1–N4	1.903(3)	1.945	Co1–N4	1.927(2)	1.955	Co1–N4	1.883(5)	1.948
Co1–N6	1.935(4)	1.995	Co1–N6	1.957(2)	1.980	Co1–N6	1.899(4)	1.994
Co1–N7	1.911(4)	1.959	Co1–N7	1.924(2)	1.242	Co1–N7	1.904(4)	1.955
Co1–N9	1.941(3)	1.976	Co1–N9	1.936(2)	1.978	Co1–N9	1.943(4)	1.970
N2–N3	1.292(4)	1.278	N2–N3	1.281(3)	1.283	N2–N3	1.288(5)	1.273
N5–N6	1.296(5)	1.282	N5–N6	1.288(3)	1.275	N5–N6	1.277(6)	1.278
N8–N9	1.289(5)	1.277	N8–N9	1.288(3)	1.280	N8–N9	1.286(5)	1.271
N1–O1	1.251(4)	1.243	N1–O1	1.252(3)	1.249	N1–O1	1.267(5)	1.246
N4–O2	1.263(4)	1.251	N4–O2	1.265(3)	1.251	N4–O2	1.278(5)	1.250
N7–O3	1.261(4)	1.251	N7–O3	1.267(3)	1.242	N7–O3	1.272(5)	1.255
C7–N1	1.343(5)	1.352	C7–N1	1.350(4)	1.354	C7–N1	1.330(5)	1.355
C30–N4	1.361(5)	1.357	C28–N4	1.337(3)	1.353	C20–N4	1.357(6)	1.358
C53–N7	1.353(5)	1.352	C49–N7	1.345(4)	1.356	C33–N4	1.337(6)	1.351
N1–Co1–N3	80.78(15)	80.92	N1–Co1–N3	80.71(10)	79.72	N1–Co1–N3	80.16(19)	80.750
N4–Co1–N6	80.37(16)	80.13	N4–Co1–N6	79.95(9)	80.07	N4–Co1–N6	80.70(2)	79.912
N7–Co1–N9	80.10(15)	80.301	N7–Co1–N9	80.28(9)	80.61	N7–Co1–N9	80.19(18)	80.015

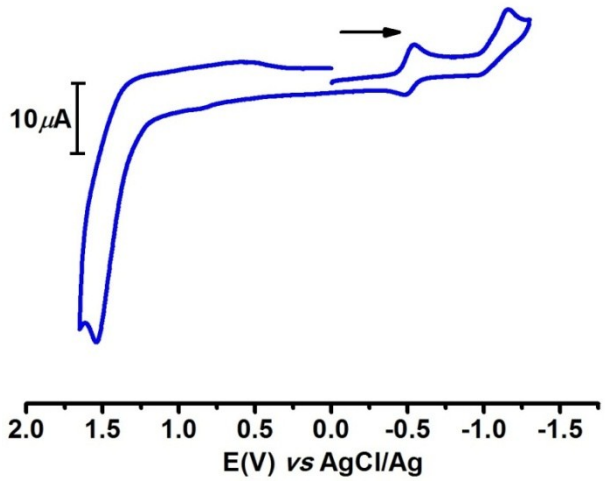


Fig. S1 Cyclic voltammogram of **2b** in dichloromethane at 298 K. Condition: Solute concentration ≈10^{-3} mol dm^{-3}; scan rate, 100 mV s^{-1}.

Table S3 Electrochemical Data for **2a**, **2b** and **2c** in dichloromethane.

Compounds	**E (V)**		
	$E_{1/2}$/V (ΔE_p/mV)	**E_{pc}**	**E_{pa}**
2a	−0.55 (75)	−1.12	+1.50
2b	−0.51 (66)	−1.16	+1.54
2c	−0.52(76)		+1.60
$E_{1/2}$ = 1/2(Ep_a+Ep_c) for reversible one-electron process, where E_{pa} and E_{pc} are the anodic and cathodic peak potentials, respectively; $\Delta E_p = E_{pa} - E_{pc}$.			

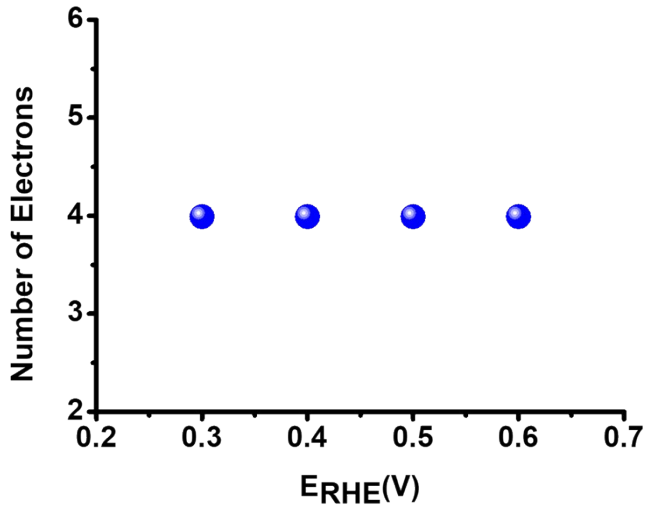


Fig. S2 Plot showing the variation in electron number for the overall oxygen reduction process at different applied voltages for Complex **2a**.

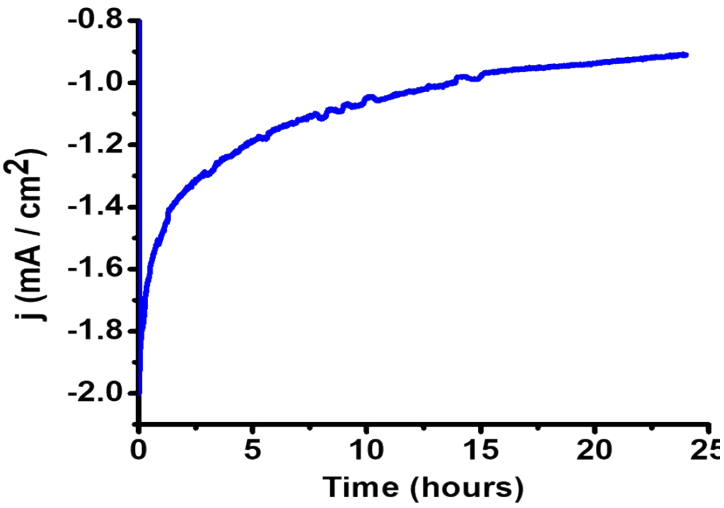


Figure S3 Chronoamperometry plot for the complex **2a**.

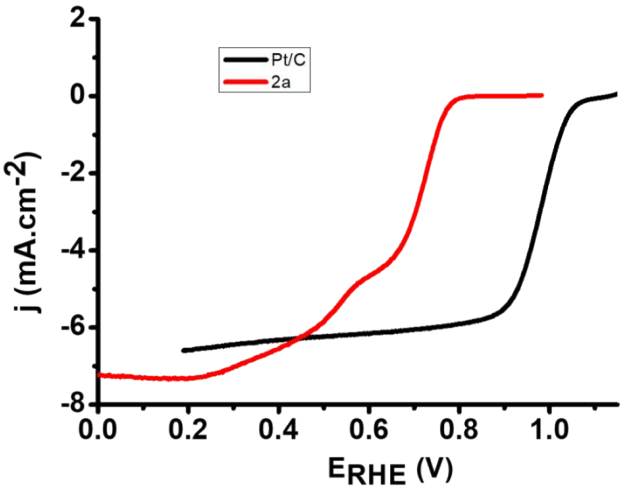


Figure S4 Comparative LSV of **2a** with Pt/C.

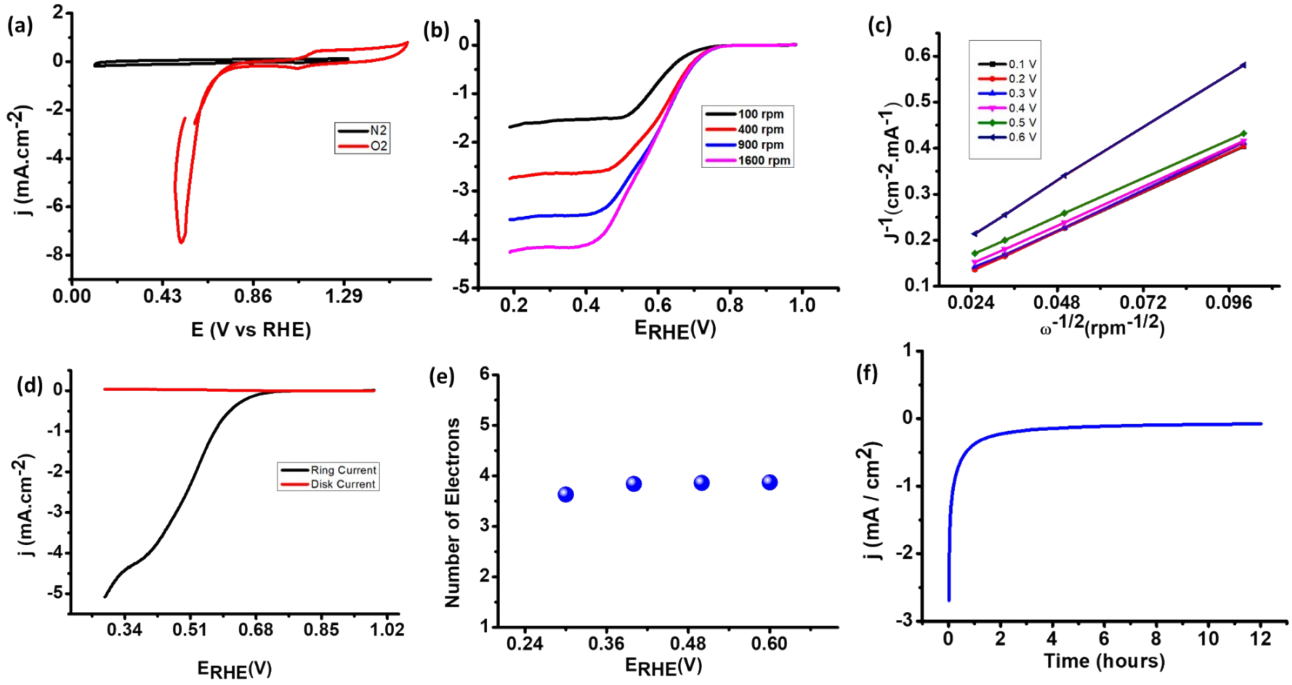


Fig. S5 ORR plots of **2c**: (a) Cyclic voltammetric in O_2 (red) and N_2 (black) saturated solution. (b) Linear sweep voltammetric curves under different rotation speeds on catalyst coated glassy carbon electrode. (c) K-L plot over a wide voltage range at different electrode rotation speeds (d) Rotating ring disk electrode plots of the complex showing the change in disk and ring currents on oxygen reduction. (e) Plot showing the variation in electron number for the overall oxygen reduction process at different applied voltages and (f) Chronoamperometric plot.

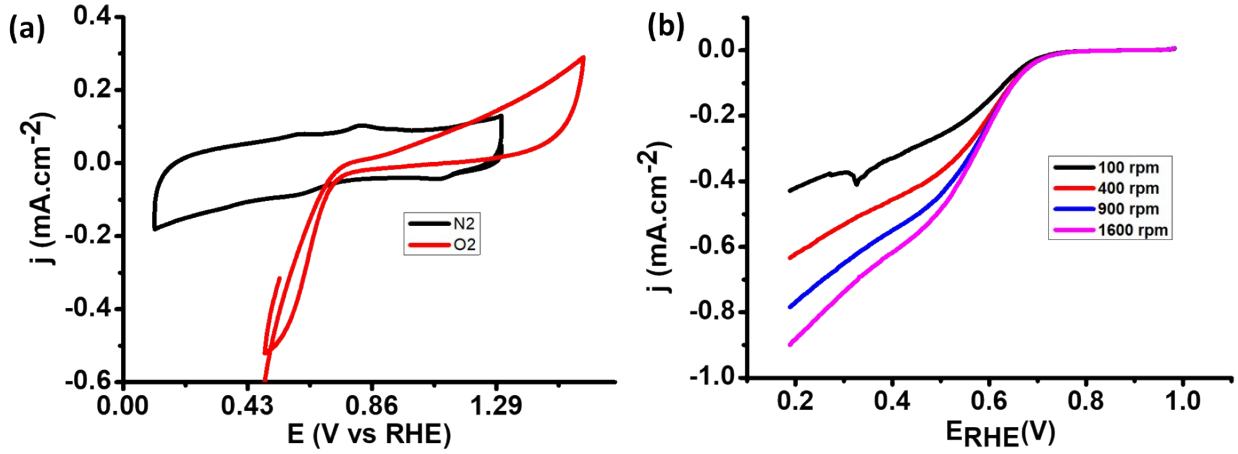


Fig. S6 ORR plots of **2d**: (a) Cyclic voltammetric in O_2 (red) and N_2 (black) saturated solution. (b) Linear sweep voltammetric curves under different rotation speeds on catalyst coated glassy carbon electrode.

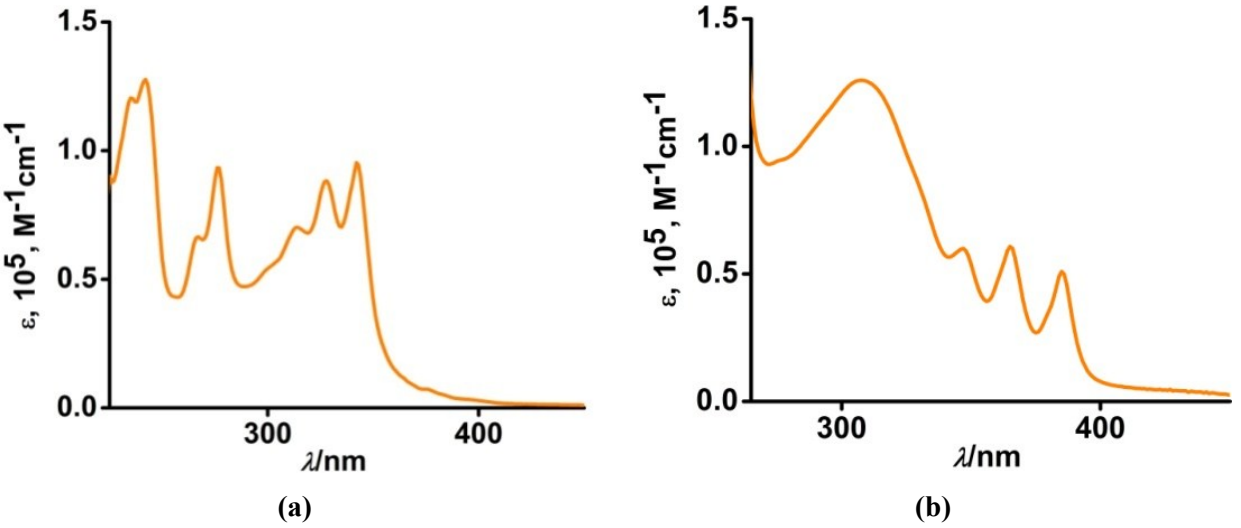


Fig. S7 Absorption spectra of (a) **1a** and (b) **1b** in CH_2Cl_2 solution at 298 K.

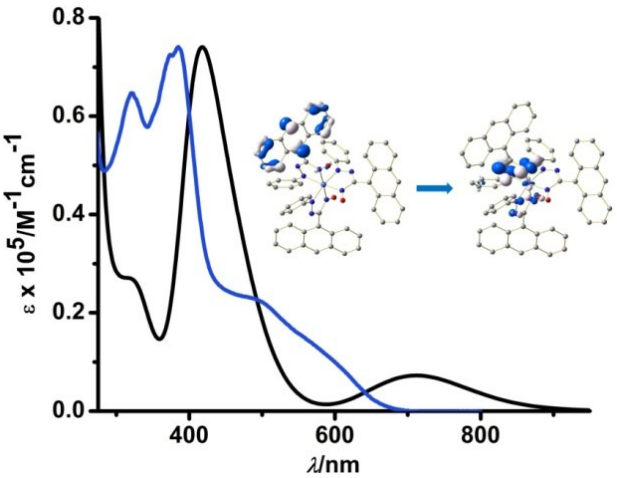


Fig. S8 Experimental (blue) and theoretical (black) absorption spectra of **2b** in CH_2Cl_2 solution at 298 K.

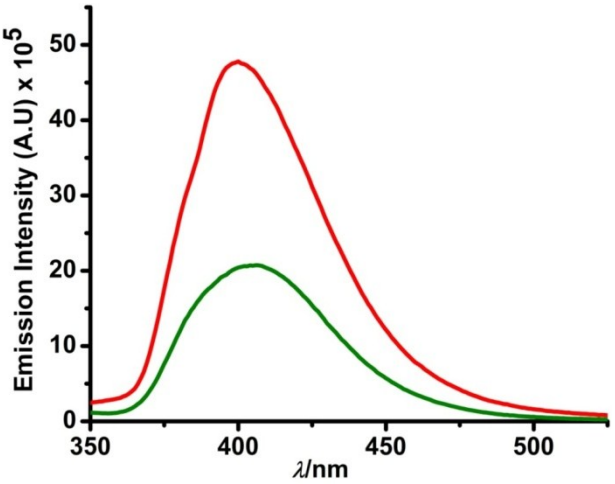


Fig. S9 Emission spectra of **1b** (red) and **2b** (green)in CH_2Cl_2 solution at 298 K.

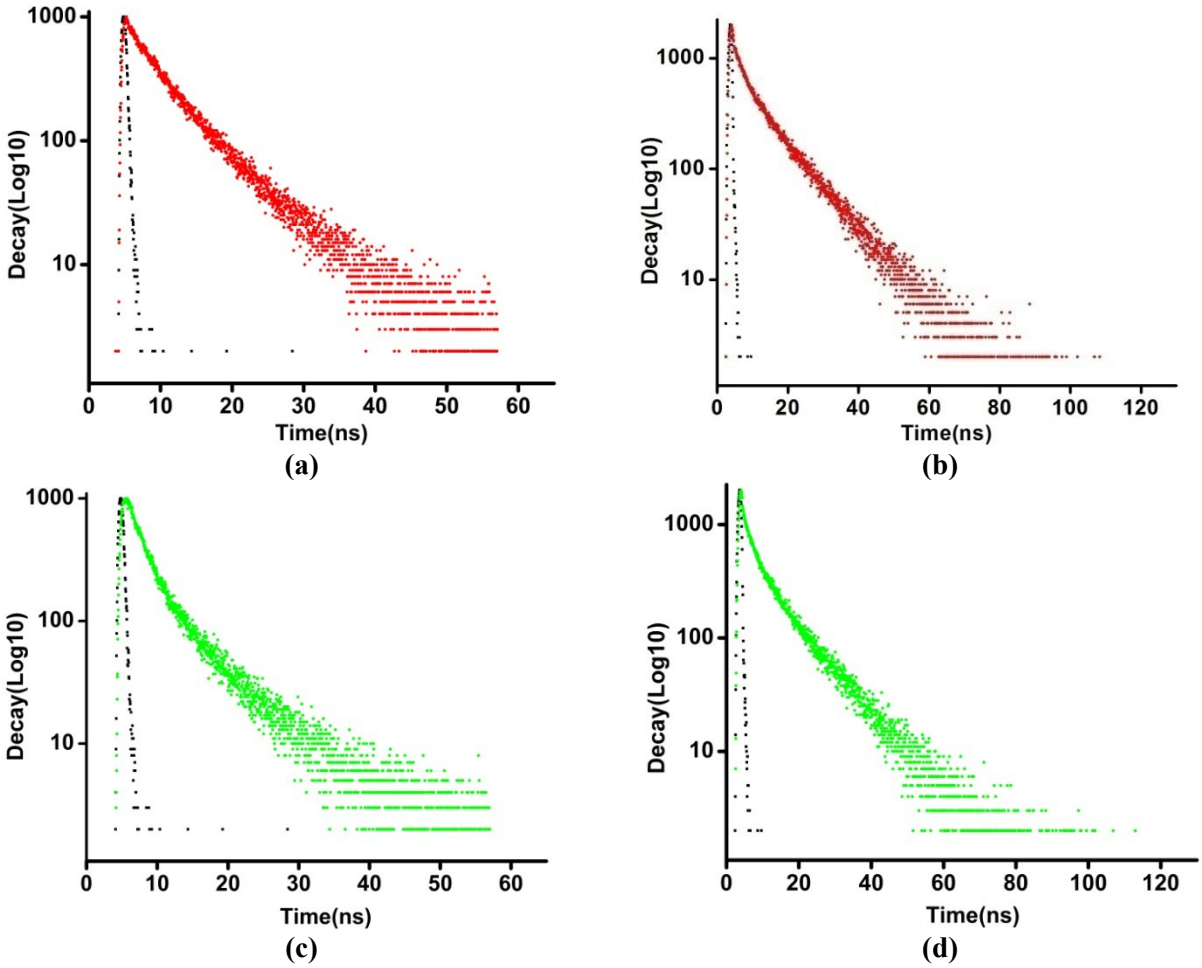
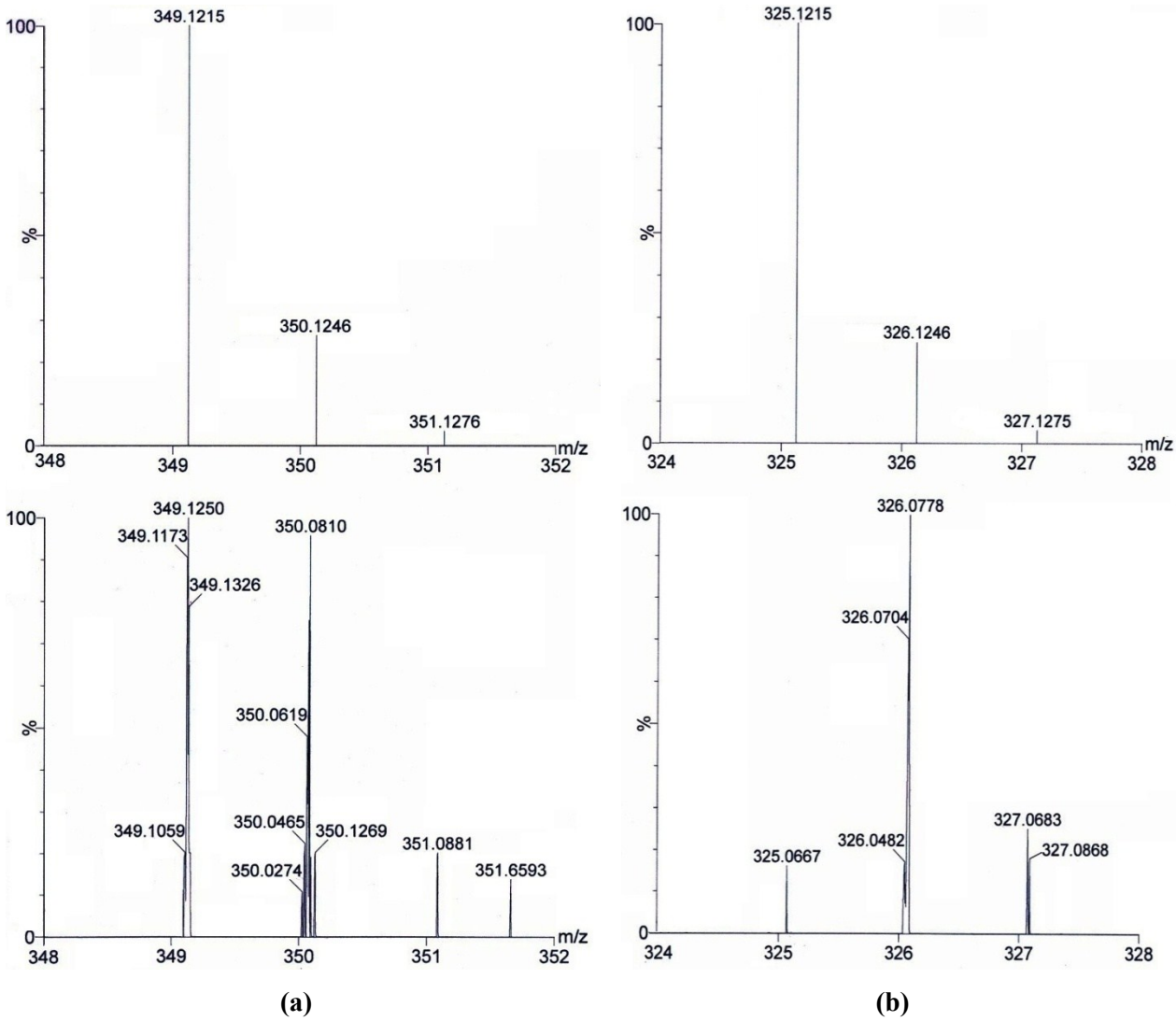


Fig. S10 Emission decays of (a)**1a**, (b) **1b**, (c) **2a** and (d) **2b**.



(a) **(b)**

Fig. S11 HRMS (ESI positive) of (a) **1a** and (b) **1b**; top (simulated), bottom (experimental).

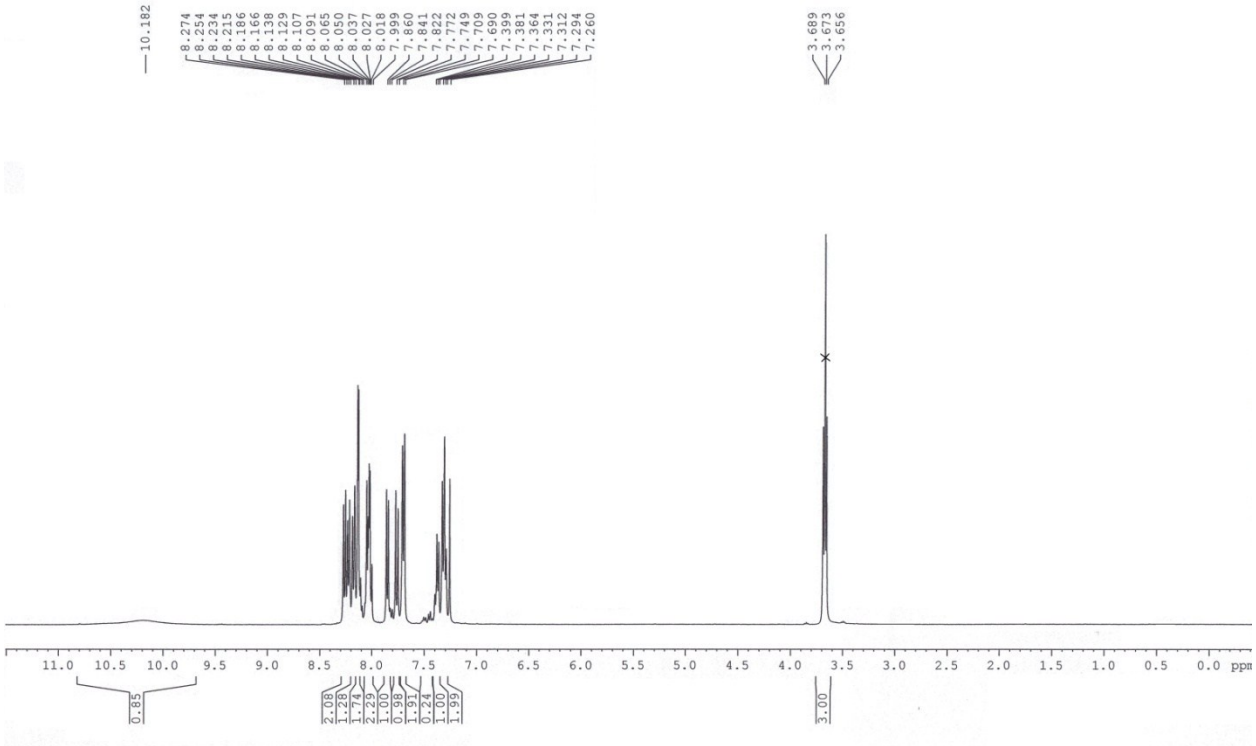


Fig. S12 ^{1}H-NMR (400 MHz, $CDCl_3$) spectrumof **1a**.

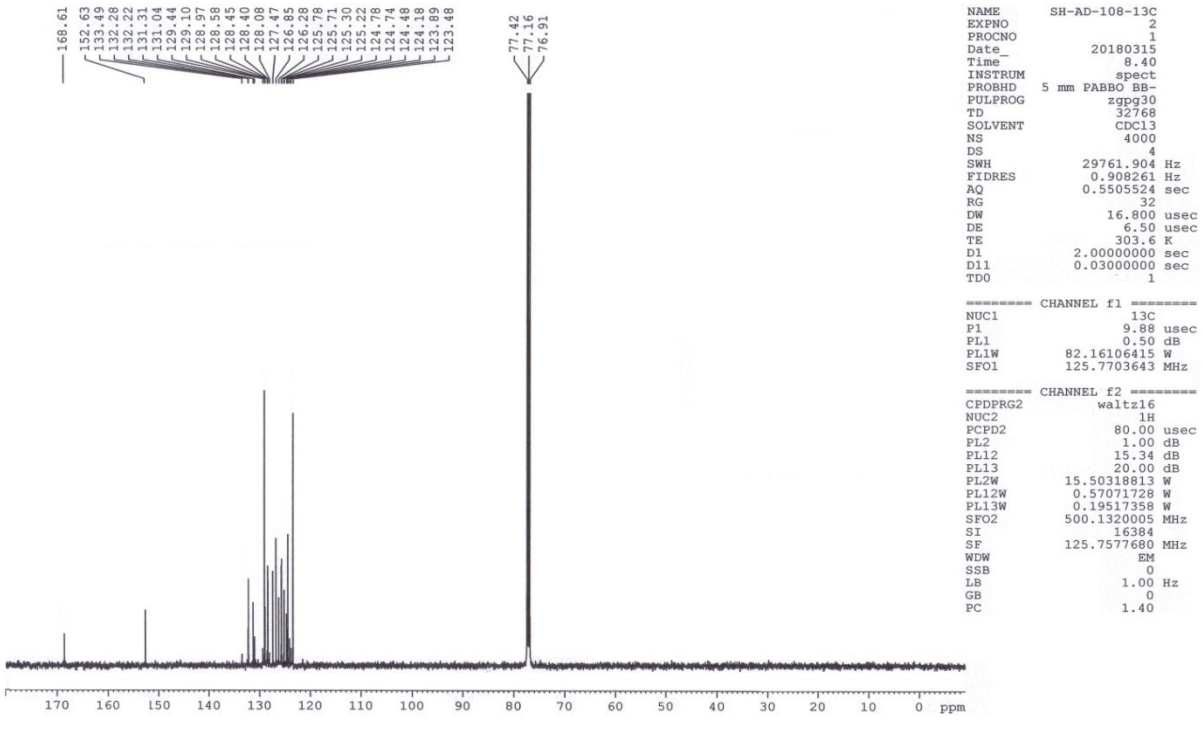


Fig. S13 ^{13}C-NMR(500 MHz, $CDCl_3$) spectrum of **1a**.

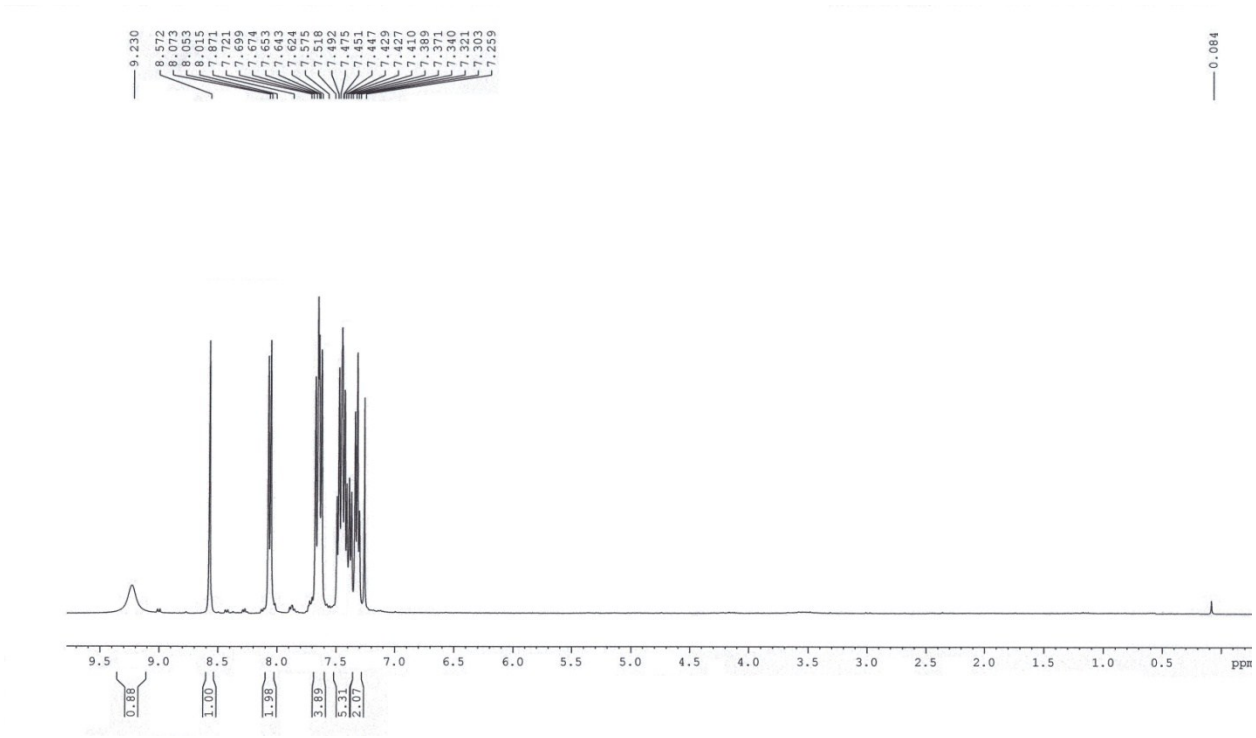


Fig. S14 ^{1}H-NMR(400 MHz, $CDCl_3$) spectrum of **1b**.

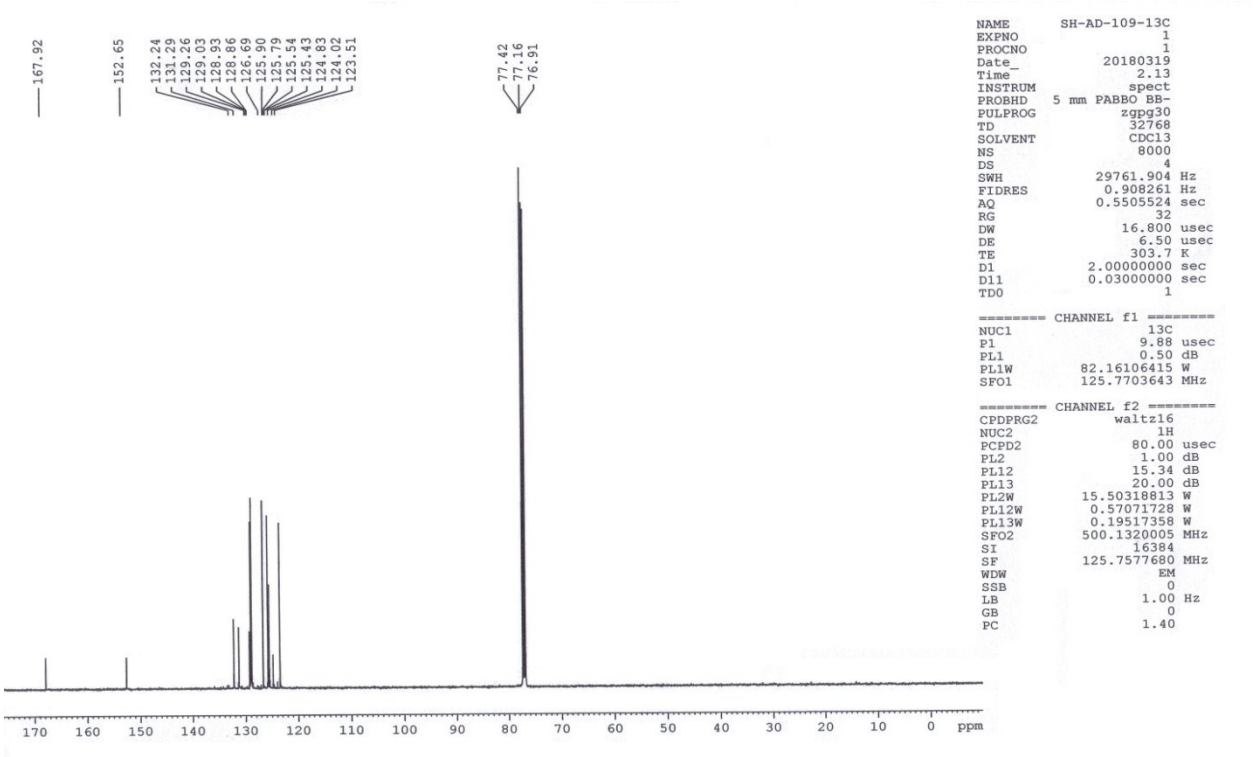


Fig. S15 ^{13}C-NMR(500 MHz, $CDCl_3$) spectrum of **1b**.

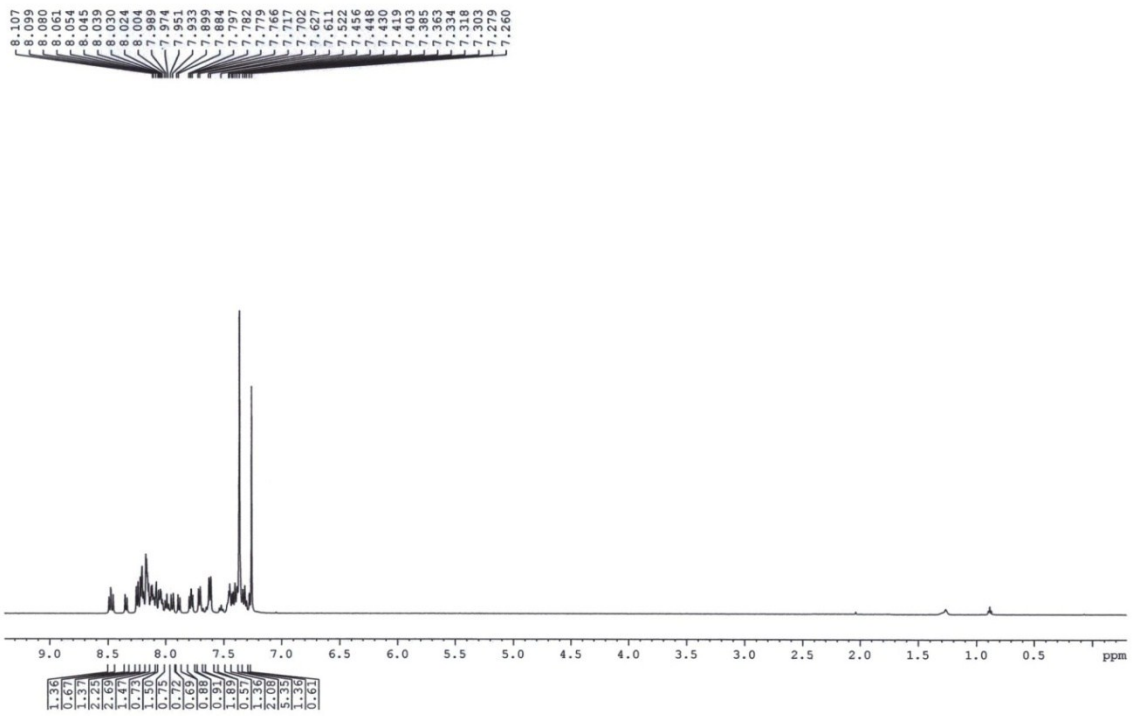


Fig. S16 ^{1}H-NMR(500 MHz, $CDCl_3$) spectrum of **2a**.

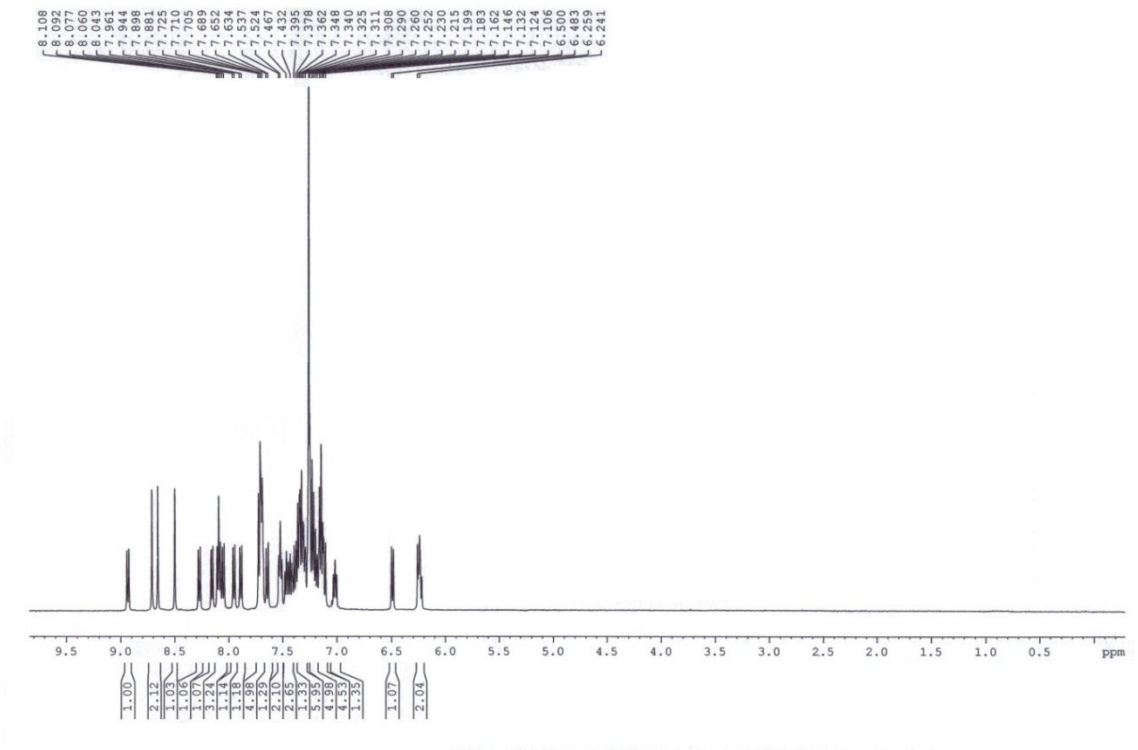


Fig. S17 ^{1}H-NMR(500 MHz, $CDCl_3$) spectrum of **2b**.

Fig. S18 Gas phase optimized geometries of **1a**(left) and **1b** (right).

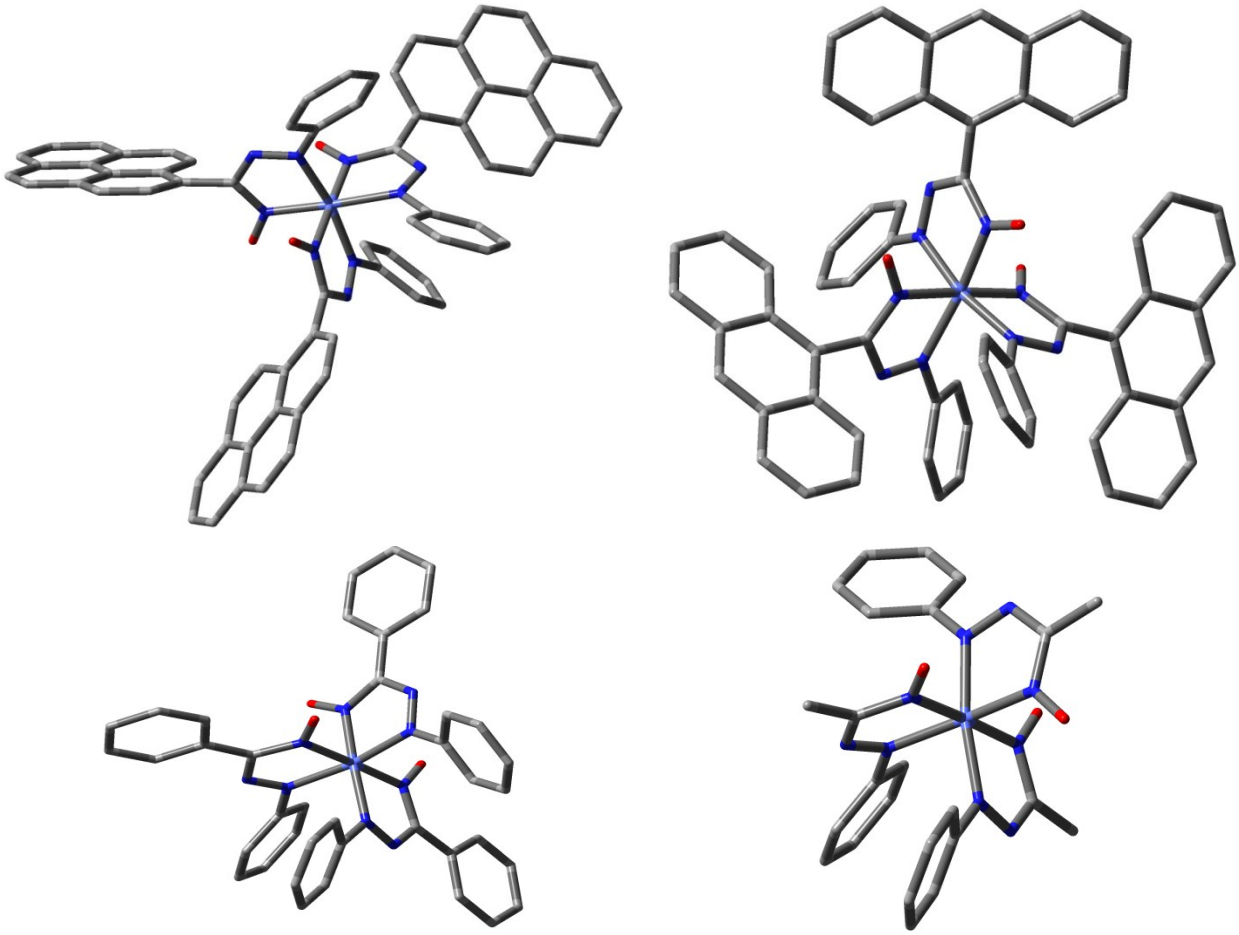


Fig. S19 Gas phase optimized geometries of **2a**(top-left), **2a**(top-right), **2c**(bottom-left) and **2d** (bottom-right) (Hs are omitted for clarity).

Table S4 Frontier Molecular Orbital Compositions (%) in the Ground State for **1a**.

Orbital	MO	Energy(EV)	% Contribution				Contribution
			Oxime	Pyrene	Azo	Ph	
97	L+5	-0.21	35	7	4	54	π*(Ph+Oxime)
96	L+4	-0.57	1	98	0	0	π*(Pyrene)
95	L+3	-0.68	2	1	1	96	π*(Ph)
94	L+2	-1.07	0	100	0	0	π*(Pyrene)
93	L+1	-1.9	1	99	0	0	π*(Pyrene)
92	LUMO	-2.66	25	0	47	28	π*(Azo+Ph+Oxime)
91	HOMO	-5.67	1	99	0	0	π(Pyrene)
90	H–1	-6.55	1	96	3	0	π(Pyrene)
89	H–2	-6.66	0	6	86	8	π(Pyrene)
88	H–3	-6.77	33	1	12	54	π(Ph+Oxime+Azo)
87	H–4	-7.2	0	100	0	0	π(Pyrene)
86	H–5	-7.35	0	0	0	100	π(Ph)

Table S5 Frontier Molecular Orbital Compositions (%) in the Ground State for **1b**

Orbital	MO	Energy(EV)	% Contribution				Contribution
			Oxime	Anthracene	Azo	Ph	
91	L+5	-0.22	36	6	4	54	π*(Ph+Oxime)
90	L+4	-0.25	1	97	0	2	π*(Anthracene)
89	L+3	-0.67	2	7	1	90	π*(Ph)
88	L+2	-0.74	0	93	0	7	π*(Anthracene)
87	L+1	-2.07	0	99	1	0	π*(Anthracene)
86	LUMO	-2.67	25	0	46	28	π*(Azo+Ph+Oxime)
85	HOMO	-5.57	1	98	1	0	π(Anthracene)
84	H–1	-6.66	-1	5	90	7	π(Azo)
83	H–2	-6.76	24	26	9	41	π(Ph+Anthracene+oxime)
82	H–3	-6.8	9	75	3	14	π(Anthracene+Ph)
81	H–4	-7.21	1	99	0	0	π(Anthracene)
80	H–5	-7.34	0	0	0	100	π(Ph)

Table S6 Frontier Molecular Orbital Compositions (%) in the Ground State for **1c**.

Orbital	MO	Energy(EV)	% Contribution				Contribution
			oxime	Ph(oxime)	Azo	Ph(azo)	
63	L+3	-0.68	5	91	0	4	π*(Ph(oxime))
62	L+2	-0.80	0	1	1	98	π*(Ph(Azo))
61	L+1	-1.41	22	62	7	8	π*(Oxime+Ph(oxime))
60	LUMO	-2.79	16	5	51	28	π*(Oxime+Azo+Ph(Azo))
59	HOMO	-6.79	40	9	34	16	π(Oxime+Azo+Ph(Azo))
58	H-1	-6.99	10	45	42	4	π(Oxime+Ph(oxime)+Azo)
57	H-2	-7.29	1	58	8	33	π(Ph(oxime)+Ph(Azo))
56	H-3	-7.39	1	54	11	35	π(Ph(oxime)+Ph(Azo))

Table S7 Frontier Molecular Orbital Compositions (%) in the Ground State for **1d**.

Orbital	MO	Energy	% Contribution				Contribution
			oxime	Methyl	Azo	Ph	
47	L+3	0.11	7	12	0	89	π*(Ph+Methyl)
46	L+2	-0.16	29	12	4	54	π*(Ph+Oxime+Methyl)
45	L+1	-0.69	1	0	0	99	π*(Ph)
44	LUMO	-2.58	15	1	52	31	π*(Ph+Oxime+Azo)
43	HOMO	-6.53	23	2	60	15	π(Ph+Oxime+Azo)
42	H-1	-6.98	22	2	36	41	π(Ph+Oxime+Azo)
41	H-2	-7.39	0	0	0	99	π(Ph)
40	H-3	-7.7	44	4	10	41	π(Ph+Oxime+Azo)

Table S8 Frontier Molecular Orbital Composition (%) in the Ground State for **2a**.

Orbital	MO	Energy (EV)	Contribution (%)					Contribution
			Co	Oxime	Pyrene	Azo	Ph	
286	L+5	-1.94	15	10	69	4	1	dz^2+π*(Pyrene+Oxime)
285	L+4	-2.11	32	18	41	5	4	dz^2 +π*(Pyrene+Oxime)
284	L+3	-2.26	53	9	4	24	10	dz^2 +π*(Azo)
283	L+2	-2.93	6	38	3	43	10	π*(Azo+Oxime)
282	L+1	-3.12	6	39	5	39	11	π*(Azo+Oxime+Ph)
281	LUMO	-3.26	5	41	3	40	11	π*(Oxime+Azo+Ph)
280	HOMO	-5.43	0	4	94	1	1	π(Pyrene)
279	H–1	-5.49	0	5	92	2	1	π(Pyrene)
278	H–2	-5.61	0	7	89	2	2	π(Pyrene)
277	H–3	-6.22	1	19	52	11	17	π(Pyrene+Oxime+Ph+Azo)
276	H–4	-6.24	1	19	53	9	19	π(Pyrene+Oxime+Ph)
275	H–5	-6.34	3	19	62	6	10	π(Pyrene+Oxime+Ph)

Table S9 Frontier Molecular Orbital Composition (%) in the Ground State for **2b**.

			Contribution (%)					
Orbital	**MO**	**Energy (EV)**	**Co**	**Oxime**	**Anthracene**	**Azo**	**Ph**	**Contribution**
268	L+5	-2.09	1	1	94	3	2	π*(Anthracene)
267	L+4	-2.25	27	13	52	5	3	d_z^2 +π*(Anthracene+Oxime)
266	L+3	-2.3	50	8	12	22	8	d_z^2 +π*(Anthracene+Azo)
265	L+2	-2.96	5	38	4	42	11	π*(Azo+Ph+Oxime)
264	L+1	-3.09	6	38	6	39	11	π*(Azo+Oxime+Ph)
263	LUMO	-3.2	5	40	4	40	10	π*(Oxime+Azo+Ph)
262	HOMO	-5.38	1	4	95	1	0	π(Anthracene)
261	H–1	-5.5	1	6	91	1	1	π(Anthracene)
260	H–2	-5.57	0	4	94	1	1	π(Anthracene)
259	H–3	-6.24	1	26	29	15	29	π(Anthracene+Oxime+Ph+Azo)
258	H–4	-6.25	2	27	27	13	31	π(Anthracene+Oxime+Ph+Azo)
257	H–5	-6.42	3	24	31	13	29	π(Anthracene+Oxime+Ph+Azo)

Table S10 Frontier Molecular Orbital Composition (%) in the Ground State for **2c**.

Orbital	MO	Energy(EV)	Contribution (%)					Contribution
			Co	Oxime	Ph_{oxime}	Azo	Ph_{azo}	
190	L+5	-1.27	1	22	57	8	12	π*(Oxime+Ph_{azo}+Ph_{oxime})
189	L+4	-1.98	54	34	2	6	4	dz^2 +π*(Oxime)
188	L+3	-2.2	55	10	1	23	11	dz^2 +π*(Oxime+Azo+Ph)
187	L+2	-2.9	6	38	1	45	11	π*(Azo+Oxime)
186	L+1	-3.08	6	39	1	41	13	π*(Azo+Oxime+Ph)
185	LUMO	-3.2	5	41	0	43	10	π*(Oxime+Ph_{azo}+Ph_{oxime})
184	HOMO	-5.89	1	42	35	11	11	π(Oxime+Azo+Ph)
183	H-1	-5.95	1	42	31	10	16	π(Oxime+Azo+Ph)
182	H-2	-6.08	2	39	36	12	12	π(Oxime+Azo+Ph)
181	H-3	-6.43	10	75	4	6	5	π(Oxime)
180	H-4	-6.84	7	42	45	4	2	dz^2 +π(Oxime)
179	H-5	-6.88	5	28	58	5	4	π(Ph)

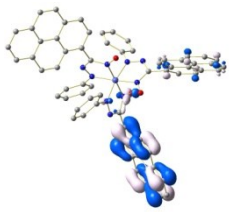
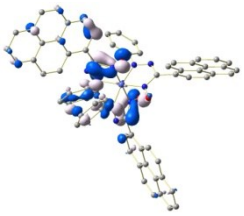
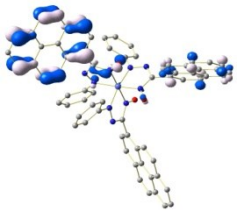
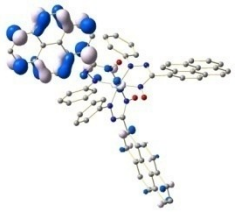
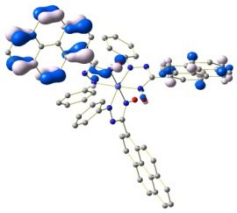
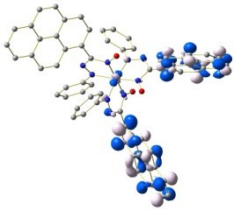
Table S11 Frontier Molecular Orbital Composition (%) in the Ground State for **2d**.

Orbital	**MO**	**Energy (EV)**	Contribution (%)					**Contribution**
			Co	**Oxime**	**Methyl**	**Azo**	**Ph**	
142	L+5	-0.72	1	0	0	0	98	π*(Ph)
141	L+4	-1.93	54	32	4	6	3	dz^2 +π*(Oxime)
140	L+3	-2.18	55	10	1	23	11	dz^2 +π*(Oxime+Azo+Ph)
139	L+2	-2.86	5	39	1	44	11	π*(Azo+Oxime)
138	L+1	-3.04	6	40	0	41	13	π*(Azo+Oxime+Ph)
137	LUMO	-3.15	6	42	0	41	11	π*(Oxime+Azo+Ph)
136	HOMO	-6.07	1	53	3	16	27	π(Oxime+Azo+Ph)
135	H−1	-6.13	2	50	3	17	28	π(Oxime+Azo+Ph)
134	H−2	-6.3	3	48	4	17	28	π(Oxime+Azo+Ph)
133	H−3	-6.5	12	70	4	8	5	π(Oxime)
132	H−4	-6.93	14	69	3	9	4	dz^2 +π(Oxime)
131	H−5	-7.22	1	7	1	2	89	π(Ph)

Table S12 Main Optical Transition at the TD-DFT/B3LYP/6-31+G(d,p) Level for the Complex **2a** with Composition in Terms of Molecular Orbital Contribution of the Transition, Computed Vertical Excitation Energies, and Oscillator Strength in Dichloromethane.

Transition	**CI**	**Composition**	**E (eV)**	**Oscillator strength (*f*)**	λ_{theo} **(nm)**
$S_0 \rightarrow S_1$	0.62034	HOMO → LUMO (77%)	1.8157	0.0470	682.84
$S_0 \rightarrow S_{15}$	0.50414	H–3 → L+1 (51%)	2.5025	0.0228	495.44
$S_0 \rightarrow S_{45}$	0.37454	HOMO → L+5 (28%)	3.2869	0.6212	377.20
$S_0 \rightarrow S_{59}$	–0.35893 0.36044 0.27586	HOMO → L+6 (26%), HOMO → L+7 (26%) H–1→ L+6 (15%)	3.4087	0.0563	363.73
$S_0 \rightarrow S_{101}$	0.31481	H–3 → L+6 (20%)	3.9652	0.0288	312.68
$S_0 \rightarrow S_{116}$	0.52195	H–5 → L+6 (54%)	4.1320	0.0263	300.05
$S_0 \rightarrow S_{200}$	0.34067	H–3 → L+8 (23%)	4.7597	0.0466	260.48

Table S13 Natural Transition Orbitals (NTOs) for Complex **2a**Illustrating the Nature of Singlet Excited States in the Absorption Bands in the Range 250–700 nm. For Each State, the Respective Number of the State, Transition Energy (eV), and the Oscillator Strength (in parentheses) are Listed. Shown are Only Occupied (holes) and Unoccupied (electrons) NTO Pairs that Contribute More Than 15% to Each Excited State.

		Hole	Electron
525 nm	S_1 w = 0.7696 1.8157 (0.0470) 495.85 nm ILCT π(Pyr+Oxime) → π*(Azo+Oxime)		
	380*nm* S_{15} w = 0.280 2.5025 (0.0228) 495.44 nm ILCT π(oxime + Ph) → π*(azo + oxime)		
349 nm	S_{45} w = 0.87 1.7730 (0. 6212) 377.20 ILCT π(pyrene+ oxime) → π*(pyrene)		
277 nm	S_{59} w = 0.257 3.4087 (0.0563) 363.73nm ILCT		

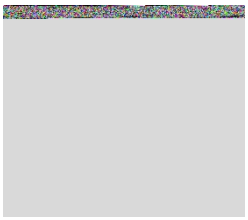
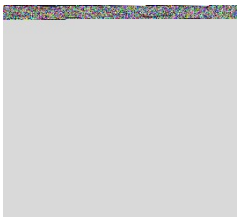
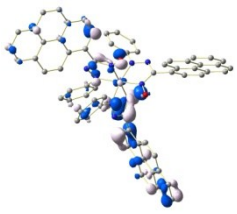
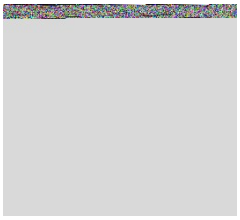
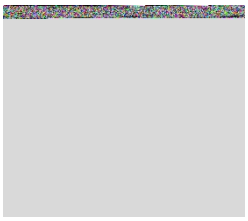
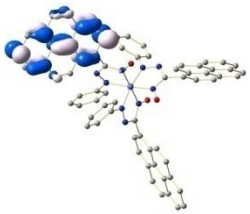
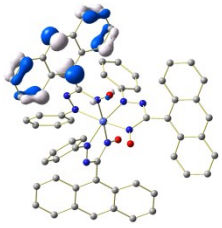
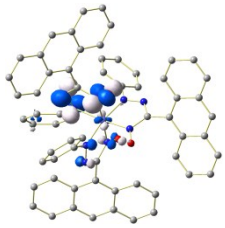
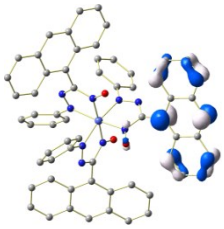
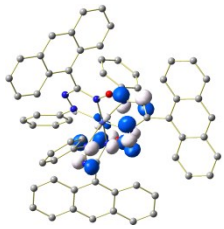
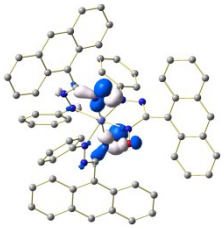
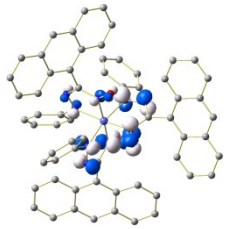
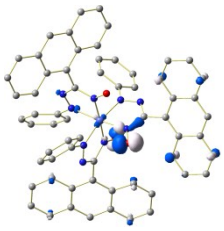
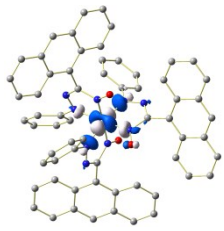
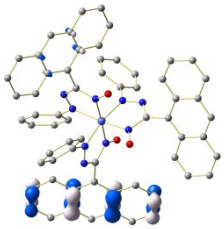
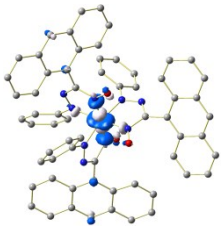
	π(oxime + pyrene) → π*(pyrene)		
	S_{101} w = 0.198 4.1320 (0.0263) 312.68 nm ILCT π (oxime) → π*(pyrene)		
239 nm	S_{116} w = 0.545 4.1320 (0.0263) 300.05 nm ILCT π(oxime) → π*(pyrene)		
	S_{200} w = 0.232 4.7597 (0.0466) 260.48 nm ILCT π(oxime + Ph) → π*(pyrene)		

Table S14 Main Optical Transition at the TD-DFT/B3LYP/6-31+G(d,p) Level for the Complex **2b** with Composition in Terms of Molecular Orbital Contribution of the Transition, Computed Vertical Excitation Energies, and Oscillator Strength in Dichloromethane

Transition	**CI**	**Composition**	**E (eV)**	**Oscillator strength (*f*)**	λ_{theo} **(nm)**
$S_0 \rightarrow S_1$	0.58759 0.13139	H–2 →LUMO (69%) H–2→L+2(22%)	1.7089	0.0369	725.51
$S_0 \rightarrow S_2$	0.49954 0.33768	HOMO → L+1 (50%) HOMO →LUMO(23%)	1.7391	0.0255	712.91
$S_0 \rightarrow S_{30}$	0.02333 0.28975	H–5 → L+2 (16%) H–4 → L+3(15%)	2.9065	0.1755	426.57
$S_0 \rightarrow S_{37}$	0.34052 0.33913	H–3 → L+3 (26%), HOMO → L+6 (23%)	3.0539	0.1790	405.98
$S_0 \rightarrow S_{101}$	0.05735	H–9 → L+3 (32%)	3.9342	0.0115	315.35
$S_0 \rightarrow S_{109}$	0.31278 0.26567 0.25100	H–7 → L+4 (20%) H–5 → L+6 (14%) H–6→ L+5 (13%)	4.0321	0.0374	307.49

Table S15 Natural Transition Orbitals (NTOs) for Complex **2b** Illustrating the Nature of Singlet Excited States in the Absorption Bands in the Range 250–700 nm. For Each State, the Respective Number of the State, Transition Energy (eV), and the Oscillator Strength (in parentheses) are Listed. Shown are Only Occupied (holes) and Unoccupied (electrons) NTO Pairs that Contribute More Than 15% to Each Excited State.

		Hole	Electron
590 nm	S_1 w = 0.6905 1.7089 (0.0369) 725.51nm ILCT π(Anc) → π*(Azo+Oxime)		
	S_2 w = 0.4990 1.7391 (0.0255) 712.91 nm ILCT π(Anc) → π*(Azo+Oxime)		
385 nm	S_{30} w = 0.5164 2.9065 (0.1755) 426.57 ILCT π(Oxime) → π*(Azo+Oxime)		
320 nm	S_{101} w = 0.0065 3.9342 (0.0115) 315.14nm ILCT π(Azo+oxime) → σ*(Co-N_{azo})		

S_{109} w = 0.1956 4.0321 (0.0374) 307.49nm ILCT π (Anc) → σ*(Co-N_{oxime})		

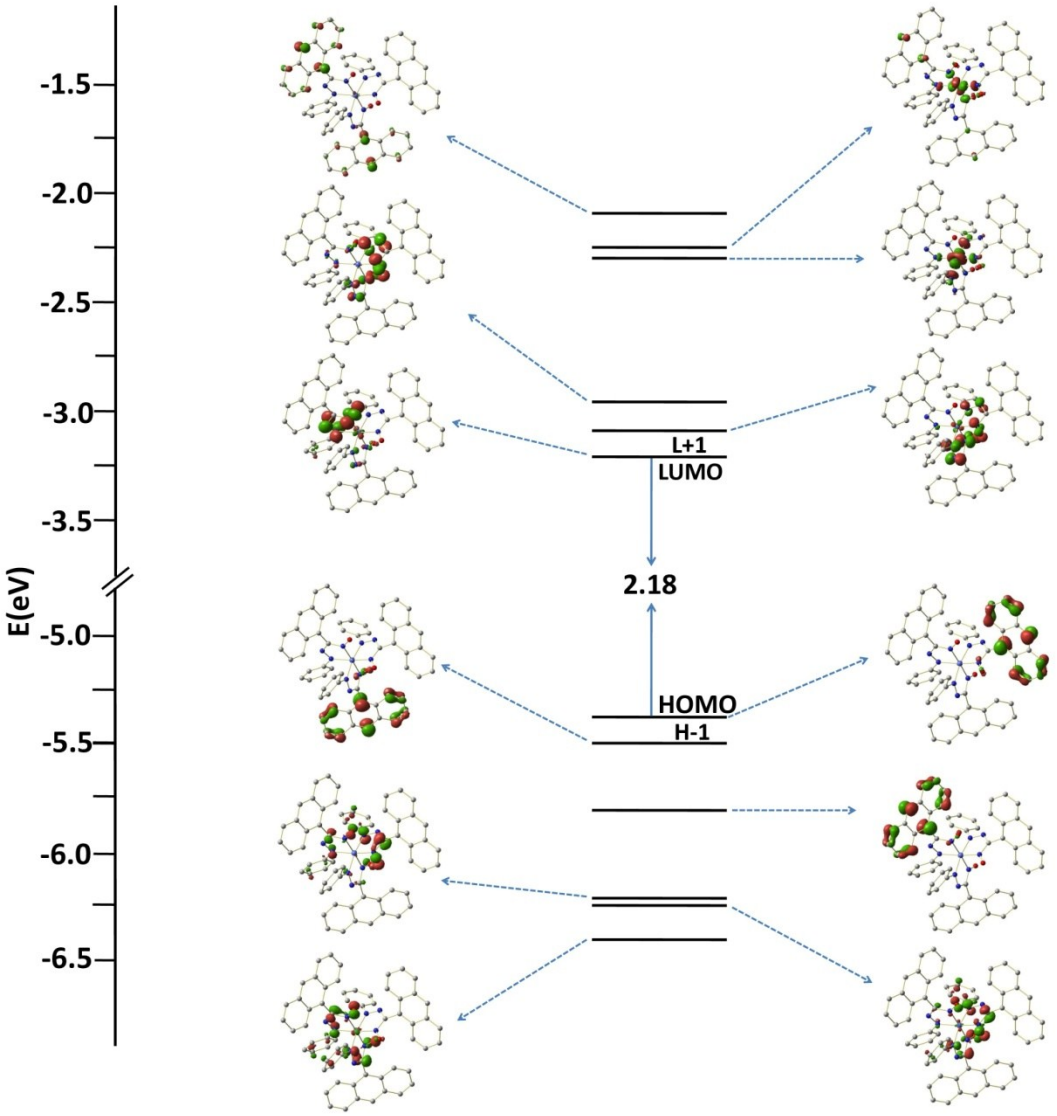


Figure S20 Partial MO diagram and isodensity surface plots(isovalue = 0.06) of selected FMOs for the complex **2b**.

Table S16 Coordinates of Optimized Geometry of **1a**.

Tag	Symbol	X	Y	Z
1	C	1.846433	7.413422	3.768741
2	C	0.447491	7.358255	3.873691
3	H	-0.14753	7.299972	2.971638
4	C	-0.14324	7.37762	5.129314
5	H	-1.2232	7.334609	5.216558
6	C	0.645279	7.452288	6.282707
7	H	0.174154	7.466987	7.259146
8	C	2.033808	7.507272	6.177651
9	H	2.645891	7.565232	7.070285
10	C	2.634874	7.487528	4.922265
11	H	3.711706	7.528603	4.809163
12	N	2.563624	7.396951	2.546207
13	N	1.85327	7.340252	1.51344
14	C	2.595461	7.324624	0.310149
15	N	1.822172	7.262525	-0.71891
16	O	2.530206	7.252524	-1.90839
17	H	1.833001	7.213688	-2.5736
18	C	4.086007	7.35616	0.275364
19	C	4.783651	8.579552	0.291646
20	C	4.784671	6.149087	0.23158
21	C	6.210643	8.560206	0.265579
22	C	4.11814	9.85239	0.332008
23	C	6.172735	6.126428	0.20611
24	H	4.23203	5.216653	0.217868
25	C	6.942741	9.784482	0.280903
26	C	6.909641	7.318203	0.223264
27	C	4.817417	11.01735	0.346746
28	H	6.696934	5.177382	0.172268
29	C	6.252236	11.0311	0.322466
30	C	8.369127	9.766797	0.255164

31	C	8.345426	7.331664	0.197912
32	H	4.292903	11.96669	0.377464
33	C	6.992569	12.22236	0.336968
34	C	9.066786	10.98356	0.271119
35	C	9.041511	8.498512	0.213279
36	H	8.86837	6.381546	0.165292
37	C	8.383794	12.19563	0.311551
38	H	6.467175	13.17101	0.368517
39	H	10.15143	10.97096	0.251637
40	H	10.12634	8.490334	0.19365
41	H	8.940052	13.12624	0.323346
42	H	3.034552	9.874314	0.347774

Table S17 Coordinates of Optimized Geometry of **1b**.

Tag	Symbol	X	Y	Z
1	C	1.845003	6.522537	3.536559
2	C	0.44315	6.523948	3.614259
3	H	-0.13404	6.769875	2.732461
4	C	-0.17314	6.210423	4.817472
5	H	-1.25546	6.209755	4.883543
6	C	0.592681	5.895175	5.94525
7	H	0.101597	5.651613	6.880739
8	C	1.984102	5.894039	5.867235
9	H	2.578512	5.650167	6.740168
10	C	2.610635	6.207344	4.664476
11	H	3.690253	6.21481	4.573028
12	N	2.587897	6.824403	2.368241
13	N	1.900661	7.106241	1.356976
14	C	2.672768	7.400625	0.209692
15	N	1.925974	7.685676	-0.80102
16	O	2.665825	7.975449	-1.93341
17	H	1.987794	8.165609	-2.59238
18	C	4.165993	7.372317	0.209246
19	C	4.833156	6.169514	-0.08692
20	C	4.141015	4.958531	-0.40148
21	H	3.05744	4.960425	-0.41811
22	C	4.823158	3.806992	-0.68214
23	H	4.277949	2.899869	-0.91749
24	C	6.246334	3.784159	-0.66911
25	H	6.768863	2.861554	-0.89516
26	C	6.947479	4.919114	-0.37337
27	H	8.032429	4.91043	-0.36163
28	C	6.274906	6.143629	-0.07217
29	C	6.977777	7.310579	0.235414
30	H	8.063295	7.286802	0.245724

31	C	6.321103	8.50722	0.530684
32	C	7.04108	9.70056	0.847103
33	H	8.125442	9.662296	0.852855
34	C	6.385112	10.86386	1.136172
35	H	6.943353	11.76211	1.374613
36	C	4.962258	10.90308	1.12502
37	H	4.453057	11.83203	1.355868
38	C	4.235517	9.783835	0.826191
39	H	3.152836	9.830529	0.818266
40	C	4.879533	8.545073	0.51758

Table 18 Coordinates of Optimized Geometry of **1c**.

Tag	Symbol	X	Y	Z
1	C	-2.36077	1.923684	2.317369
2	C	-0.97112	1.8687	2.382002
3	C	-0.20826	2.843922	1.742765
4	C	-0.83647	3.875737	1.037332
5	C	-2.22157	3.939662	0.972578
6	C	-2.98833	2.960809	1.621145
7	H	-2.98066	1.1765	2.79848
8	H	-0.48547	1.066301	2.925149
9	H	0.874227	2.800987	1.786549
10	H	-0.23826	4.62775	0.535026
11	H	-2.72198	4.72871	0.426514
12	C	-6.39904	3.821593	1.054726
13	N	-4.41005	2.915652	1.622495
14	N	-4.97674	3.91195	1.131328
15	N	-6.85262	2.710909	0.594974
16	O	-8.23935	2.700324	0.417703
17	H	-8.3836	1.854816	-0.02146
18	C	-7.11358	5.068787	1.410855
19	C	-8.38711	5.047749	2.000295
20	C	-6.48645	6.306446	1.193423
21	C	-9.01344	6.237733	2.357882
22	H	-8.88004	4.103619	2.180184
23	C	-7.12589	7.492573	1.539495
24	H	-5.50054	6.329687	0.749226
25	C	-8.3904	7.462871	2.124736
26	H	-9.99441	6.206564	2.818505
27	H	-6.6335	8.440722	1.354986
28	H	-8.88631	8.387271	2.3989

Table 19 Coordinates of Optimized Geometry of **1d**.

Tag	Symbol	X	Y	Z
1	O	12.76334	27.2344	2.822703
2	N	11.6505	27.94738	3.291717
3	N	9.348774	27.90236	3.466564
4	N	9.353533	28.51907	4.554062
5	C	10.57299	27.27742	3.117528
6	C	8.156606	29.22075	4.858739
7	C	7.066475	29.35839	3.986032
8	H	7.113385	28.9043	3.000766
9	C	5.950014	30.07437	4.394965
10	H	5.10306	30.18598	3.721103
11	C	5.909374	30.65705	5.666362
12	H	5.030722	31.21818	5.977543
13	C	6.994034	30.52389	6.531147
14	H	6.965451	30.97915	7.518489
15	C	8.118411	29.80929	6.126857
16	H	8.981591	29.69348	6.777695
17	C	10.46633	25.93227	2.467395
18	H	10.94037	25.17109	3.099535
19	H	9.416131	25.66984	2.316739
20	H	10.99186	25.92269	1.505617
21	H	13.49121	27.86111	2.93917

Table 20 Coordinates of Optimized Geometry of **2a**.

Tag	**Symbol**	**X**	**Y**	**Z**
1	Co	11.32059	29.3431	4.454591
2	O	10.83261	27.54581	6.591743
3	O	11.08205	30.95702	6.796668
4	O	12.7838	27.37579	2.955354
5	N	11.68177	28.21934	5.982376
6	N	13.8063	28.97413	5.548255
7	N	13.25083	29.67316	4.632816
8	N	10.93853	30.90062	5.555235

9	N	10.86271	30.66397	3.030837
10	C	9.618813	37.22567	6.994136
11	H	10.38181	37.65051	7.642444
12	C	8.502964	37.94285	6.679048
13	H	8.365181	38.94787	7.071568
14	N	11.66024	27.76527	3.344044
15	N	9.37899	27.59591	3.573932
16	N	9.476398	28.65479	4.281403
17	C	12.99198	28.21954	6.326372
18	C	14.15381	30.35768	3.767685
19	C	15.31932	29.71318	3.324319
20	H	15.50171	28.68777	3.624798
21	C	16.20834	30.39018	2.4907
22	H	17.10528	29.88475	2.14245
23	C	15.94594	31.70726	2.097309
24	H	16.64109	32.23169	1.447138
25	C	14.78427	32.34544	2.542726
26	H	14.5768	33.37122	2.250255
27	C	13.88441	31.67406	3.371684
28	H	12.99767	32.18057	3.731808
29	C	13.56874	27.40032	7.416627
30	C	13.17856	27.55869	8.768373
31	C	12.23434	28.55823	9.193925
32	H	11.80687	29.22893	8.456234
33	C	11.8809	28.68363	10.50485
34	H	11.16713	29.44849	10.80296
35	C	12.43268	27.83034	11.52063
36	C	13.38887	26.84274	11.13281
37	C	13.76595	26.7098	9.76016
38	C	14.74084	25.73317	9.387797
39	C	15.30862	24.89173	10.40626
40	H	16.04599	24.14909	10.10963
41	C	14.93846	25.01268	11.71287

42	H	15.37646	24.36685	12.4708
43	C	13.96936	25.99201	12.12478
44	C	13.57907	26.13953	13.46753
45	H	14.0193	25.49062	14.22142
46	C	12.64072	27.10457	13.83651
47	H	12.35096	27.20496	14.8794
48	C	12.07391	27.94296	12.87548
49	H	11.34609	28.696	13.16938
50	C	15.11747	25.62802	8.038346
51	H	15.86151	24.89025	7.747326
52	C	14.54041	26.44811	7.074911
53	H	14.8325	26.34589	6.033527
54	C	10.50252	31.96455	4.834965
55	N	10.43431	31.78194	3.489008
56	C	10.73713	30.50644	1.620519
57	C	9.673959	31.10282	0.921314
58	H	8.929331	31.67069	1.468056
59	C	9.588072	30.9567	-0.46172
60	H	8.758969	31.41146	-0.99744
61	C	10.55829	30.22594	-1.15778
62	H	10.48792	30.11505	-2.23651
63	C	11.61652	29.63851	-0.45825
64	H	12.3818	29.08115	-0.99207
65	C	11.70783	29.76819	0.928465
66	H	12.53848	29.32487	1.46471
67	C	10.19907	33.29058	5.418963
68	C	11.14381	33.86916	6.282776
69	H	12.03619	33.31019	6.543293
70	C	10.96387	35.14449	6.802505
71	H	11.71842	35.57134	7.458917
72	C	9.821897	35.89782	6.483165
73	C	7.482478	37.39374	5.828374
74	C	6.321272	38.11351	5.495116

75	H	6.191163	39.11931	5.888177
76	C	5.343386	37.55255	4.672604
77	H	4.452174	38.12391	4.426123
78	C	5.501593	36.2613	4.167809
79	H	4.73419	35.82628	3.531423
80	C	6.647504	35.50592	4.472952
81	C	7.657104	36.07246	5.309138
82	C	8.832527	35.32207	5.627943
83	C	9.01373	34.00255	5.098067
84	C	7.960812	33.45298	4.284391
85	H	8.057134	32.43813	3.917267
86	C	6.838826	34.16839	3.987228
87	H	6.056089	33.72175	3.377971
88	C	10.53229	27.06584	3.087581
89	C	8.230171	29.19842	4.714118
90	C	7.122844	29.19168	3.850282
91	H	7.234072	28.79322	2.847169
92	C	5.899933	29.69426	4.292727
93	H	5.045181	29.69175	3.621204
94	C	5.773527	30.20034	5.591388
95	H	4.819689	30.59324	5.933067
96	C	6.87906	30.2002	6.447151
97	H	6.785706	30.58253	7.459853
98	C	8.110248	29.70497	6.015111
99	H	8.957241	29.67525	6.689514
100	C	10.49611	25.79711	2.325129
101	C	9.961322	24.61583	2.89837
102	C	9.897474	23.4281	2.09991
103	C	10.38233	23.43692	0.75566
104	C	10.9291	24.62336	0.238027
105	H	11.30419	24.6362	-0.78274
106	C	10.98581	25.77659	1.011586
107	H	11.40278	26.68554	0.590158

108	C	10.29883	22.23202	-0.02415
109	H	10.66906	22.25308	-1.04675
110	C	9.77078	21.08726	0.495145
111	H	9.713854	20.18404	-0.10841
112	C	9.282288	21.03927	1.846522
113	C	9.354741	22.22304	2.645599
114	C	8.88604	22.19392	3.994506
115	C	8.988063	23.39274	4.779017
116	H	8.653037	23.36564	5.813378
117	C	9.499287	24.54571	4.260879
118	H	9.571348	25.42596	4.89037
119	C	8.355209	20.999	4.511535
120	H	8.000803	20.97849	5.539611
121	C	8.282846	19.85002	3.722818
122	H	7.86911	18.93479	4.138446
123	C	8.741762	19.86742	2.404921
124	H	8.685976	18.96775	1.796055

Table S21. Coordinates of Optimized Geometry of **2b**.

Tag	**Symbol**	**X**	**Y**	**Z**
1	C	0.691089	9.062026	18.88734
2	Co	0.132939	10.29912	16.46288
3	N	-0.20836	9.919671	18.35039
4	O	-1.13275	10.42347	19.02637
5	C	2.599634	8.465071	15.96558
6	N	1.632771	8.587102	18.0235
7	O	-0.75957	7.727166	15.66394
8	C	3.891237	8.24954	16.47598
9	H	4.105359	8.502982	17.50858
10	N	1.575413	8.988089	16.81381
11	O	0.013636	10.24249	13.58999
12	C	4.87642	7.705186	15.6541
13	H	5.874947	7.542263	16.05164

14	N	-1.08233	8.907963	15.87595
15	C	4.582615	7.370044	14.32702
16	H	5.352495	6.945284	13.68834
17	N	-2.54096	10.67689	15.93649
18	C	3.295705	7.585093	13.82668
19	H	3.056762	7.320778	12.80036
20	N	-1.52963	11.36215	16.31972
21	C	2.300966	8.134175	14.63713
22	H	1.297187	8.265614	14.25558
23	N	0.560525	10.73782	14.59799
24	C	0.747704	8.649417	20.31452
25	N	2.000202	12.19618	15.64573
26	C	-0.36469	8.02637	20.93559
27	N	1.478054	11.77504	16.73975
28	C	-1.59062	7.751128	20.25109
29	H	-1.68277	8.019306	19.20755
30	C	-2.65631	7.170912	20.89226
31	H	-3.57943	6.995111	20.34705
32	C	-2.57091	6.801729	22.26594
33	H	-3.4264	6.345161	22.75673
34	C	-1.40649	7.01678	22.9549
35	H	-1.31714	6.727651	23.99971
36	C	-0.27526	7.624118	22.32126
37	C	0.920212	7.818158	23.01864
38	H	0.987345	7.495435	24.05611
39	C	2.032497	8.416929	22.41888
40	C	3.248912	8.603883	23.14996
41	H	3.290958	8.247569	24.17689
42	C	4.332219	9.218262	22.57797
43	H	5.251293	9.354033	23.14202
44	C	4.243155	9.69765	21.23986
45	H	5.091156	10.21455	20.79817
46	C	3.094744	9.5321	20.50568

47	H	3.052037	9.935248	19.50178
48	C	1.947515	8.865236	21.0465
49	C	-2.33216	9.37261	15.62829
50	C	-1.85219	12.66745	16.79901
51	C	-3.0307	12.86377	17.53815
52	H	-3.65902	12.01045	17.76577
53	C	-3.36292	14.14021	17.98667
54	H	-4.27026	14.28287	18.5676
55	C	-2.52956	15.22893	17.70473
56	H	-2.79041	16.2228	18.05849
57	C	-1.35675	15.02991	16.9714
58	H	-0.70545	15.86859	16.74084
59	C	-1.01141	13.75368	16.52357
60	H	-0.10923	13.61522	15.94337
61	C	-3.42402	8.58865	14.99198
62	C	-3.97486	7.450811	15.6298
63	C	-3.49685	6.948469	16.88136
64	H	-2.67325	7.453393	17.36996
65	C	-4.04053	5.828224	17.4586
66	H	-3.63781	5.456932	18.39695
67	C	-5.1201	5.136707	16.83586
68	H	-5.53781	4.251511	17.30831
69	C	-5.6239	5.592973	15.64597
70	H	-6.45082	5.079688	15.16011
71	C	-5.07506	6.750282	15.00648
72	C	-5.58983	7.217739	13.79317
73	H	-6.42936	6.695318	13.33765
74	C	-5.04554	8.32948	13.1422
75	C	-5.5677	8.782007	11.88843
76	H	-6.41946	8.254238	11.46481
77	C	-5.00336	9.84332	11.22958
78	H	-5.40398	10.17433	10.2749
79	C	-3.87135	10.50276	11.78973

80	H	-3.40196	11.31877	11.24649
81	C	-3.35128	10.10825	12.99741
82	H	-2.46642	10.60267	13.37813
83	C	-3.92411	9.022297	13.73631
84	C	1.500959	11.70626	14.48403
85	C	2.077965	12.32305	17.91363
86	C	1.28678	12.56887	19.04462
87	H	0.231791	12.32581	19.03691
88	C	1.858751	13.15962	20.17244
89	H	1.23727	13.35244	21.04248
90	C	3.213218	13.50156	20.1853
91	H	3.653868	13.95552	21.0688
92	C	4.002219	13.24842	19.05675
93	H	5.058331	13.50595	19.05947
94	C	3.442966	12.66238	17.92324
95	H	4.045699	12.4694	17.04246
96	C	1.984573	12.25936	13.19097
97	C	1.10029	12.99378	12.3631
98	C	-0.27015	13.23369	12.70262
99	H	-0.66602	12.83369	13.62847
100	C	-1.09451	13.96094	11.88095
101	H	-2.12867	14.12984	12.17014
102	C	-0.60976	14.50069	10.65381
103	H	-1.27824	15.07063	10.01387
104	C	0.697279	14.30288	10.29173
105	H	1.083644	14.71531	9.362279
106	C	1.591021	13.55837	11.12658
107	C	2.9347	13.38634	10.77757
108	H	3.300901	13.82246	9.849793
109	C	3.821776	12.67385	11.59146
110	C	5.197001	12.51437	11.22747
111	H	5.540945	12.97	10.3015
112	C	6.060915	11.80474	12.02073

113	H	7.103204	11.69059	11.73453
114	C	5.586614	11.20164	13.22169
115	H	6.269498	10.62007	13.83541
116	C	4.275178	11.33294	13.60577
117	H	3.935991	10.84529	14.51247
118	C	3.34094	12.08397	12.82101

Table S22 Coordinates of Optimized Geometry of **2c**.

Tag	Symbol	X	Y	Z
1	Co	11.30179	29.34604	4.516285
2	O	10.93361	27.57732	6.675322
3	O	11.20045	30.95146	6.859314
4	O	12.71506	27.4363	2.933367
5	N	11.76694	28.23242	6.020154
6	N	13.84017	29.02609	5.473583
7	N	13.22172	29.70947	4.594596
8	N	10.96011	30.90576	5.632678
9	N	10.72819	30.65381	3.123381
10	N	11.5926	27.78671	3.372028
11	N	9.330136	27.61549	3.685946
12	N	9.464183	28.64013	4.427261
13	C	13.09406	28.23606	6.293829
14	C	14.05947	30.41925	3.683761
15	C	15.1941	29.79027	3.148854
16	H	15.39959	28.75919	3.41389
17	C	16.0188	30.4897	2.268283
18	H	16.89175	29.99748	1.847677
19	C	15.72104	31.81185	1.920155
20	H	16.36572	32.3538	1.233392
21	C	14.58913	32.43309	2.457352
22	H	14.35671	33.46301	2.200448
23	C	13.75292	31.73984	3.333478
24	H	12.89152	32.23201	3.767959
25	C	10.44473	31.95856	4.946509
26	N	10.29369	31.75459	3.60738
27	C	10.48019	30.47095	1.731683
28	C	9.326751	31.00563	1.132802
29	H	8.609965	31.54179	1.745462
30	C	9.112285	30.82915	-0.23274

31	H	8.21403	31.23498	-0.69082
32	C	10.03999	30.12391	-1.00861
33	H	9.867256	29.98446	-2.07235
34	C	11.18492	29.59274	-0.40762
35	H	11.91125	29.04607	-1.00264
36	C	11.40818	29.75771	0.960087
37	H	12.30277	29.35389	1.419398
38	C	10.45926	27.09495	3.118062
39	C	8.247073	29.17588	4.946252
40	C	7.101683	29.23433	4.137027
41	H	7.157187	28.88692	3.110459
42	C	5.916032	29.75017	4.658493
43	H	5.032047	29.80562	4.028553
44	C	5.866413	30.20123	5.982355
45	H	4.941574	30.60499	6.385632
46	C	7.010304	30.13361	6.78379
47	H	6.974987	30.47278	7.815402
48	C	8.205604	29.62719	6.271647
49	H	9.086063	29.54817	6.89795
50	C	13.77765	27.50004	7.372769
51	C	15.15232	27.74341	7.587873
52	C	13.12884	26.55504	8.193021
53	C	15.85006	27.06525	8.583946
54	H	15.66574	28.46928	6.967445
55	C	13.83985	25.8779	9.187285
56	H	12.07627	26.35378	8.052761
57	C	15.19831	26.1259	9.390747
58	H	16.90702	27.27282	8.731231
59	H	13.31967	25.1516	9.806759
60	H	15.74365	25.59727	10.16849
61	C	10.05245	33.27164	5.496542
62	C	9.508934	34.23645	4.618392
63	C	10.19626	33.61483	6.856818
64	C	9.121385	35.49016	5.08376
65	H	9.394232	33.99321	3.568304
66	C	9.803989	34.87654	7.312645
67	H	10.6151	32.89863	7.548903
68	C	9.26583	35.81976	6.436158
69	H	8.705415	36.2131	4.386362
70	H	9.925579	35.11793	8.365639
71	H	8.964092	36.79923	6.798378
72	C	10.32364	25.86647	2.313021
73	C	9.04596	25.27411	2.196237
74	C	11.40759	25.25006	1.654312
75	C	8.861019	24.11513	1.447286
76	H	8.20243	25.72889	2.70276

77	C	11.20987	24.08745	0.904584
78	H	12.39629	25.6784	1.734656
79	C	9.942463	23.51348	0.793975
80	H	7.86784	23.67874	1.375962
81	H	12.06089	23.62929	0.406723
82	H	9.797229	22.60789	0.210452

Table S23 Coordinates of Optimized Geometry of **2d**.

Tag	Symbol	X	Y	Z
1	Co	11.24376	29.39017	4.470009
2	O	10.88698	27.71567	6.743073
3	O	11.164	31.14845	6.745239
4	O	12.5562	27.32579	2.938619
5	N	11.68799	28.33794	6.018452
6	N	13.78941	29.0406	5.429648
7	N	13.18634	29.70149	4.511584
8	N	10.94134	30.99556	5.523479
9	N	10.69269	30.65852	3.015682
10	N	11.47759	27.78643	3.384438
11	N	9.203629	27.69536	3.700643
12	N	9.373625	28.73629	4.425817
13	C	13.01113	28.33032	6.274199
14	C	14.03976	30.32467	3.5582
15	C	15.17811	29.6485	3.090477
16	H	15.37533	28.64262	3.443525
17	C	16.01884	30.26751	2.166459
18	H	16.89373	29.73682	1.799977
19	C	15.73429	31.55708	1.703516
20	H	16.39052	32.03541	0.98129
21	C	14.59913	32.22631	2.171524
22	H	14.37491	33.23118	1.823739
23	C	13.74858	31.61374	3.092774
24	H	12.88203	32.1426	3.469664
25	C	13.58535	27.59608	7.440372
26	C	10.44205	32.01365	4.789387
27	N	10.27887	31.79078	3.466804
28	C	10.43844	30.43423	1.634339
29	C	9.310322	30.99366	1.008784

30	H	8.61748	31.58575	1.596772
31	C	9.09239	30.77533	-0.35025
32	H	8.214239	31.20318	-0.82709
33	C	9.990753	30.00308	-1.09639
34	H	9.816307	29.83378	-2.15561
35	C	11.11118	29.44806	-0.47055
36	H	11.81926	28.85463	-1.04282
37	C	11.33766	29.65526	0.89093
38	H	12.21613	29.23625	1.367238
39	C	10.09615	33.33118	5.403187
40	C	10.31612	27.14919	3.152838
41	C	8.180278	29.31248	4.948248
42	C	7.018145	29.37105	4.162283
43	H	7.044385	28.99053	3.146512
44	C	5.852938	29.92285	4.693081
45	H	4.956794	29.97539	4.080184
46	C	5.837444	30.41066	6.004811
47	H	4.927343	30.83921	6.41622
48	C	6.996612	30.34268	6.784563
49	H	6.98725	30.7042	7.80941
50	C	8.17156	29.79971	6.262555
51	H	9.061659	29.71739	6.874758
52	C	10.24616	25.89032	2.352936
53	H	10.97848	33.7926	5.863445
54	H	9.696722	33.99877	4.636402
55	H	9.352902	33.20396	6.199436
56	H	10.86029	25.10529	2.810817
57	H	9.209707	25.55067	2.295155
58	H	10.63535	26.05029	1.34011
59	H	14.67211	27.70545	7.440999
60	H	13.18103	27.98867	8.381409
61	H	13.32507	26.53169	7.397859

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