Supporting information

Self-assembly of a redox active water soluble Pd_6L_8 'molecular dice'

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Materials and methods: All the chemicals and solvents were purchased from various commercial sources and used without further purification. NMR spectra were recorded in a Bruker 400 MHz spectrometer. The NMR chemical shifts (δ) are reported in ppm (parts per million) and calculated with respect to either solvent signal originated due to incomplete deuteration of the solvents (δ = 4.79 for D_2O, δ = 2.50 for DMSO-d_6 in ^1H NMR) or the internal standard tetramethylsilane protons signal (δ = 0). ESI MS analyses were done on Agilent 6538 Ultra-High Definition (UHD) Accurate Mass Q-TOF spectrometer. Elemental analyses (C, H, N) were carried out in a Perkin Elmer 240C elemental analyser. FTIR spectra were recorded in a Bruker ALPHA spectrometer. Single crystal X-Ray data of **MC-1**·$(NO_3)_{36}$ was collected in synchrotron radiation source and the structure was solved by direct methods using SHELX-2014 software package incorporated in WinGX.[1] All the non-hydrogen atoms in the main fragment were refined with anisotropic displacement coefficients and the hydrogen atoms were fixed at the geometric positions suggested by the software. Appropriate restraints were used in order to stabilize the model during refinement. SQUEEZ option in PLATON[2] was used in the last refinement to model the scattering contribution of the disordered anions and solvent molecules to the calculated structure factor which suggested the formula unit to be $(Pd_6C_{336}H_{312}N_{48})\cdot 36(NO_3)\cdot 245(H_2O)$. Cyclic voltammograms were recorder in a CHI617 instrument.

Experimental Section:

Synthesis of L·$(NO_3)_3$**:** 2000 mg (12.8 mmol) 4,4′-bipyridine was taken in a 250 mL round bottom flask and dissolved in 10 mL acetonitrile then heated at 70 °C. A solution of 1,3,5-tris(bromomethyl)-2,4,6-trimethylbenzene (**3**) (850 mg, 2.13 mmol) in 150 mL acetonitrile was added to it very slowly for 3h with vigorous stirring. A pale yellow solid started to form after sometime. The solution was refluxed at 85 °C for another 24 h. The heavy solid formed was isolated by filtration followed by washing with chloroform and dried under vacuum. The

product (**1**, 2 mmol) was dissolved in 50 mL water and a concentrated aqueous solution of silver nitrate (1020 mg, 6 mmol) was added to it to get heavy precipitate. The solution was stirred overnight in dark and was diluted with 50 mL water after the reaction and filtered through celite. Evaporation of the solvent gave **L**·$(NO_3)_3$ as dirty white powder. Yield: 1550 mg, 89.4% with respect to **3**. ^{1}H NMR (400 MHz, D_2O): δ= 8.81 (6H, d, *J* = 6.73 Hz), 8.73 (6H, d, *J* =6.17 Hz), 8.39 (6H, d, *J* = 6.79 Hz), 7.85 (6H, d, *J* = 6.29 Hz), 2.34 (9H, s); ^{13}C NMR (100 MHz, D_2O): δ= 154.7, 150.4, 144.6, 144.2, 142.7, 129.2, 126.7, 122.8, 59.1, 16.7; ESI MS: m/z= 344.4 [**L**·$(NO_3)_3$–$2NO_3^-$]$^{+2}$; Anal Calc for $C_{42}H_{39}N_9O_9$: C, 61.99; H, 4.83; N, 15.49. Found: C, 61.69; H, 4.92; N, 15.80.

Synthesis of MC-1·$(NO_3)_{36}$**:** 100 mg (0.12 mmol) of **L**·$(NO_3)_3$ was dissolved in 10 mL water and 22.9 mg (0.09 mmol) of solid $Pd(NO_3)_2$·H_2O was added to it. The brown clear solution was then heated at 60 °C for 12h. The final solution was concentrated to 1 mL and treated with 50 mL acetone to obtain brown precipitate. The product was collected by filtration and dried under vacuum to get 113 mg of **MC-1**·$(NO_3)_{36}$. Isolated yield: 92 %. ^{1}H NMR (400 MHz, D_2O): δ= 9.15 (48H, d, *J* = 6.60 Hz), 8.87 (48H, d, *J* = 6.73 Hz), 8.41 (48H, d, *J* = 6.84 Hz), 8.11(48H, d, *J* = 6.76 Hz), 2.28 (72H, s); ^{13}C NMR (100 MHz, D_2O): δ= 152.6, 151.7, 146.0, 145.6, 144.4, 128.0, 126.9, 124.1, 59.1, 16.8; ESI MS: m/z= 1668.48 [**MC-1**·$(PF_6)_{36}$–$6PF_6^-$]$^{+6}$, 1215.12 [**MC-1**·$(PF_6)_{36}$–$8PF_6^-$]$^{+8}$; Anal Calc for $C_{336}H_{422}N_{84}O_{163}Pd_6$ (including 55 H_2O molecules): C, 45.43; H, 4.79; N, 13.24. Found: C, 45.44; H, 4.61; N, 12.26.

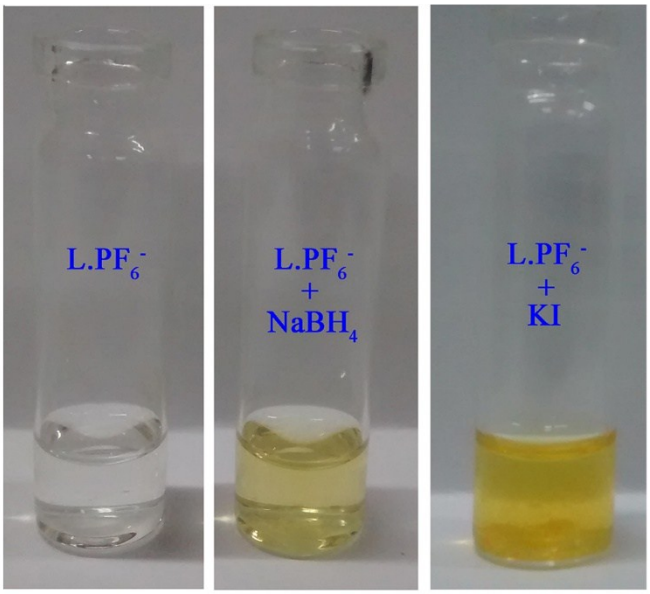

Figure S1: **L**·$(PF_6)_3$ (left), **L**·$(PF_6)_3$ + $NaBH_4$ (middle) and **L**·$(PF_6)_3$ + KI (right) in MeCN. The colouration appears due to the reduction of **L**.$(PF_6)_3$ as well as oxidation of I^- to I_2 in the case of treatment with KI.

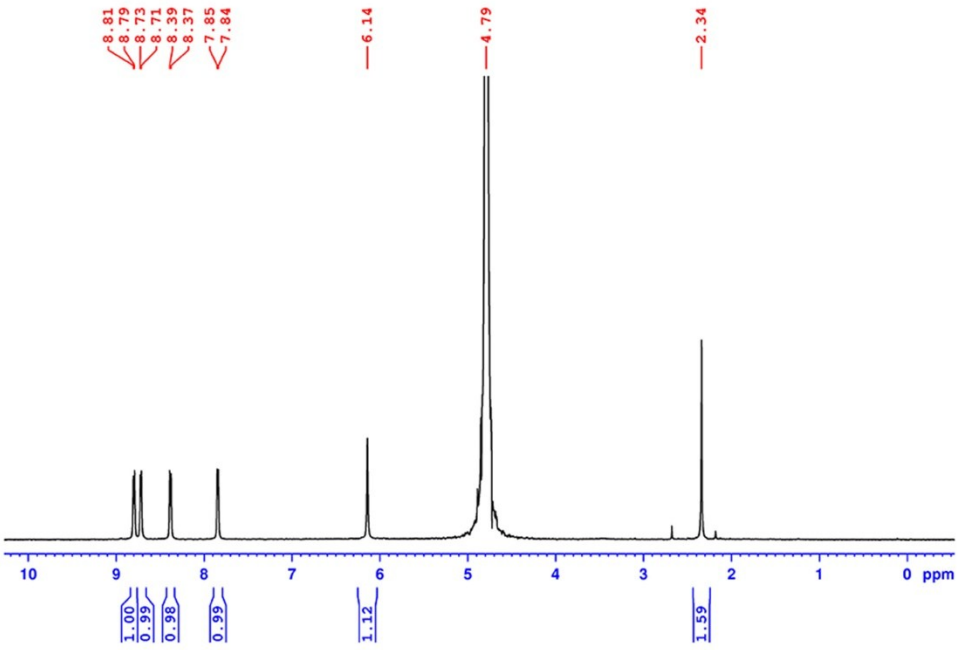

Figure S2: ^{1}H NMR spectra of **L**· **$(NO_3)_3$** in D_2O.

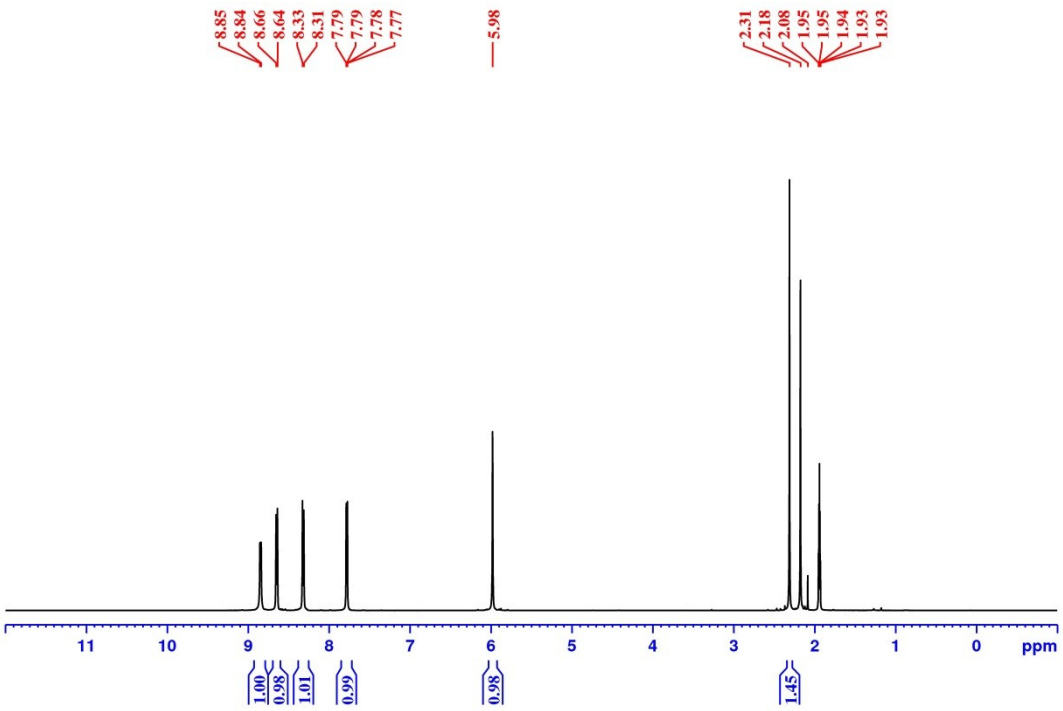

Figure S3: ^{1}H NMR spectra of L· $(PF_6)_3$ in CD_3CN.

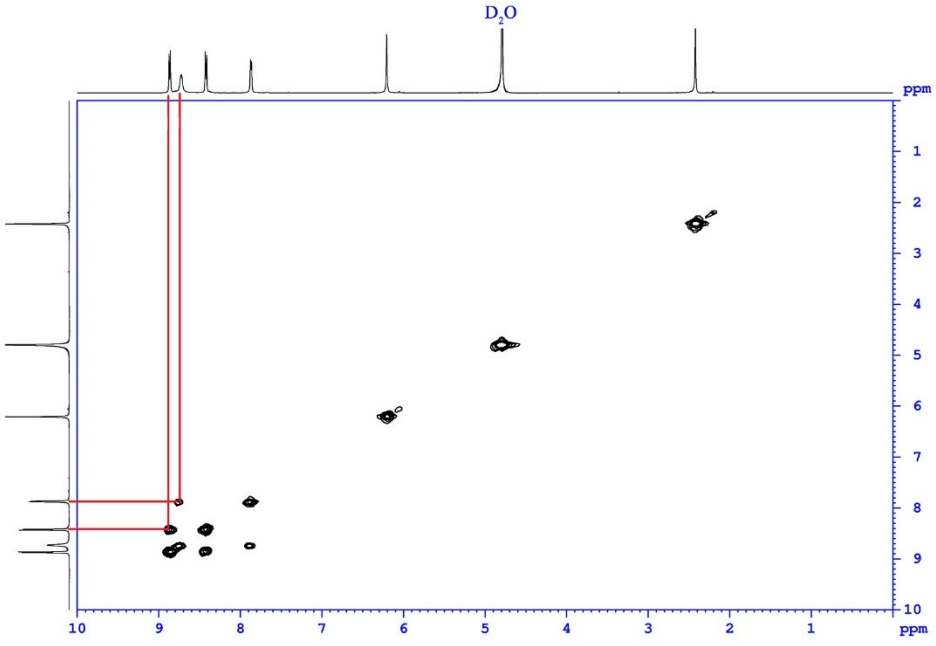

Figure S4: ^{1}H-^{1}H COSY spectra of **L·$(NO_3)_3$** in D_2O.

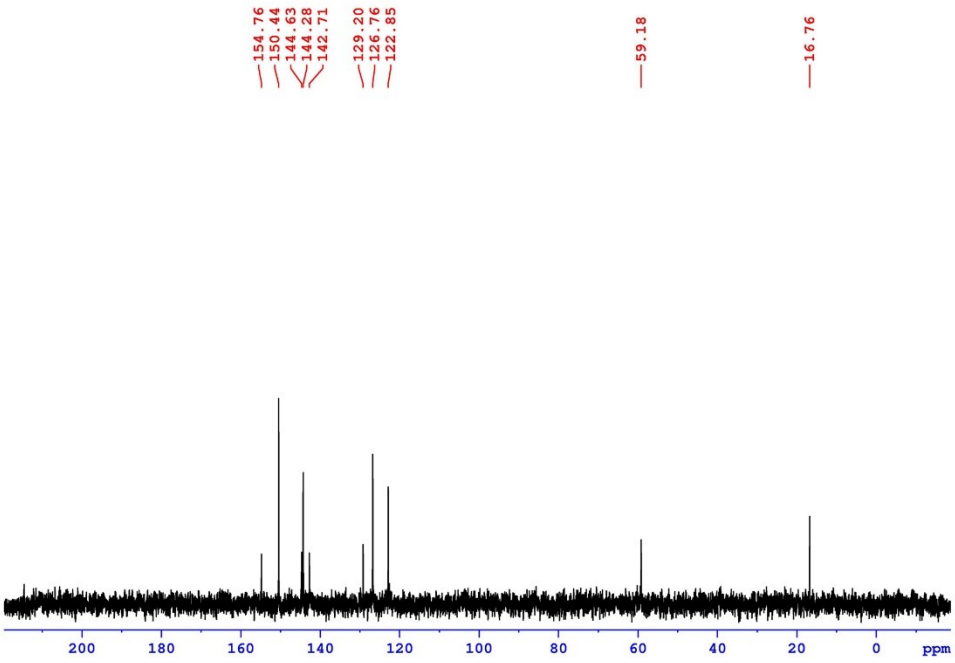

Figure S5: ^{13}C NMR spectra of **L·(NO$_3$)$_3$** in D_2O.

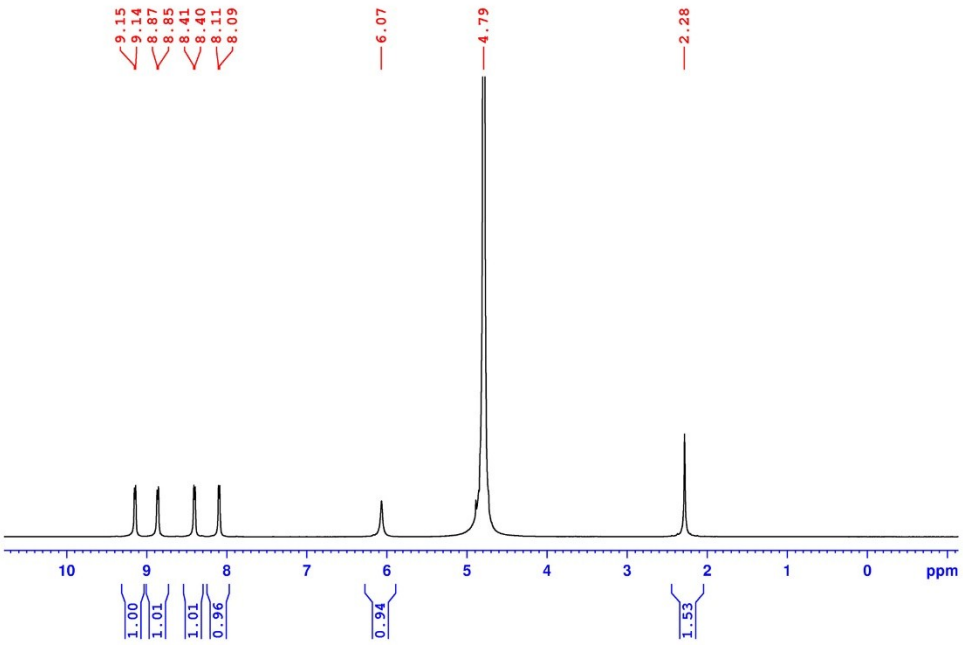

Figure S6: ^{1}H NMR spectra of [**MC-1**· **(NO$_3$)$_{36}$]** in D_2O.

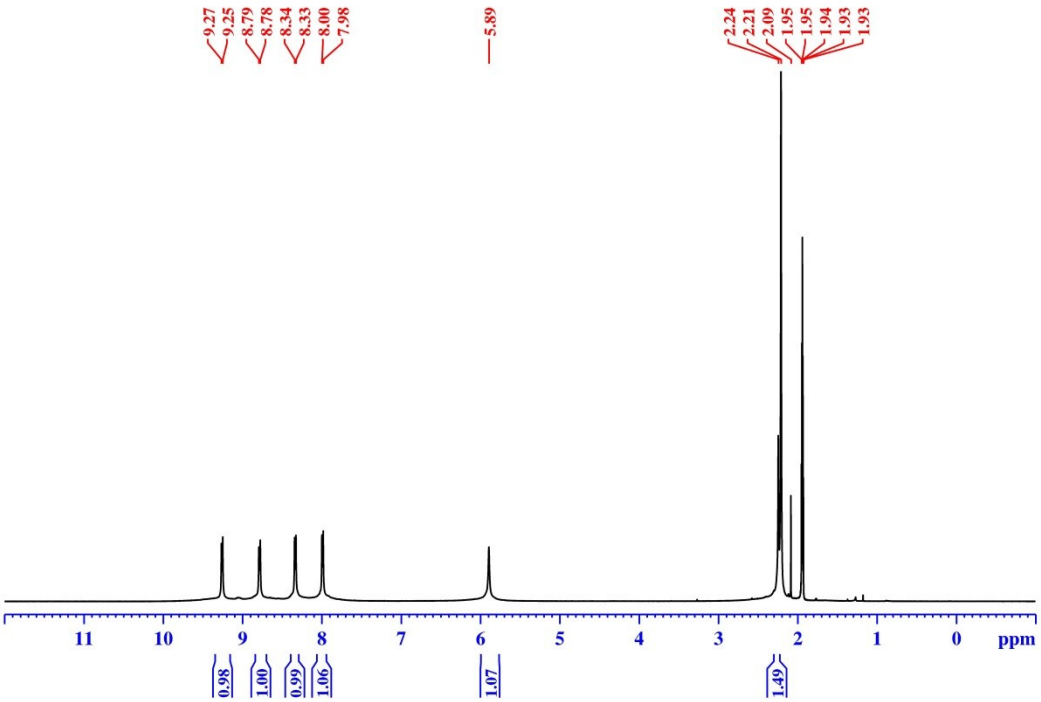

Figure S7: ^{1}H NMR spectra of **[MC-1·(PF$_6$)$_{36}$]** in CD_3CN.

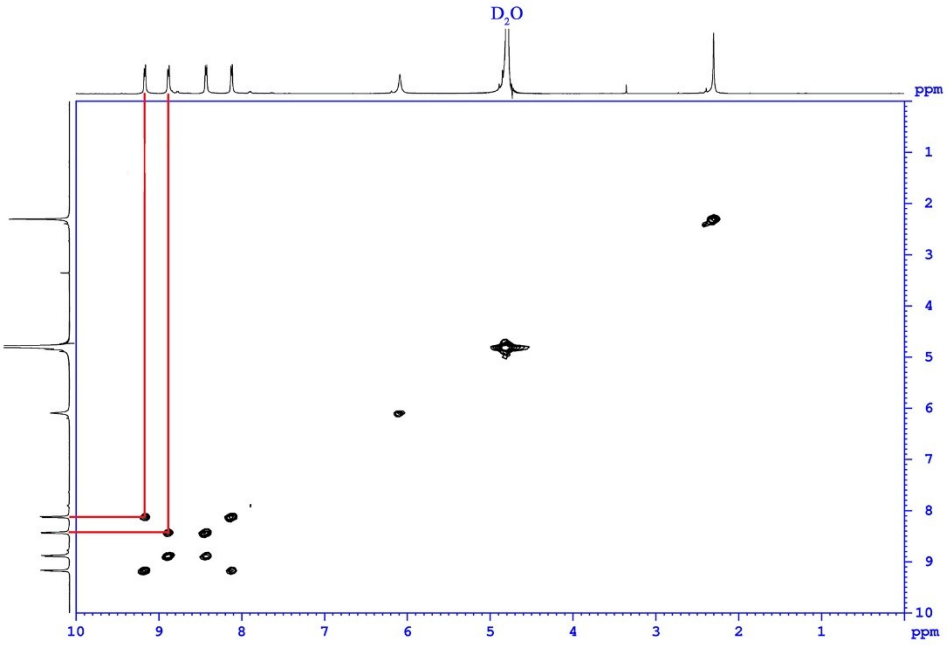

Figure S8: ^{1}H-^{1}H COSY spectra of [**MC-1**· **(NO$_3$)$_{36}$]** in D_2O.

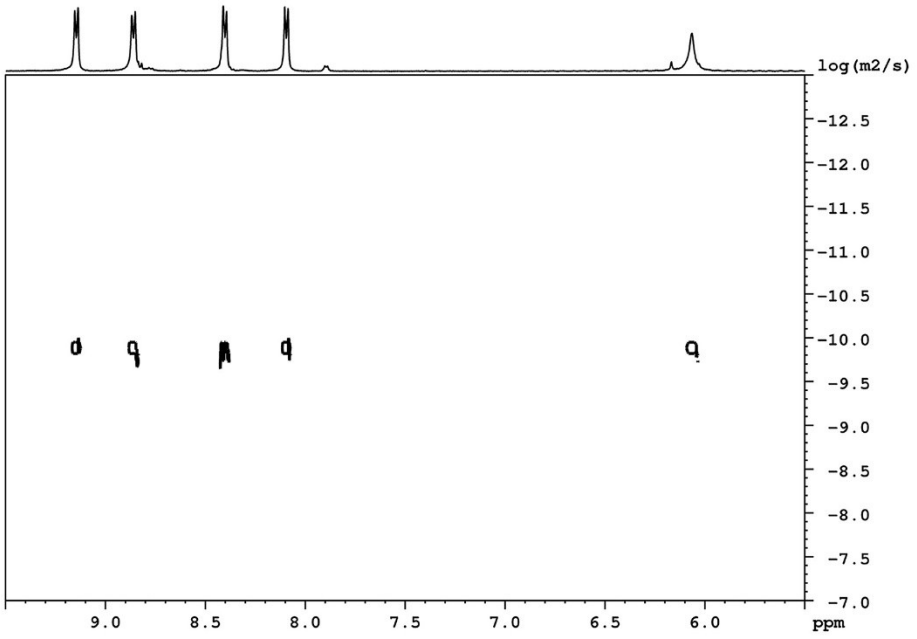

Figure S9: Partial DOSY spectra of [**MC-1**· **$(NO_3)_{36}$**] in D_2O.

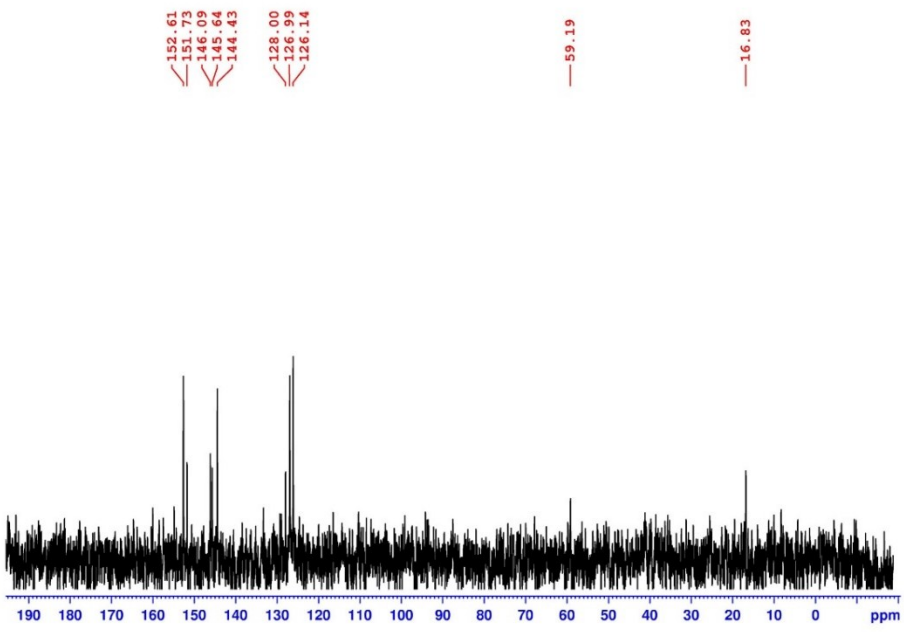

Figure S10: ^{13}C NMR spectra of [**MC-1**· **$(NO_3)_{36}$**] in D_2O.

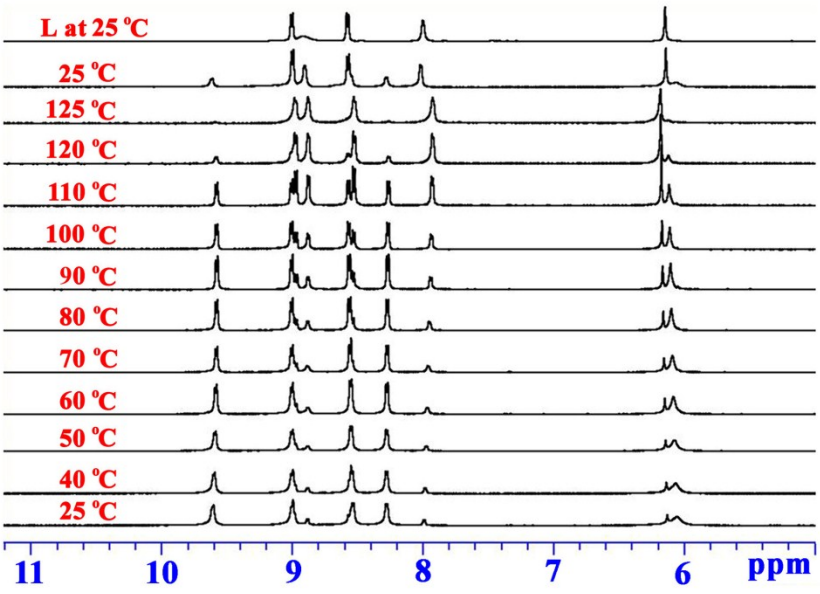

Figure S11: Variable temperature (VT) ^{1}H NMR spectra of **[MC-1·(NO$_3$)$_{36}$]** in DMSO-d$_6$ stacked by keeping the solvent peak position fixed at δ = 2.50 ppm.

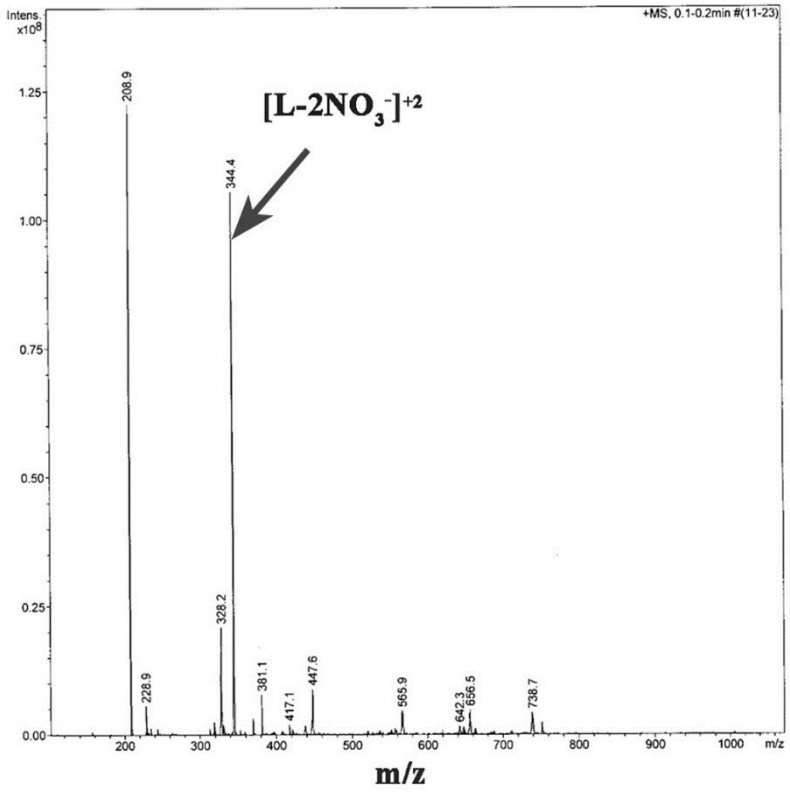

Figure S12: ESI MS spectra of **L·(NO$_3$)$_3$**.

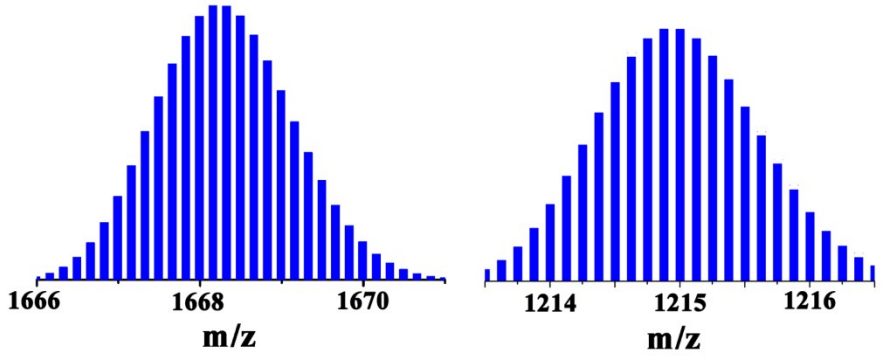

Figure S13: Calculated isotopic distribution pattern for the +6 and +8 charged fragments of **[MC-1·(PF$_6$)$_{36}$]**.

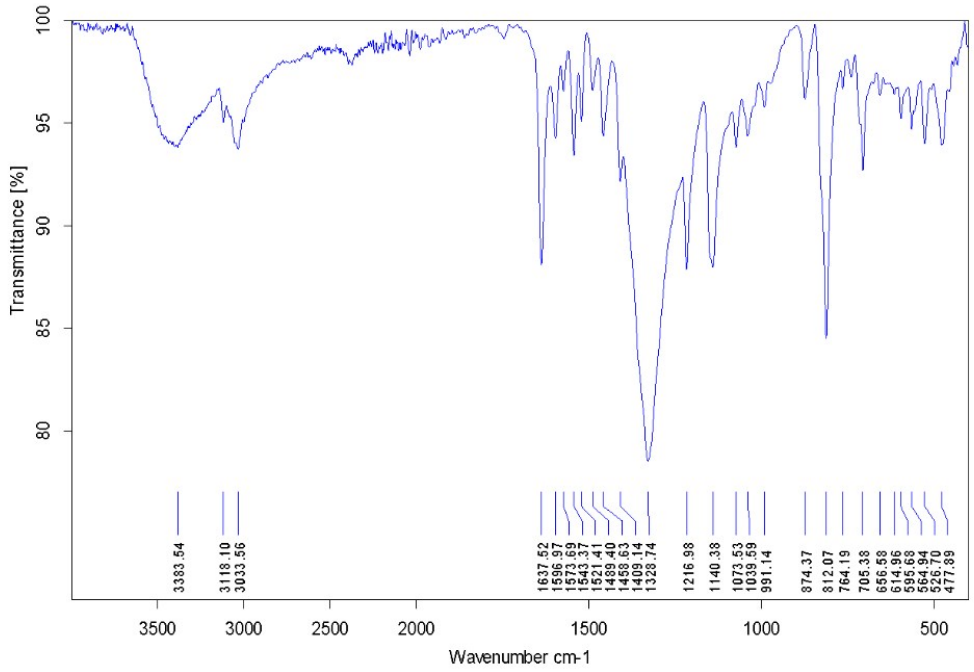

Figure S14: FTIR spectra of **L·(NO$_3$)$_3$**.

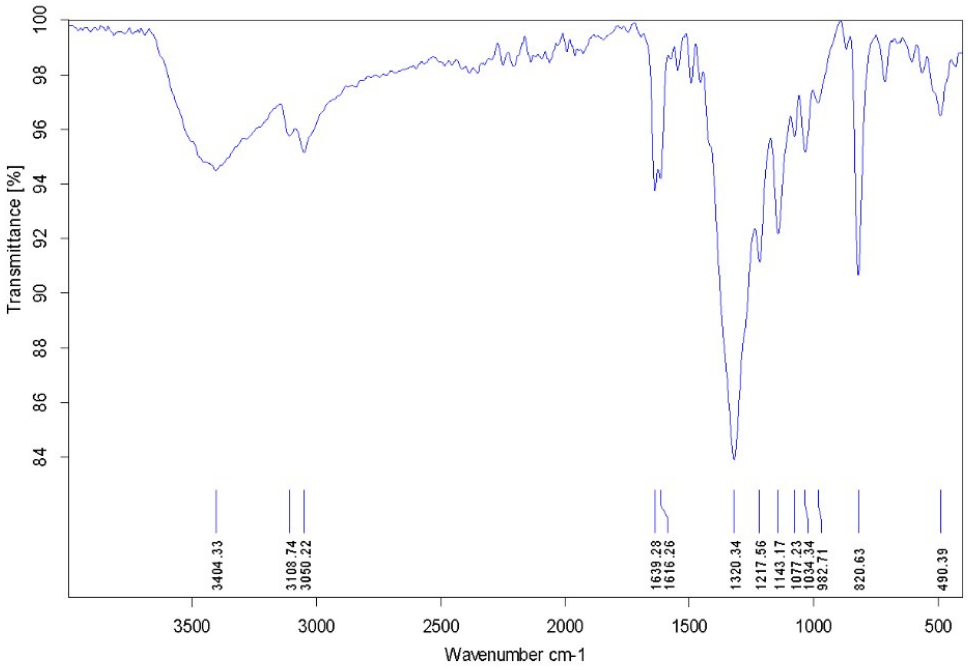

Figure S15: FTIR spectra of [**MC-1·$(NO_3)_{36}$**].

Crystallographic table:

Identification code	**[MC-1.$(NO_3)_{36}$]**
Empirical formula	$C_{336}H_{312}N_{48}O_{38}Pd_6$
Formula weight	6268.72
Temperature (k)	100 (2)
wavelength	0.77000
Crystal system	tetragonal
Space group	I4/m
Unit cell dimension	
a (Å)	33.231(3)
b (Å)	33.231(3)
c (Å)	28.780(2)
α (°)	90
β = 90°	90
γ = 90°	90
Volume ($Å^3$)	31782(7)
Z	2
ρ (g/cm^{-3})	0.655
μ (mm^{-1})	0.223
F(000)	6488.0
2θ range for data collection	1.87° to 37.28°
Reflections collected	29461
Independent reflections	4703
GooF	1.104
Final R indexes [$I \geq 2s(I)$]	R_1[a] = 0.0800; wR_2[b] = 0.2384
Final R indexes [all data]	R_1[a] = 0.0973; wR_2[b] = 0.2563
CCDC no.	1445058

[a]$R_1 = \Sigma||F_o| - |F_c||\Sigma|F_o|$. [b]$wR_2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$.

Important bond distances and bond angles:

Pd2-Pd2 (Å)	**20.2462(28)**	**N4-Pd2-N4 (°)**	**89.77(4)**
Pd1-Pd1 (Å)	**20.9618(24)**	**N2-Pd1-N6 (°)**	**90.3(3)**
Pd1-Pd2 (Å)	**14.5714(17)**	**N6-Pd1-N6 (°)**	**89.6(4)**
Pd1-Pd1 (Å)	**14.8222(23)**	**N2-Pd1-N2 (°)**	**89.9(4)**
Pd2-N4 (Å)	**1.985(9)**		
Pd1-N2 (Å)	**2.009(8)**		
Pd1-N6 (Å)	**2.038(9)**		

Cyclic voltammetry study:

10^{-4} M solution of [**MC-1·$(PF_6)_{36}$**] was used for recording CV while 8×10^{-4} M solution was used in case of **L·$(PF_6)_3$**. NH_4PF_6 was used as supporting electrolyte in 10^{-2} M concentration. The potential was applied with respect to Ag/AgCl electrode while glassy carbon and platinum were used as working and counter electrodes respectively. The voltage was swept from positive to negative potential with the mentioned scan rate.

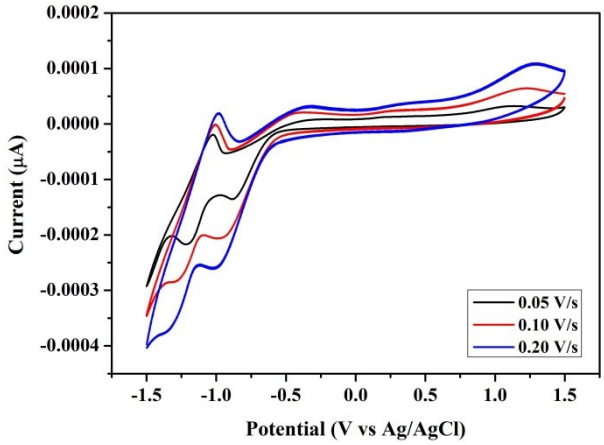

Figure S16: CV spectra of [**MC-1·$(PF_6)_{36}$**] ($1x10^{-4}$ M) at different scan rate recorded in acetonitrile.

DFT calculation:

Syn and *anti* conformation of L·$(NO_3)_3$ (without counter ions):

The geometries of the conformers were optimized using B3LYP method and 6-311G** basis set in Gaussian 09 package. Frequency calculations were also carried out for the optimized geometries to assure that the geometries had attained the global minima.

Calculation of free energy change (ΔG) for the formation of the model complex MC-1':

The geometries of **L'** and **ML-1'** were optimized in gas phase using 6-31+G** basis set for C, H and N atoms and LANL2DZ basis set for Pd atom. As the original complex **MC-1·$(NO_3)_{36}$** has a fixed geometry, the frequency calculations for the model compounds were carried out with the gas phase optimized structures in solvent medium using polarization continuum model (PCM).

DMSO solvent medium:

Sum of electronic and thermal free energies for **MC-1'** complex= –2266.430555 Hartree

Sum of electronic and thermal free energies for **L'**= –535.014675 Hartree

Sum of electronic and thermal free energies for $\mathbf{Pd^{+2}}$ ion= –126.259811 Hartree

ΔG_{DMSO}= -2266.430555-{4×(-535.014675)+(-126. 259811)} Hartree = -0.112044 Hartree = **-70.3** Kcal/mol.

Aqueous medium:

Sum of electronic and thermal free energies for **MC-1'** complex= –2266.450423 Hartree

Sum of electronic and thermal free energies for **L'**= –535.015451 Hartree

Sum of electronic and thermal free energies for $\mathbf{Pd^{+2}}$ ion= –126.265698 Hartree

ΔG_{H2O}= –2266.450423 –{4×(–535.015451)+(–126.265698)} Hartree = –0.122921 Hartree = –**77.1** Kcal/mol.

❖ Optimized coordinates of *syn*-conformer of **L·(NO$_3$)$_3$** (without counter ions):

C	0.47756300	3.31949700	-0.40251400
H	0.08136300	2.32939000	-0.22807400
C	0.70835800	4.21525800	0.61653000
H	0.49403800	3.90773200	1.63089600
C	1.23836200	5.49505400	0.35171200
C	1.51506600	5.78545700	-1.00121000
H	1.90062700	6.75246700	-1.29489800
C	1.26700200	4.85844000	-1.98321700
H	1.45361400	5.06471700	-3.02926700
C	1.48780900	6.47101900	1.41926500
C	0.71261900	6.48079200	2.58938200
H	-0.11558400	5.79723300	2.73223400
C	0.98357100	7.43653200	3.56416700
H	0.38800900	7.48062400	4.47038400
C	2.70406700	8.32809400	2.34716400
H	3.49420100	9.06975900	2.29030100
C	2.50627700	7.42940200	1.30187500
H	3.16365600	7.46412600	0.44167900
C	-8.78488900	-1.76410000	2.45371400
H	-9.81454800	-1.42518200	2.40316000
C	-7.91069200	-1.51803600	1.39787400
H	-8.26277800	-0.96534800	0.53538900
C	-6.58096600	-1.95274000	1.50779000
C	-6.20799600	-2.62771700	2.68058500
H	-5.21008600	-3.02666700	2.81719800
C	-7.16816100	-2.83797500	3.66596300
H	-6.91404200	-3.37415500	4.57470300
C	-5.61349600	-1.71329000	0.43020300
C	-6.01026200	-1.63017200	-0.92114200
H	-7.04485100	-1.76505000	-1.20650600
C	-5.08507400	-1.41175700	-1.91210900
H	-5.36268700	-1.36330300	-2.95716800
C	-3.34663200	-1.33379600	-0.34312500
H	-2.28783800	-1.19480400	-0.17785100
C	-4.23534300	-1.55319800	0.68447900
H	-3.85671700	-1.57778200	1.69713600

C	-2.81488100	-1.10517900	-2.78973800
H	-3.30984100	-0.42599300	-3.48207700
H	-2.77618400	-2.07695900	-3.27938200
C	2.67428200	0.84911600	-2.56759700
H	3.01372600	0.98667300	-3.60097500
H	3.37405200	0.16729700	-2.08600700
H	2.78433900	1.80688700	-2.05999000
C	-1.40838100	-0.60404300	-2.50742300
C	-0.34048200	-1.52476700	-2.47752400
C	0.98708800	-1.04512200	-2.51125500
C	1.24896300	0.33952800	-2.51835400
C	0.17144400	1.25040900	-2.53852100
C	-1.15928900	0.78566100	-2.51570800
C	-2.31745900	1.76156200	-2.56156900
H	-3.20195400	1.37278500	-2.05883700
H	-2.60447100	1.99348000	-3.59377300
H	-2.08247800	2.70708000	-2.07335600
C	0.44758200	2.71271200	-2.84324000
H	-0.40022200	3.15542000	-3.36352400
H	1.30154300	2.78987800	-3.51427600
C	-0.61007600	-3.01620600	-2.46555900
H	0.17797300	-3.57114700	-1.95710700
H	-0.68820800	-3.42040900	-3.48127100
H	-1.53706200	-3.26383100	-1.94889800
C	2.11988900	-2.01472900	-2.80063400
H	1.73951100	-2.87943300	-3.34202000
H	2.85311300	-1.53725800	-3.44891700
C	2.57750700	-2.33988100	-0.34465800
H	1.72402700	-1.69912300	-0.17519500
C	3.31038900	-2.88690300	0.68429800
H	3.02487000	-2.65424600	1.70108100
C	4.42847200	-3.70527800	0.42339800
C	4.73771000	-3.92141600	-0.93649700
H	5.56348800	-4.55778400	-1.22476900
C	3.97500000	-3.35548700	-1.92773900
H	4.18328400	-3.51697200	-2.97767900
C	4.64650900	-4.62812300	2.73750400
H	3.58903000	-4.48809600	2.92646200
C	5.44650400	-5.20159700	3.72144100
H	5.02155500	-5.48351100	4.67946300
C	7.30576200	-5.12307200	2.38963800

H	8.36784000	-5.32287200	2.29128800
C	6.59405600	-4.56447500	1.33080000
H	7.11577100	-4.31058500	0.41611900
C	5.22647000	-4.30076400	1.50200700
N	-3.76367200	-1.26180500	-1.62875500
N	2.90414400	-2.56899900	-1.63745200
N	-8.42907400	-2.41219800	3.56466100
N	1.96048200	8.33940600	3.45523500
N	6.74966600	-5.44084600	3.56037300
N	0.75480200	3.63340000	-1.68954900

Energy: -1952.04481272 Hartree

- Optimized coordinates of *anti*-conformer of **L·$(NO_3)_3$** (without counter ions):

C	2.55523800	-2.71011600	0.22562200
H	2.25351700	-1.74047900	-0.14351800
C	3.58794200	-3.42522800	-0.33633700
H	4.12429100	-2.98790200	-1.16735100
C	3.96495800	-4.68216600	0.18005800
C	3.22114600	-5.14894700	1.28505700
H	3.42687200	-6.11553400	1.72467000
C	2.19692900	-4.39968800	1.80924000
H	1.60999100	-4.73852300	2.65313000
C	5.06771600	-5.46067300	-0.39597700
C	5.39379300	-5.36040700	-1.75755400
H	4.82333600	-4.73907400	-2.43733600
C	6.44555700	-6.12612400	-2.25204600
H	6.70857400	-6.08329400	-3.30410900
C	6.87690900	-7.03375500	-0.19604900
H	7.49627000	-7.69890700	0.39687300
C	5.83283300	-6.32904800	0.39780600
H	5.65987800	-6.43342900	1.46201000
C	-10.42036900	-0.73682600	-1.01410200
H	-11.16060100	-1.02166800	-1.75470400
C	-9.06406800	-0.76691900	-1.32768700
H	-8.75476500	-1.10079600	-2.31054800
C	-8.13428900	-0.41262400	-0.33761900
C	-8.63047100	-0.03630600	0.92060000

H	-7.97482100	0.28205800	1.72197700
C	-10.00770600	-0.02324400	1.12076300
H	-10.42045500	0.27991400	2.07758500
C	-6.69264300	-0.43706400	-0.60913600
C	-6.17415700	-0.22335400	-1.90443100
H	-6.82999300	-0.00627200	-2.73665600
C	-4.82087400	-0.25780600	-2.13483800
H	-4.40201600	-0.09714700	-3.11966400
C	-4.39743800	-0.70094100	0.12701400
H	-3.65332400	-0.89033500	0.88740600
C	-5.74382900	-0.67517100	0.40729200
H	-6.06029900	-0.87227900	1.42248000
C	-2.47653200	-0.62089600	-1.48232600
H	-2.30553000	0.08094300	-2.29729800
H	-2.35234700	-1.61830500	-1.89751200
C	1.58617600	0.33323800	2.61878000
H	1.20798500	0.25050800	3.64402500
H	2.02324400	1.32458400	2.51428400
H	2.41256500	-0.37103900	2.52074200
C	-1.48982400	-0.37471000	-0.35525200
C	-1.21196600	0.94292200	0.06572300
C	-0.22929900	1.15812700	1.05482700
C	0.49578300	0.07741800	1.59706600
C	0.17009800	-1.23990800	1.20701600
C	-0.81742800	-1.47292600	0.22564800
C	-1.14690500	-2.88297600	-0.22292200
H	-2.22223400	-3.07355400	-0.22403300
H	-0.69933700	-3.64591300	0.40803300
H	-0.78352400	-3.06918900	-1.23861400
C	0.77676100	-2.40311200	1.97238100
H	0.00163400	-3.12522400	2.22563800
H	1.20087900	-2.06093600	2.91370400
C	-1.97837400	2.11688400	-0.50733600
H	-1.35569800	3.00494300	-0.61758300
H	-2.82138100	2.39138800	0.13636900
H	-2.39008600	1.90991800	-1.49301200
C	-0.06641900	2.54222000	1.65833700
H	-0.98760400	3.11233700	1.54924600
H	0.12916000	2.46056600	2.72611400
C	1.63272200	3.18114800	-0.08319200
H	1.33143500	2.28242600	-0.60210500

C	2.58494000	4.03895100	-0.58456000
H	3.05124600	3.79342200	-1.52895300
C	2.96759300	5.19495400	0.12689500
C	2.32118600	5.40559900	1.36366300
H	2.53683700	6.28026000	1.96239100
C	1.37544300	4.52201700	1.82153800
H	0.85449300	4.67215900	2.75834600
C	4.17421400	6.29938200	-1.76508400
H	3.56391800	5.78513900	-2.49765000
C	5.14163200	7.20267600	-2.19592000
H	5.30084500	7.37223000	-3.25596400
C	5.73684800	7.73454500	-0.05114700
H	6.38429900	8.31249100	0.60032600
C	4.78460100	6.87322400	0.48768200
H	4.71222000	6.76894400	1.56337700
C	3.97977600	6.12556600	-0.38582100
N	-3.93551400	-0.49190300	-1.13006900
N	1.03316200	3.41564700	1.10830400
N	-10.88917600	-0.36905500	0.18009300
N	7.17929600	-6.94246800	-1.49267800
N	5.91422000	7.90335800	-1.36299100
N	1.86248500	-3.19015800	1.28532000

Energy: -1952.04930731 Hartree

- Optimized coordinates of model ligand **L'**:

N	-4.06043300	-0.00202500	0.00462000
C	-3.36919000	1.09349400	-0.33222500
H	-3.95524900	1.96642100	-0.60793900
C	-3.36632900	-1.09646100	0.33921100
H	-3.95008600	-1.97037200	0.61668900
C	-1.97137700	-1.15272700	0.34523200
H	-1.47407000	-2.06758700	0.65091000
C	-1.24732300	0.00021800	0.00002200
C	0.22805700	0.00109200	-0.00236800
C	-1.97431600	1.15194100	-0.34297500
H	-1.47950400	2.06745200	-0.65070500
N	3.02720100	0.00453000	-0.01430200
C	2.34793200	-1.12226600	-0.34513600

H	2.94625800	-1.98456800	-0.61425300
C	2.34807700	1.12885700	0.32490900
H	2.94656200	1.99232500	0.58990300
C	0.96817000	-1.14895700	-0.34638300
H	0.47029600	-2.06368300	-0.64525400
C	0.96825300	1.15242500	0.33689300
H	0.47055400	2.06761700	0.63465500
C	4.51000800	-0.00718500	0.02365700
H	4.84553700	-0.30643300	1.01933800
H	4.87986800	-0.71164600	-0.72072200
H	4.88068500	0.99035800	-0.20987200

Energy: -535.09614669 Hartree

❖ Optimized coordinates of model complex **ML-1'**:

N	0.04592500	6.54104700	6.52466800
C	1.04650100	5.63095900	6.47520100
H	1.82316300	5.71984500	7.22717500
C	0.03754100	7.58334500	7.59914100
H	-0.50029600	7.18983800	8.46568400
H	1.06599400	7.82120200	7.86987100
C	0.02894700	4.55665500	4.55644800
C	1.06260500	4.63642300	5.50624400
H	1.88044500	3.92476500	5.52707500
C	-0.96435200	6.49098600	5.62535800
H	-1.73412100	7.24992100	5.71484700
C	0.02290400	3.49870500	3.49973800
C	1.21198400	3.04713800	2.89879900
H	2.17691700	3.46676100	3.16412400
C	1.16915300	2.06068200	1.91658700
H	2.08545400	1.71563200	1.44967700
C	-1.17153300	2.90368300	3.05453000
H	-2.13279500	3.17413200	3.47929800
N	0.01220800	1.49827400	1.49896200
C	-1.13974700	1.92106300	2.06780400
H	-2.05949600	1.45749600	1.72796700
C	-0.99741200	5.51406600	4.63913600
H	-1.81927200	5.53819600	3.93224400

Pd	-0.00000300	0.00000100	0.00000000
N	-0.01221600	-1.49826900	1.49896100
C	-1.16915900	-2.06067900	1.91658500
H	-2.08546100	-1.71563000	1.44967700
C	1.13974100	-1.92105700	2.06780000
H	2.05948900	-1.45748800	1.72796500
C	1.17152900	-2.90367900	3.05452500
H	2.13279200	-3.17412800	3.47929100
C	-0.02290700	-3.49870400	3.49973200
C	-0.02894700	-4.55665600	4.55644000
C	-1.21198700	-3.04713800	2.89879600
H	-2.17692000	-3.46676200	3.16412000
N	-0.04591900	-6.54105200	6.52465700
C	0.96435900	-6.49098600	5.62534700
H	1.73413000	-7.24991900	5.71483400
C	-1.04649700	-5.63096700	6.47519100
H	-1.82315900	-5.71985800	7.22716400
C	0.99741600	-5.51406500	4.63912600
H	1.81927500	-5.53819100	3.93223400
C	-1.06260400	-4.63643000	5.50623500
H	-1.88044600	-3.92477400	5.52706900
C	-0.03752600	-7.58334600	7.59913300
H	0.50032700	-7.18984000	8.46566600
H	0.45910300	-8.47688300	7.22165100
N	-0.01221600	-1.49826900	-1.49896100
C	-1.16915900	-2.06067900	-1.91658500
H	-2.08546100	-1.71563000	-1.44967700
C	1.13974100	-1.92105700	-2.06780000
H	2.05948900	-1.45748800	-1.72796500
C	1.17152900	-2.90367900	-3.05452500
H	2.13279200	-3.17412800	-3.47929100
C	-0.02290700	-3.49870400	-3.49973200
C	-0.02894700	-4.55665600	-4.55644000
C	-1.21198700	-3.04713800	-2.89879600
H	-2.17692000	-3.46676200	-3.16412000
N	-0.04591900	-6.54105200	-6.52465700
C	0.96435900	-6.49098600	-5.62534700
H	1.73413000	-7.24991900	-5.71483400

C	-1.04649700	-5.63096700	-6.47519100
H	-1.82315900	-5.71985800	-7.22716400
C	0.99741600	-5.51406500	-4.63912600
H	1.81927500	-5.53819100	-3.93223400
C	-1.06260400	-4.63643000	-5.50623500
H	-1.88044600	-3.92477400	-5.52706900
C	-0.03752600	-7.58334600	-7.59913300
H	0.50032700	-7.18984000	-8.46566600
H	0.45910300	-8.47688300	-7.22165100
N	0.04592500	6.54104700	-6.52466800
C	1.04650100	5.63095900	-6.47520100
H	1.82316300	5.71984500	-7.22717500
C	0.03754100	7.58334500	-7.59914100
H	-0.50029600	7.18983800	-8.46568400
H	1.06599400	7.82120200	-7.86987100
C	0.02894700	4.55665500	-4.55644800
C	1.06260500	4.63642300	-5.50624400
H	1.88044500	3.92476500	-5.52707500
C	-0.96435200	6.49098600	-5.62535800
H	-1.73412100	7.24992100	-5.71484700
C	0.02290400	3.49870500	-3.49973800
C	1.21198400	3.04713800	-2.89879900
H	2.17691700	3.46676100	-3.16412400
C	1.16915300	2.06068200	-1.91658700
H	2.08545400	1.71563200	-1.44967700
C	-1.17153300	2.90368300	-3.05453000
H	-2.13279500	3.17413200	-3.47929800
N	0.01220800	1.49827400	-1.49896200
C	-1.13974700	1.92106300	-2.06780400
H	-2.05949600	1.45749600	-1.72796700
C	-0.99741200	5.51406600	-4.63913600
H	-1.81927200	5.53819600	-3.93224400
H	-0.45909900	8.47687800	-7.22166400
H	-1.06597600	-7.82119600	-7.86987900
H	-1.06597600	-7.82119600	7.86987900
H	-0.45909900	8.47687800	7.22166400

Energy: -2264.94969916 Hartree