Supporting Information

Fluxional motion in dinuclear copper(I) complex with a propeller-type ligand: metal hopping on both sides

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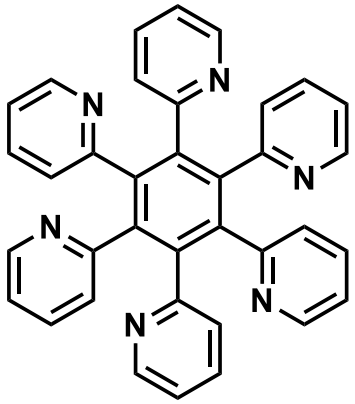
1. General Information

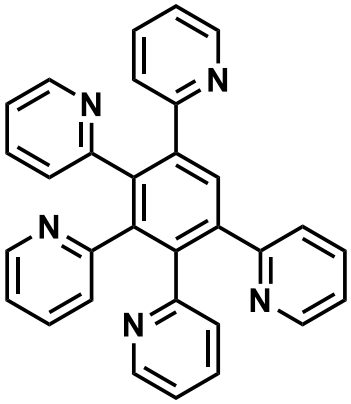
Reagents. 2-Phenylpyridine, triphenylphosphine, potassium carbonate, 2-bromopyridine, 2-bromo-5-fluoropyridine, copper(I) chloride, and triethylamine were purchased from commercial sources and used as received without further purification. $[(\eta^6\text{-}C_6H_6)RuCl_2]_2$ was synthesized following the procedure described in the literature.[1] *N*-methyl-2-pyrrolidone (NMP) was dried over molecular sieves (3 Å) prior to use. Tetrahydrofuran (THF) was distilled from sodium/benzophenone and stored over molecular sieves (3 Å) prior to use. Acetonitrile and d_3-acetonitrile were distilled from P_2O_5 and stored over molecular sieves (4 Å) prior to use.

Experimental equipment. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker DRX spectrometer operating at 500 MHz, 282 MHz and 125 MHz for ^{1}H, ^{19}F and ^{13}C acquisitions, respectively. Proton decoupled ^{13}C NMR spectra ($^{13}C\{^1H\}$) were recorded using a AVANCE III HD 850 spectrometer operating at 214 MHz.

2. Synthetic Procedures

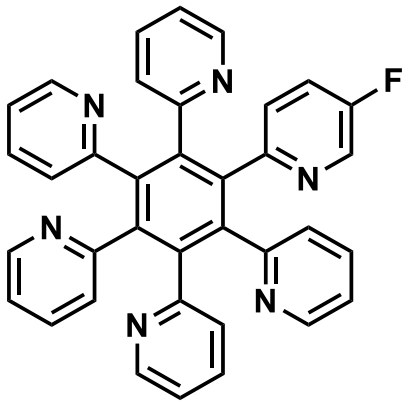


2-HPB



2-PPB

Hexa(2-pyridyl)benzene (2-HPB) and penta(2-pyridyl)benzene (2-PPB).[2] Under N_2 atmosphere, 2-phenylpyridine (0.16 g, 1.0 mmol), $[(\eta^6\text{-}C_6H_6)RuCl_2]_2$ (0.025 g, 0.050 mmol), triphenylphosphine (0.053 g, 0.20 mmol), and potassium carbonate (1.66 g, 12.0 mmol) were added into a flask containing 5 mL of *N*-methyl-2-pyrrolidone (NMP). The resulting solution was heated to 140 ℃ while stirring. At this temperature, 2-bromopyridine (1.58 g, 10.0 mmol) was added dropwise by means of a syringe pump over 24 h, and stirring was continued for 24 h at the same temperature. In order to remove NMP, water was added and the mixture was extracted with chloroform several times. Combined organic extracts were dried over anhydrous sodium sulfate and volatiles were removed *in vacuo*. The residue was purified by column chromatography on silica gel (eluting acetone:methanol:Et_3N = 20:2:1). Further purification was achieved by recrystallization from THF for each compound. Hexa(2-pyridyl)benzene (0.077 g, 14.2% yield) and penta(2-pyridyl)benzene (0.108 g, 23.3% yield). For hexa(2-pyridyl)benzene : ^{1}H NMR (500 MHz, CD_3CN): δ 8.06 (ddd, J = 5.0, 1.8, 1.0 Hz, 6H), 7.25 (td, J = 7.8, 1.8 Hz, 6H), 6.94 (d, J = 7.8, 6H), 6.84 (ddd, J = 7.2, 4.8, 1.0 Hz, 6H) ppm. ^{13}C NMR (125 MHz, CD_3CN) δ 158.2, 147.8, 140.2, 134.3, 126.7, 120.7 ppm. HR-MS : [M + H] (m/z) = 541.2139; calcd. value for $C_{36}H_{25}N_6$ = 541.2141. For penta(2-pyridyl)benzene : ^{1}H NMR (500 MHz, CD_3CN) δ 8.46 (ddd, *J* = 5.0, 1.8, 1.0 Hz, 2H), 8.17 (ddd, *J* = 5.0, 1.8, 1.0 Hz, 2H), 8.10 (ddd, *J* = 5.0, 1.8, 1.0 Hz, 1H), 8.03 (s, 1H), 7.48 (td, *J* = 7.8, 1.8 Hz, 2H), 7.34 (td, *J* = 7.8, 1.8 Hz, 2H), 7.26 (td, *J* = 7.8, 1.8 Hz, 1H), 7.14 (ddd, *J* = 8.7, 5.7, 1.2 Hz, 2H), 7.07 (dt, *J* = 9.6, 1.2 Hz, 2H), 6.98 (dt, *J* = 9.6, 1.2 Hz, 2H), 6.95 (ddd, *J* = 8.7, 5.7, 1.2 Hz, 2H), 6.91 (dt, *J* = 9.6, 1.2 Hz, 1H), 6.87 (ddd, *J* = 7.2, 4.8, 1.0 Hz, 1H). ^{13}C NMR (125 MHz, CD_3CN) δ 158.48, 158.22, 158.20, 149.07, 148.13, 147.79, 141.05, 140.48, 139.43, 135.52, 134.70, 134.34, 131.71, 126.77, 126.68, 124.65, 121.61, 121.09, 120.80. HR-MS : [M + H] (m/z) = 463.1799; calcd. value for $C_{31}H_{22}N_5$ = 463.1797.



MFHPB

Monofluorohexa(2-pyridyl)benzene (MFHPB). Under N_2 atmosphere, penta(2-pyridyl)benzene (0.231 g, 0.5 mmol), $[(\eta^6\text{-}C_6H_6)RuCl_2]_2$ (0.025 g, 0.050 mmol), triphenylphosphine (0.053 g, 0.20 mmol), and potassium carbonate (1.66 g, 12.0 mmol) were added into a flask containing 3 mL of *N*-methyl-2-pyrrolidone (NMP). The resulting solution was heated to 140 ℃ while stirring. At this temperature, 2 mL NMP solution of 2-bromo-5-fluoropyridine (0.51 g, 3.0 mmol) was added dropwise by means of a syringe pump over 24 h, and stirring was continued for 24 h at the same temperature. In order to remove NMP, water was added and the mixture was extracted with chloroform several times. Combined organic extracts were dried over anhydrous sodium sulfate and volatiles were removed *in vacuo*. The residue was purified by column chromatography on silica gel (eluting acetone : methanol : Et_3N = 20 : 2: 1). Further purification was achieved by recrystallization from THF, providing the target product as a white solid. Monofluorohexa(2-pyridyl)benzene (0.035 g, 12.5% yield) ^{1}H NMR (500 MHz, CD_3CN): δ 8.12~8.09 (m, 5H), 7.99 (d, J = 3.0 Hz, 1H), 7.32~7.27 (m, 5H), 7.08 (td, J = 8.6, 3.0 Hz, 1H), 7.02~6.96 (m, 6H), 6.91~6.86 (m, 5H) ppm. ^{13}C NMR (214 MHz, CD_3CN) δ 158.13, 158.05, 155.80 (d, *J* = 490 Hz), 147.93, 147.86, 147.84, 140.38, 140.33, 140.20, 139.31, 135.55 (d, *J* = 24 Hz), 134.48, 134.38, 134.36, 127.75, 126.66, 121.26 (d, *J* = 20 Hz), 120.76, 120.75, 120.71, 120.60 ppm. ^{13}C NMR (214 MHz, CD_3CN) δ −132.48 ppm. HR-MS : [M + H] (m/z) = 558.1970; calcd. value for $C_{36}H_{24}FN_6$ = 558.1968.

(2-HPB)$(CuCl)_2(MeCN)_2$, 1. See the reference (3).

Sample preparation for variable temperature (VT) ^{1}H NMR experiments and the 2D EXSY experiments with complexes 1 and 1a.

1. A saturated solution of complex **1** was prepared by stirring 2 mg of the complex in 1 mL of d_3-acetonitrile and filtering the resulting suspension into a screw-cap NMR tube.

1a. A stock solution of CuCl (0.2 mL, 2 equiv.) and a stock solution of MFHPB (0.4 mL) were mixed and transferred into a screw-cap NMR tube.

The stock solution of MFHPB (10 mM): 3 mg MFHPB in CD_3CN (0.6 mL) and the stock solution of CuCl (40 mM): 3.6 mg CuCl in CD_3CN (1.0 mL)).

3. NMR spectra and Interpretation

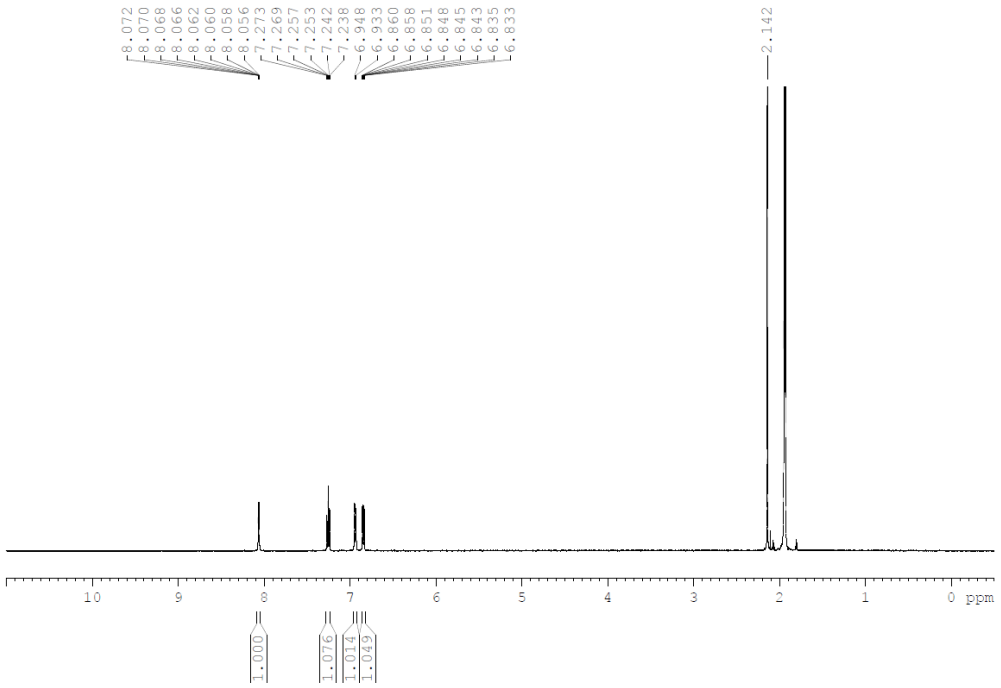


Figure S1. ^{1}H NMR spectrum of hexa(2-pyridyl)benzene (**2-HPB**) in CD_3CN.

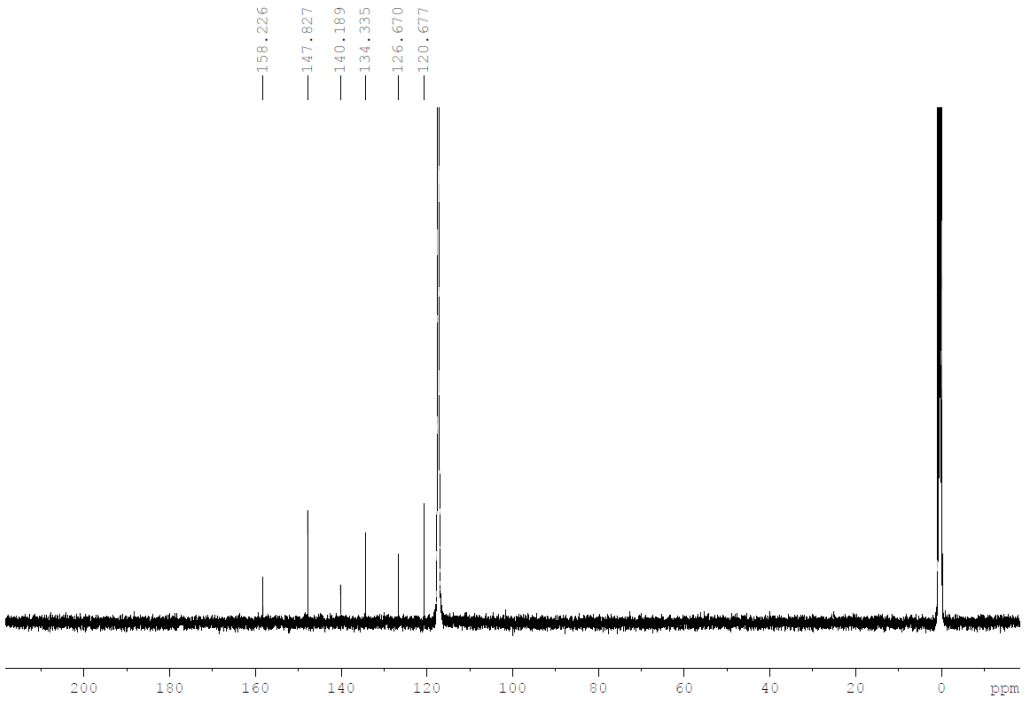


Figure S2. ^{13}C NMR spectrum of hexa(2-pyridyl)benzene (**2-HPB**) in CD_3CN.

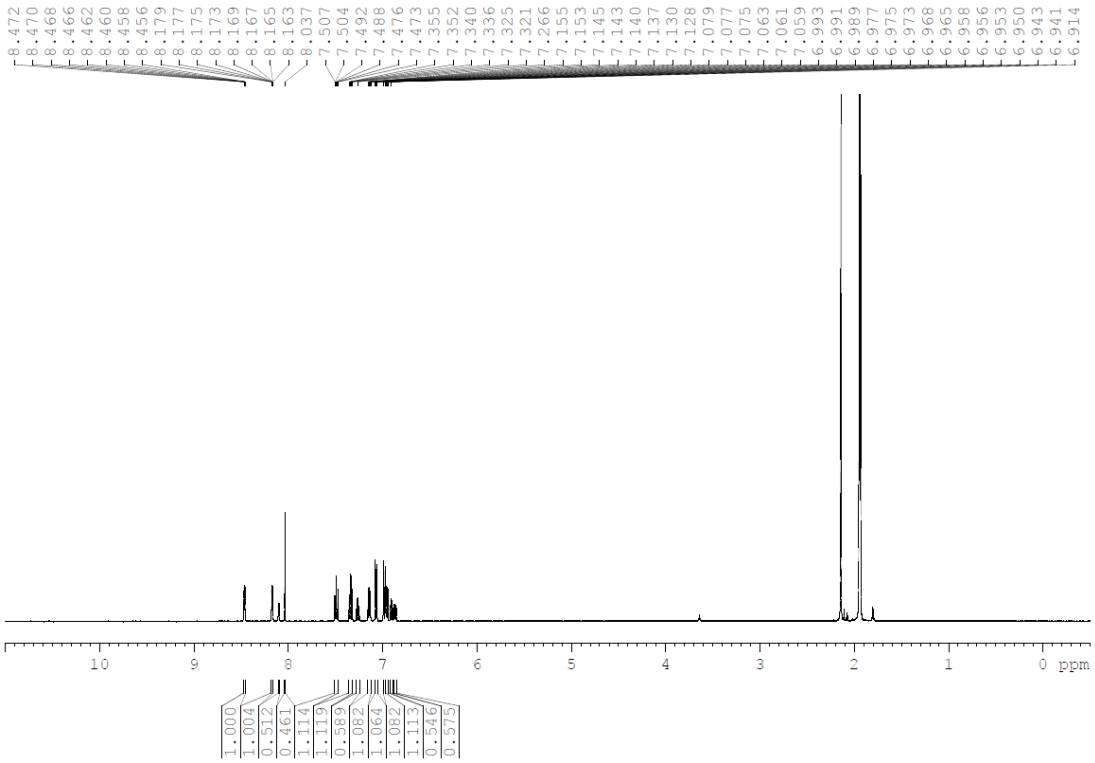


Figure S3. ^{1}H NMR spectrum of peta(2-pyridyl)benzene (**2-PPB**) in CD_3CN.

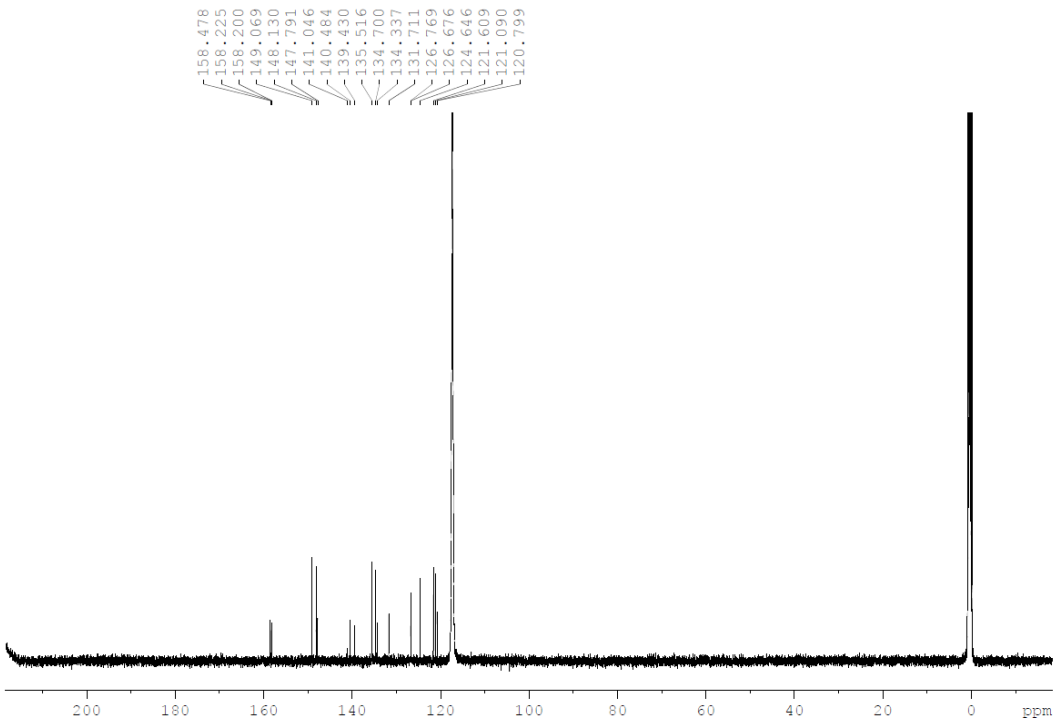


Figure S4. ^{13}C NMR spectrum of peta(2-pyridyl)benzene (**2-PPB**) in CD_3CN.

Figure S5. ^{1}H NMR spectrum of monofluorohexa(2-pyridyl)benezne (**MFHPB**) in CD_3CN.

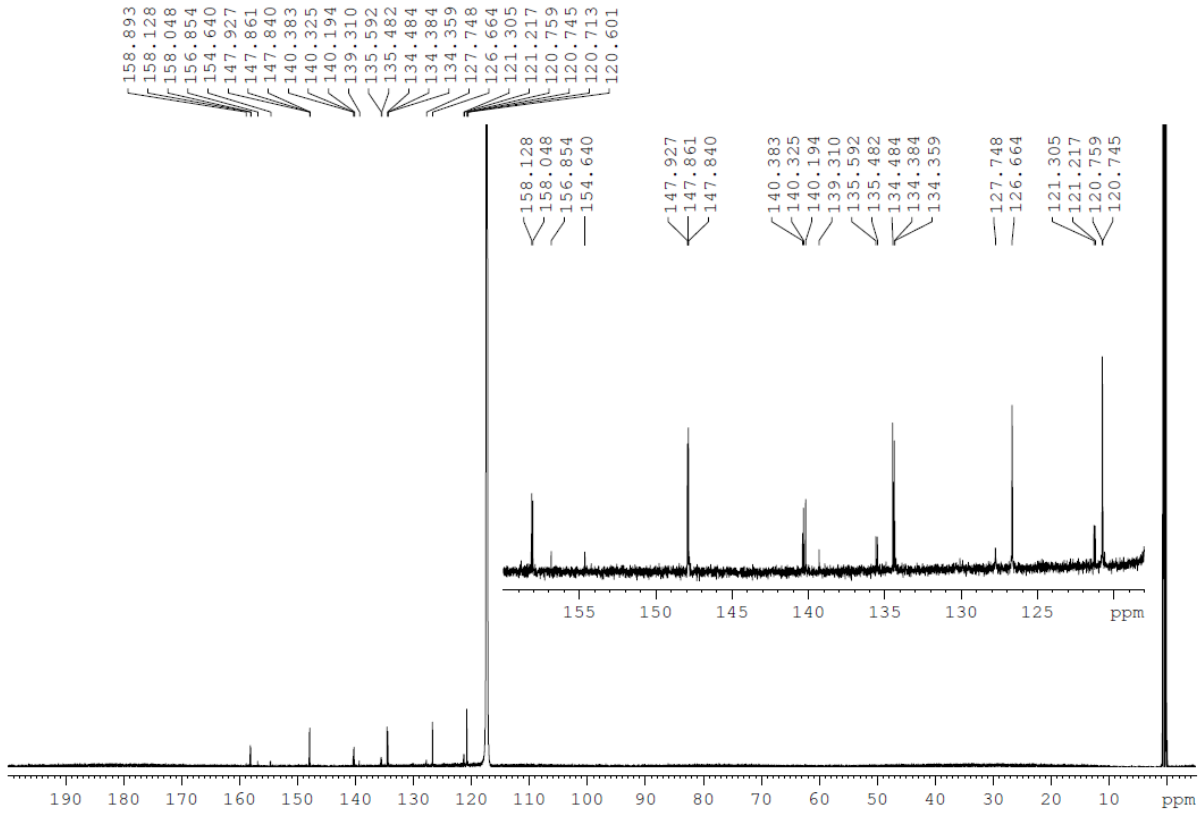


Figure S6. ^{13}C NMR spectrum of monofluorohexa(2-pyridyl)benezne (**MFHPB**) in CD_3CN.

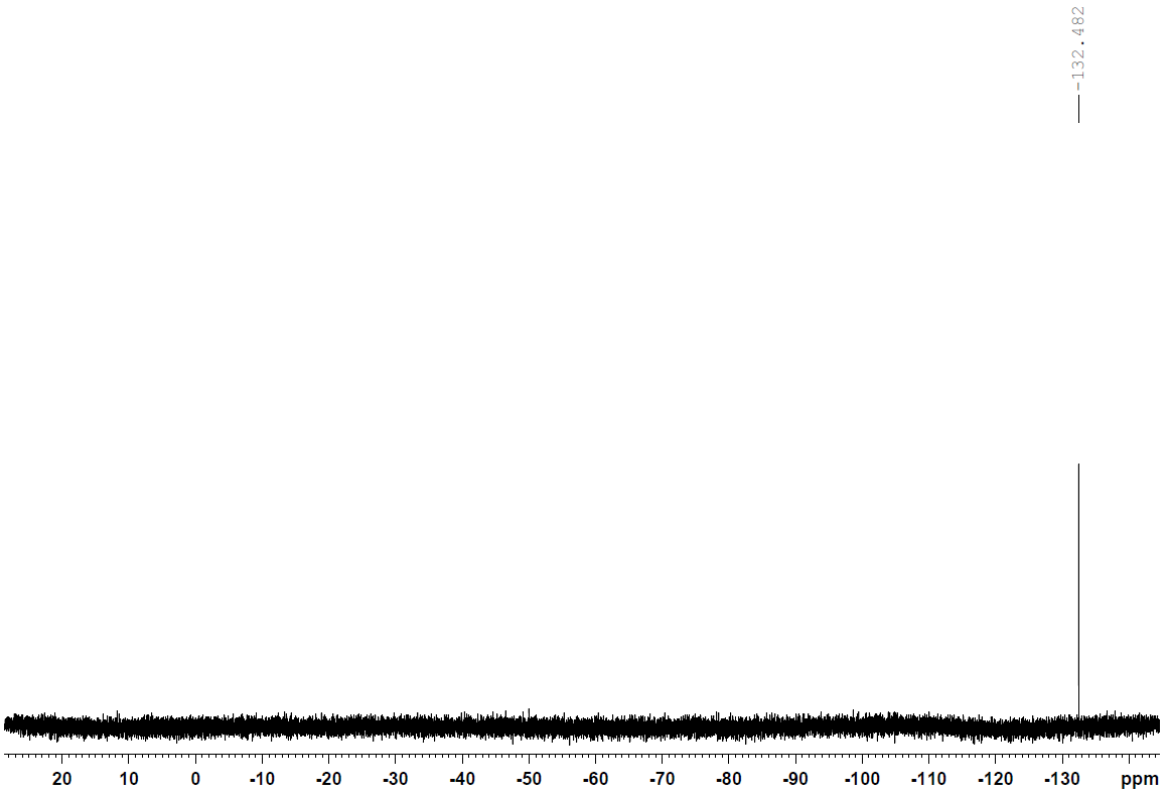


Figure S7. ^{19}F NMR spectrum of monofluorohexa(2-pyridyl)benezne (**MFHPB**) in CD_3CN.

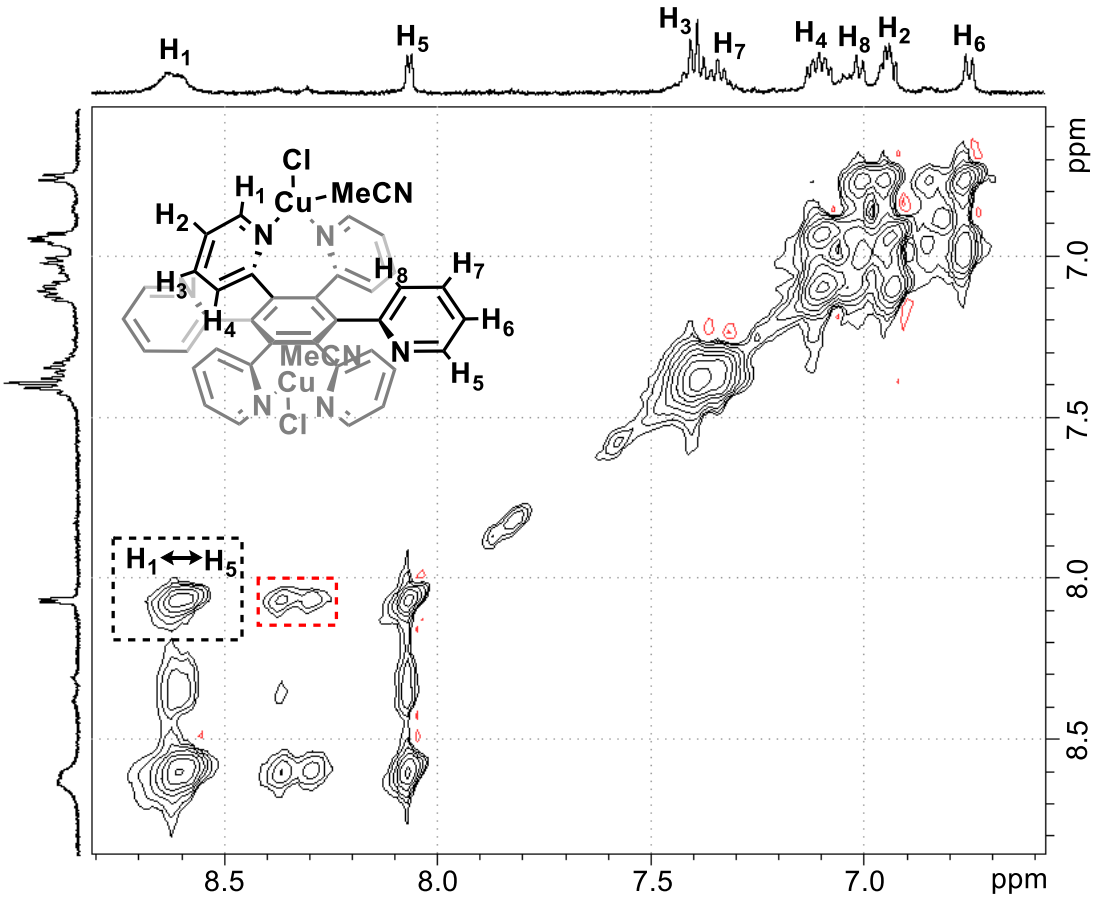


Figure S8. ^{1}H 2D EXSY spectrum of complex **1** in CD_3CN at 233 K. (τ = 0.3 sec) The exchange signals between **1** and the intermediate species are highlighted in the red dotted box.

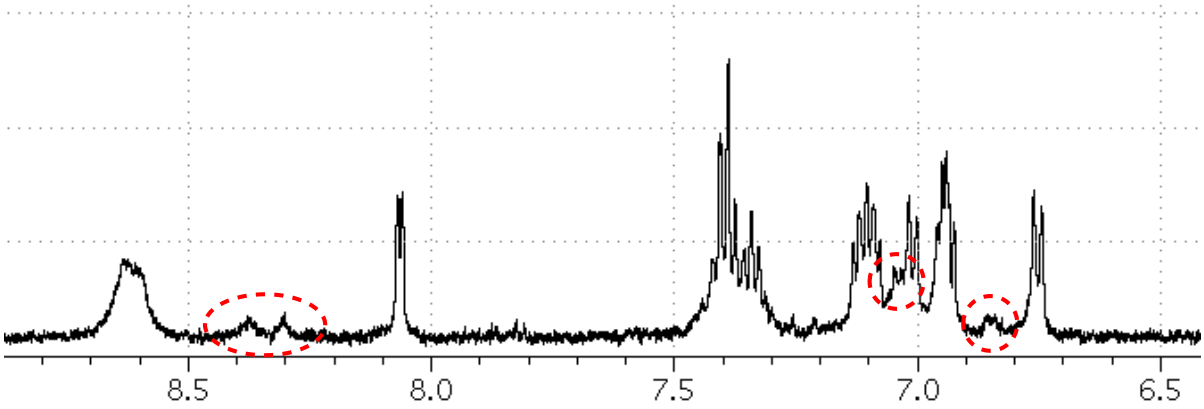


Figure S9. ^{1}H NMR spectrum of complex **1** at 223 K. The signals of the intermediate species that lay beneath the signals of **1** are highlighted in the red dotted circles.

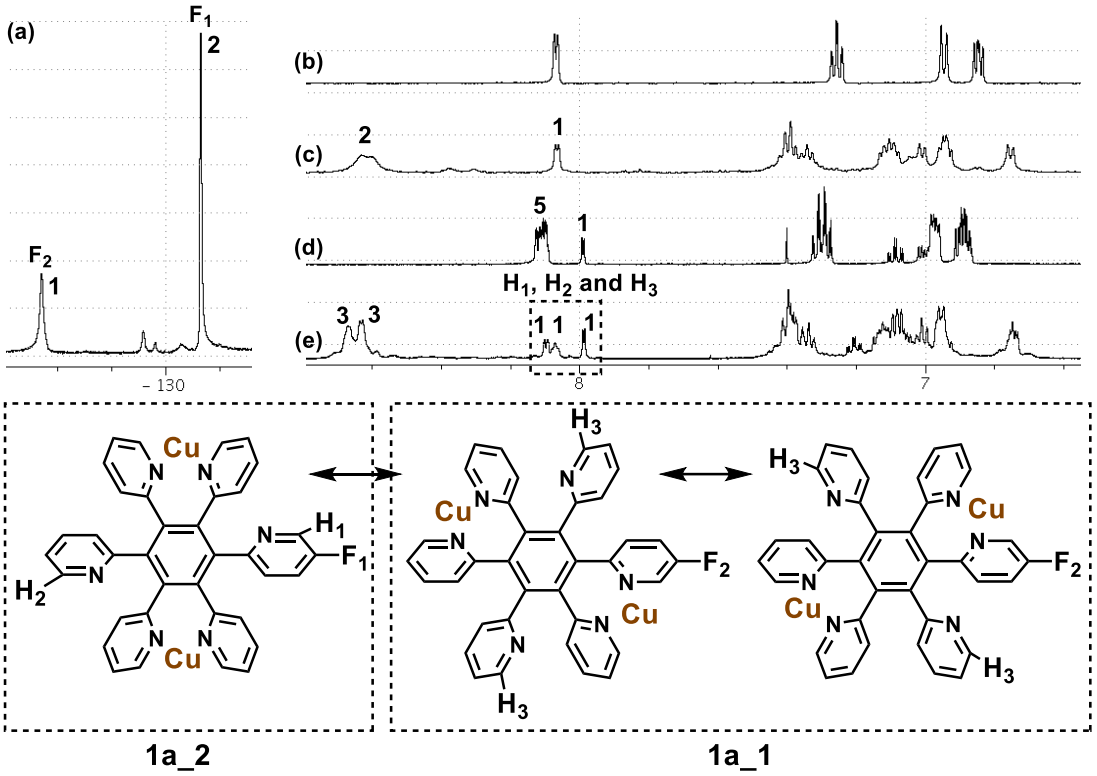


Figure S10. Analysis for the integration pattern in ^{19}F and ^{1}H NMR spectra. ^{19}F spectrum of **1a** at 223 K (a), ^{1}H NMR spectrum of **2-HPB** (b), **1** at 223 K (c), **MFHPB** (d) and **1a** (e).

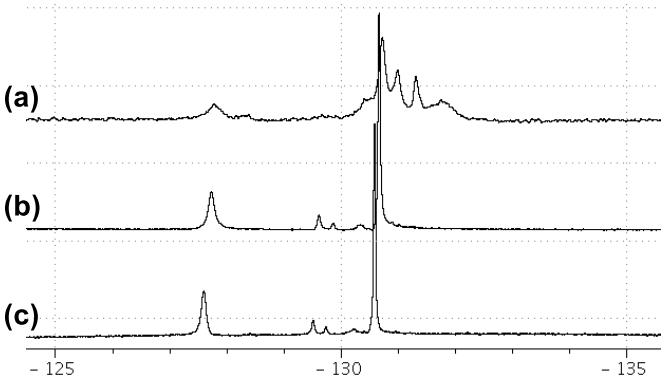


Figure S11. ^{19}F NMR spectra of **MFHPB** with 1 equivalent (a), 2 equivalents (b) and 3 equivalents (c) of copper(I) chloride in d_3-acetonitrile solution.

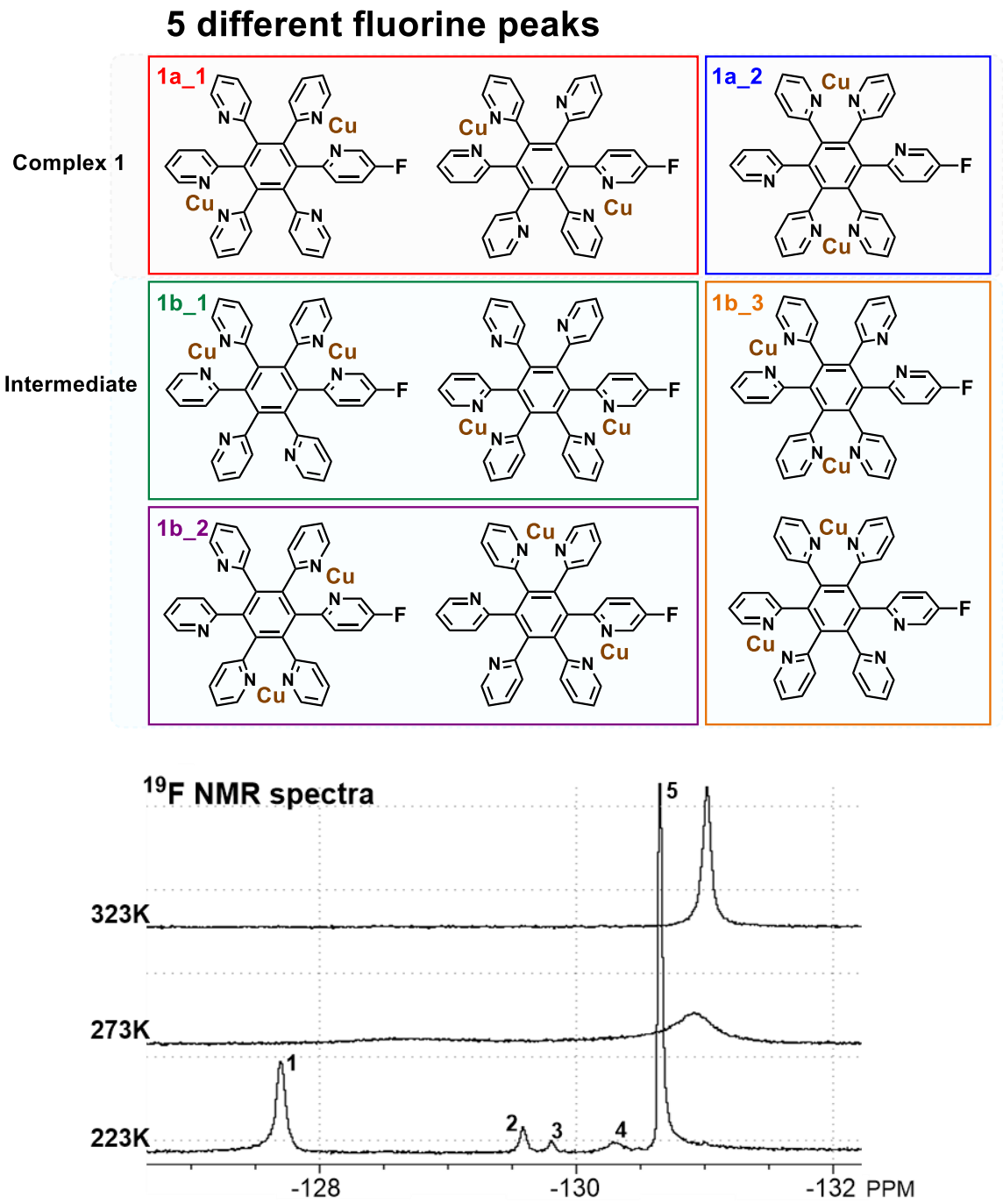


Figure S12. Proposed structures of possible isomers of **1a** (**1a_1**, **1a_2**) and intermediate species **1b** (**1b_1**, **1b_2** and **1b_3**) accounting for five different signals in ^{19}F NMR spectra.

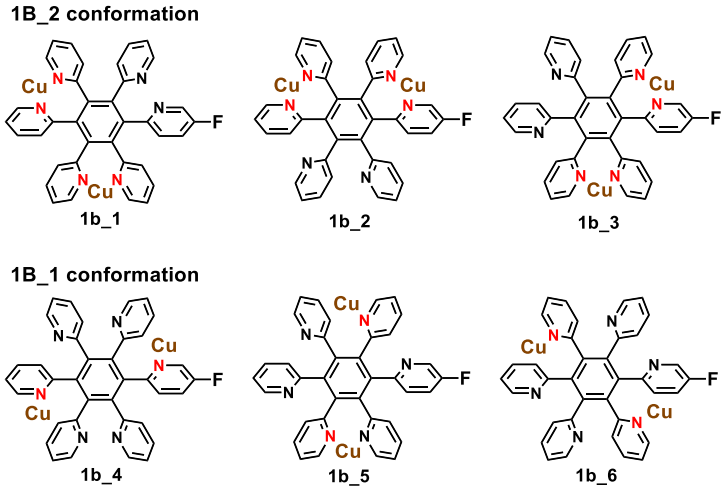


Figure S13. Three different isomers for **1B_1** (**1b_4**, **1b_5**, and **1b_6**) and **1B_2** (**1b_1**, **1b_2**, and **1b_3**) when using **MFHPB** as a ligand. **1b_5** and **1b_6** are considered as conformational isomers.

4. Structural Analysis by X-ray Crystallography

CCDC 1552119 and 1874373 contains the supplementary crystallographic data for **1** and **1a**. The data can be obtained free of charge via www.ccdc.cam.ac.uk/cgibin/catreq.cgi (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CD21EZ, UK; fax (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk). For **1** and **1a**, all the non-hydrogen atoms were refined anisotropically and hydrogen atoms were added to their ideal positions. For **1a**, the all the F1, F2 and F3 atoms were refined isotropically with U(eq) value of 0.04 and occupancies of F1, F2 and F3 are assigned to be 0.210, 0.192 and 0.110, respectively.

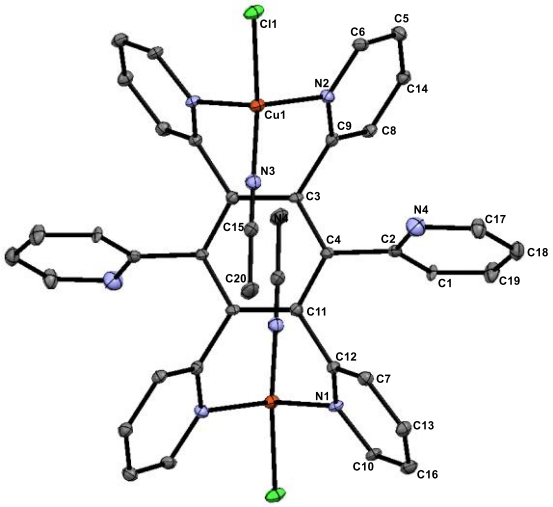


Figure S14. ORTEP diagram of $(CuCl(MeCN))_2$(**2-HPB**) (**1**), ellipsoids are shown at 50% probability level.

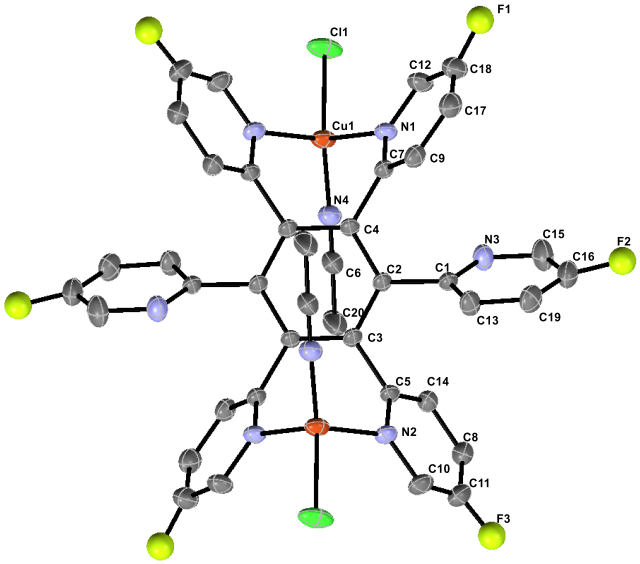


Figure S15. ORTEP diagram of $(CuCl(MeCN))_2$(**MFHPB**) (**1a**), ellipsoids are shown at 50% probability level. The occupancies of F1, F2 and F3 are assigned to be 0.210, 0.192 and 0.110, respectively.

5. UV-Vis Spectra

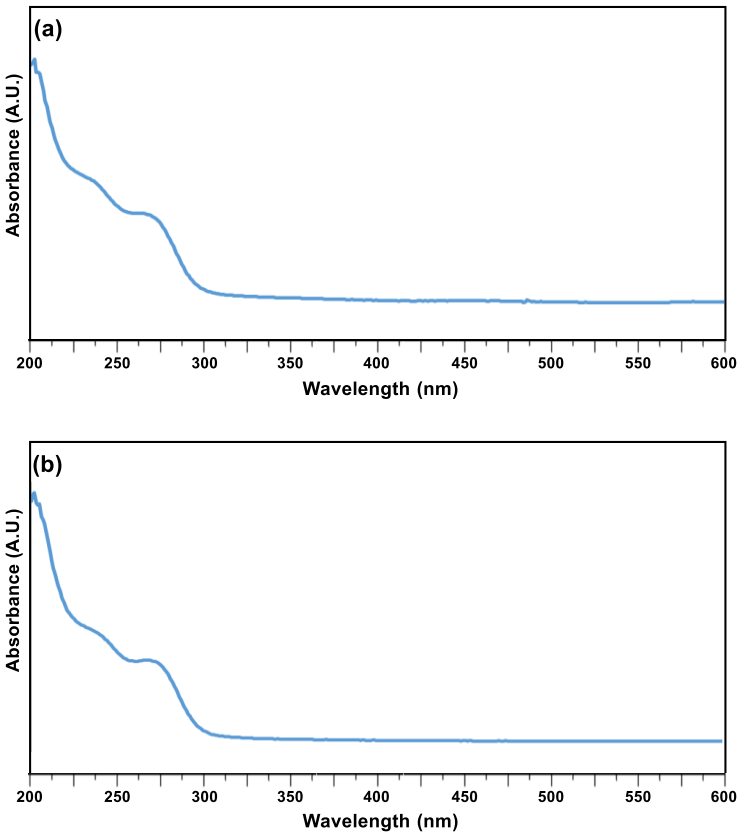


Figure S16. UV-Vis spectra of **1** (a) and **1a** (b) in acetonitrile (50 μM).

6. Rate Constant Calculations and Derivation of the Thermodynamic Parameters[4]

The rate constants at different temperatures were determined from the ^{19}F 2D EXSY spectrum. The rate constants, k_{obs}, can be calculated from the peak intensities in the spectrum according to the following equation :

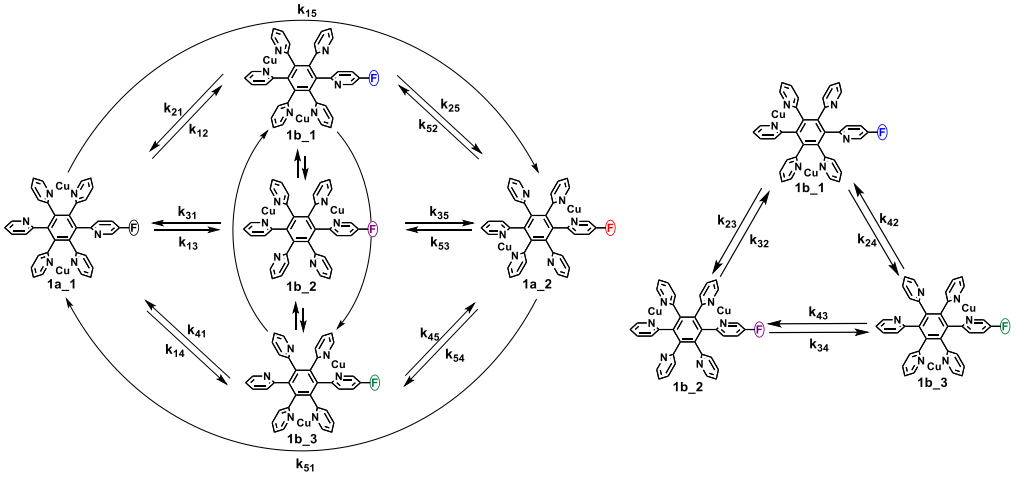
$$\mathbf{M} = \exp(\mathbf{R}t_m)\mathbf{M_0} \qquad [1]$$

Where matric **M** contains the integrated intensities of the signals in 2D EXSY spectra, $\mathbf{M_0}$ is a diagonal matrix representing the EXSY spectra acquired with a mixing time (t_m) of zero and matrix **R** contains exchange and relaxation rate constants.

For the case when the cross relaxation is neglected, **R** has the form:

$$\mathbf{R} = \begin{bmatrix} -\frac{1}{T_{11}} - k_{12} -\ldots- k_{1n} & k_{12} & \ldots & k_{1n} \\ k_{21} & -\frac{1}{T_{12}} - k_{21} -\ldots- k_{2n} & \ldots & k_{2n} \\ \ldots & \ldots & \ldots & \ldots \\ k_{n1} & k_{n2} & \ldots & -\frac{1}{T_{1n}} - k_{n1} -\ldots- k_{nn} \end{bmatrix} \quad [2]$$

The rates for the exchange between the five different species in solution were determined using equations 1 and 2.



k_{12}	3.77 ± 0.75	k_{21}	0.46 ± 0.06	k_{24}	0.22 ± 0.14	k_{42}	0.22 ± 0.26
k_{13}	0.19 ± 0.03	k_{31}	1.35 ± 0.14	k_{25}	0.19 ± 0.03	k_{52}	1.35 ± 0.14
k_{14}	5.03 ± 0.1	k_{41}	0.5 ± 0.01	k_{34}	1.15 ± 0.62	k_{43}	0.51 ± 0.15
k_{15}	0.34 ± 0.05	k_{51}	0.15 ± 0.04	k_{35}	0.15 ± 0.17	k_{53}	1.02 ± 0.19
k_{23}	1.3 ± 0.34	k_{32}	2.01 ± 1.97	k_{45}	0.26 ± 0.04	k_{54}	1.47 ± 0.25

Figure S17. Possible isomers of **1a** (**1a_1** and **1a_2**) and intermediate species (**1b_1**, **1b_2** and **1b_3**) accounting for five different signals in the ^{19}F NMR spectra.

T (K)	k_1 (s^{-1})	k_{-1} (s^{-1})
223	0.99	0.49
228	2.29	0.99
233	5.18	2.84

Table S1. The calculated rate constant of the exchange process of **1a** in CD_3CN (6 mM).

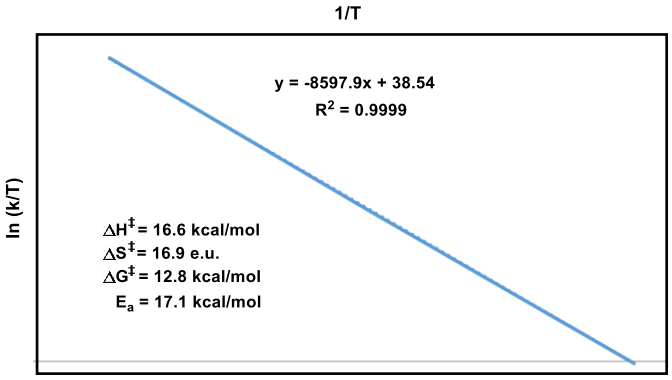


Figure S18. Arrhenius plot analysis and thermodynamic parameters of the exchange process of **1a** in CD_3CN (6 mM). The upper and lower lines represent the error bands of the linear regression with a 95% confidence level.

7. DFT Calculations

Geometry optimizations were performed using density functional theory as implemented in Gaussian 09[5] and the B3LYP functional. The atomic coordinates of simulated structures were generated by Chem3D (CambridgeSoft Corp., MA).[6,7] As for the basis sets, we used 6-31G(d,p)

for C, H, N.[8] For Cl[9] and Cu,[10] the pseudo-potential basis sets MWB10 and MDF10 was adopted, respectively. Solvent was included to the optimizations via the SMD model (acetonitrile). The rotational barriers of non-coordinated pyridine ring in **1** and **1B_2** were calculated by scanning the torsional profile for the rotation including geometrical optimization, incrementing the dihedral angle about the one C–C bond in 15 ° for each step.

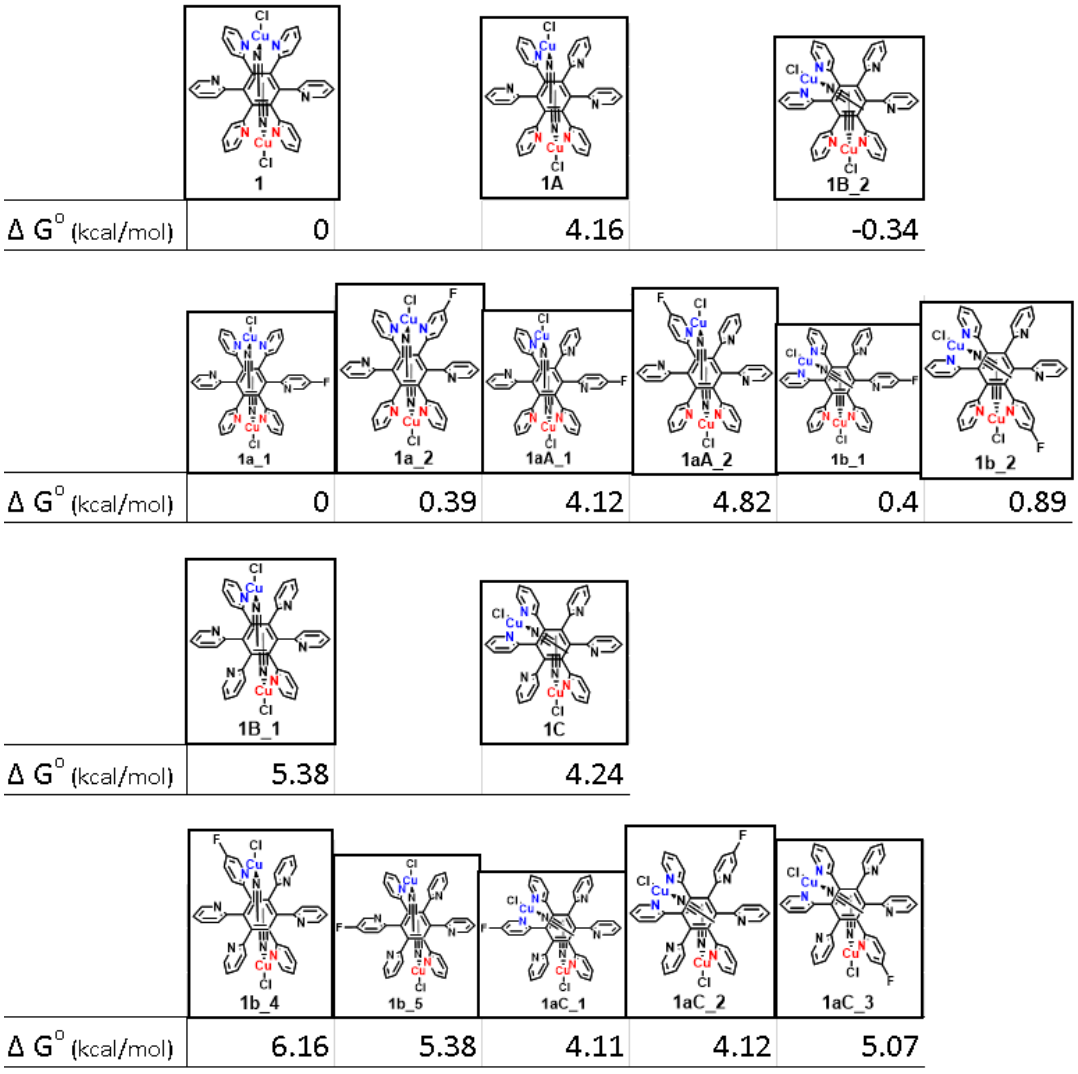


Table S2. Calculated free energies for the isomeric species of **1** (**1**, **1A**, **1B_1**, **1B_2** and **1C**) and its mono-fluorinated analog **1a** (**1a_1**, **1a_2**, **1aA_1**, **1aA_2**, **1b_1**, **1b_2**, **1b_3**, **1b_5**, **1aC_1**, **1aC_2** and **1aC_3**).

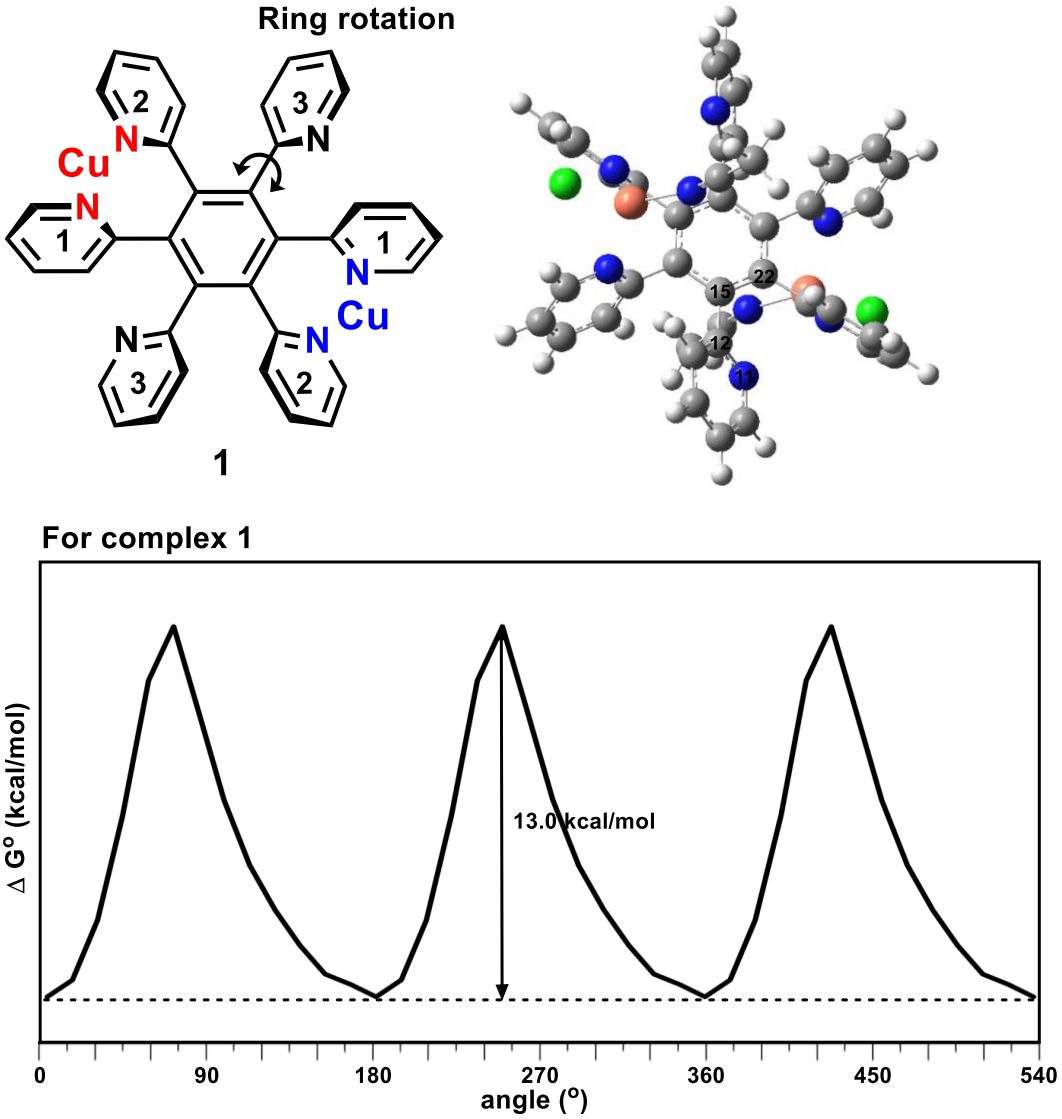


Figure S19. Calculated free energy profiles for rotation of non-coordinated pyridine ring (ring 3, dihedral angle for 11(N)–12(C)–15(C)–22(C)) in **1**.

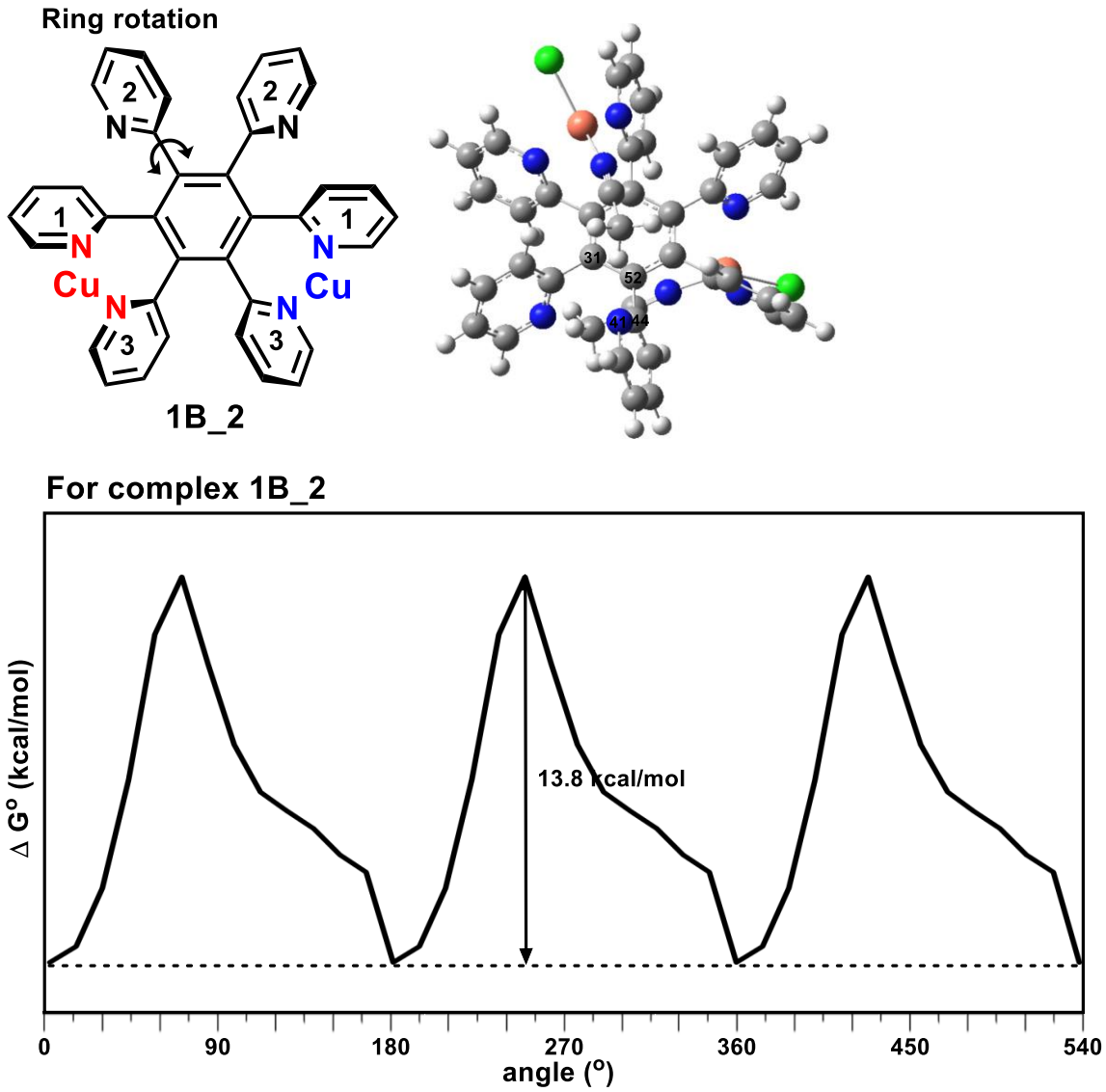
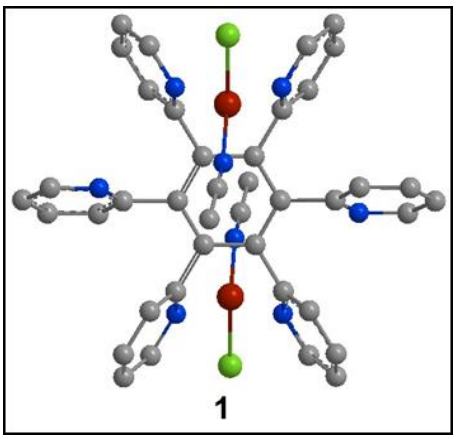


Figure S20. Calculated free energy profiles for rotation of non-coordinated pyridine ring (ring 2, dihedral angle for 41(N)–44(C)–52(C)–31(C)) in **1B_2**.

Cartesian coordinates of optimized structures

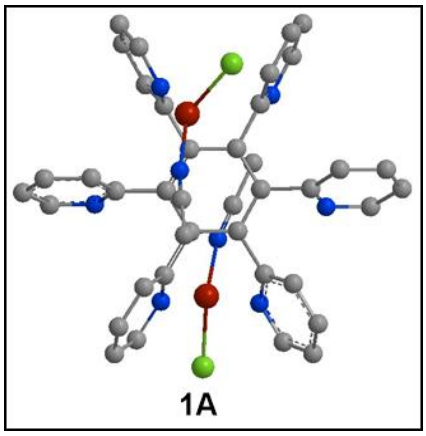
The optimized geometries of **1**, **1A**, **1B_1**, **1B_2**, **1C**, **1a_1**, **1a_2**, **1aA_1**, **1aA_2**, **1b_1**, **1b_2**, **1b_3**, **1b_5**, **1aC_1**, **1aC_2** and **1aC_3** were displayed in Cartesian coordinates (a.u.). G° represents the sum of electronic and thermal free energies in Hartree unit.



G°	-2404.781696
G° (acetonitrile)	-2405.395561

Cu	3.699935	-0.00717	-1.64284	C	-2.41195	1.45101	-0.7727
Cl	6.001217	-0.03532	-2.09357	C	1.164535	0.732215	0.312623
N	2.743127	0.063512	-3.33366	C	3.521724	2.995503	2.231859
C	2.511372	0.195424	-4.46211	C	-3.55423	2.839496	-2.37469
C	2.270184	0.37059	-5.88813	C	-0.87863	3.615668	0.89107
H	1.805678	1.342721	-6.07601	C	4.61843	2.968112	1.373157
H	1.609728	-0.4155	-6.26494	C	-0.86436	5.008044	0.869145
H	3.2199	0.323381	-6.42921	C	0.751455	4.876614	-0.89042
N	-3.46426	-1.45553	0.084085	C	-0.03185	5.65795	-0.04078
N	3.466774	-1.44893	-0.07118	H	5.395036	-2.07766	-0.39911
N	-0.76167	-3.51989	0.862225	H	-1.5264	-2.23665	-2.55874
C	0.041528	-2.89755	-0.01664	H	1.528271	-2.07523	2.613041
C	1.179989	-0.67675	0.314063	H	-5.39199	-2.06621	0.445583
C	4.561888	-2.13759	0.296316	H	5.546235	-3.38263	1.745316
C	0.013639	-1.39711	-0.01185	H	-3.55749	-3.56091	-3.16585
C	-2.40085	-2.23825	-1.91733	H	3.568845	-3.35171	3.302066
C	2.408264	-2.10612	1.980003	H	1.504342	-3.05412	-1.59977
C	-4.55603	-2.16771	-0.24161	H	-5.53458	-3.50771	-1.60858
C	4.639784	-2.84164	1.495051	H	1.479619	-5.55499	-1.57071
C	-2.39248	-1.49509	-0.73145	H	-1.42526	-5.32619	1.597406
C	2.400454	-1.43216	0.753467	H	-0.02451	-6.72209	0.075435
C	-1.17617	-0.71335	-0.33144	H	-5.40687	2.096619	0.378918
C	-3.5334	-2.97667	-2.2506	H	1.514738	2.255454	2.539965
C	3.543236	-2.82076	2.354994	H	-1.53921	2.093903	-2.63207
C	0.866684	-3.59688	-0.90999	H	5.38034	2.085163	-0.46436
C	-4.6301	-2.94923	-1.39189	H	-5.55741	3.401436	-1.76566

C	0.852376	-4.98926	-0.88797	H	3.5458	3.579733	3.147126
C	-0.76292	-4.85767	0.872062	H	-3.57954	3.370376	-3.32181
C	0.020111	-5.63908	0.022242	H	-1.51648	3.072851	1.580642
N	3.452625	1.474437	-0.10287	H	5.522902	3.526598	1.589863
N	-3.47852	1.467861	0.051628	H	-1.49182	5.573715	1.551743
N	0.750246	3.538839	-0.88067	H	1.413987	5.3452	-1.61555
C	-0.0532	2.916417	-0.00209	H	0.012746	6.740962	-0.0939
C	-1.1916	0.695611	-0.33296	Cu	-3.71198	0.027011	1.623864
C	-4.57352	2.156499	-0.31627	Cl	-6.01326	0.055255	2.073682
C	-0.02527	1.415975	-0.00696	N	-2.7542	-0.04498	3.313925
C	2.389192	2.257075	1.898566	C	-2.52038	-0.17792	4.441825
C	-2.41938	2.124874	-1.99929	C	-2.27661	-0.35442	5.867247
C	4.54439	2.186625	0.222854	H	-1.8143	-1.32789	6.053618
C	-4.65104	2.860455	-1.51508	H	-1.61326	0.429705	6.243058
C	2.380833	1.513951	0.712665	H	-3.22503	-0.30498	6.410398

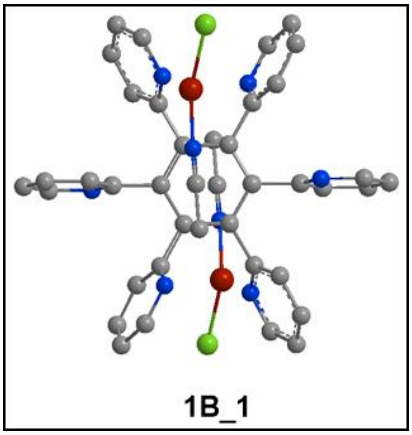


G° -2404.774653

G° (acetonitrile) -2405.38893

Cu	4.097593	3.285639	7.823951	C	6.006	4.137253	5.434792
Cl	4.285034	1.275873	8.931898	C	5.388488	5.4871	5.667389
N	2.50126	4.102051	7.094303	C	7.613721	2.737155	4.312425
C	1.66878	4.519568	6.404792	C	1.281046	8.104931	2.699327
C	0.654813	5.056566	5.509653	C	4.999485	5.862489	2.115208
H	0.284183	4.262307	4.855256	C	7.107412	1.652354	5.024838
H	1.097382	5.852158	4.895543	C	4.753981	5.147952	0.945188
H	-0.18385	5.457959	6.086308	C	3.486227	3.603978	2.260255
N	4.743086	10.5195	5.752161	C	3.979414	3.991501	1.014083
N	5.698546	4.482287	8.691829	H	5.81999	3.093438	10.19915
N	4.366088	7.623133	9.360179	H	2.039625	8.933487	6.980725
C	5.149094	8.142987	8.400243	H	7.965437	6.841627	7.892238
C	5.545504	6.147753	6.902916	H	4.976652	12.55144	5.474985
C	6.327626	3.942262	9.748613	H	8.021805	3.930501	11.07287
C	5.066821	7.464074	7.060804	H	1.232144	11.29609	7.194666

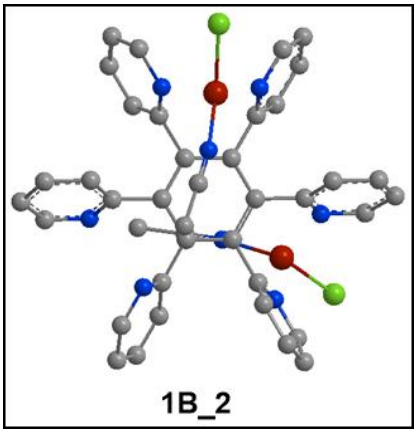
C	2.659272	9.767702	6.67282	H	9.139979	5.831812	9.860878
C	7.525794	6.01569	8.441379	H	6.598403	9.635684	7.824549
C	4.299605	11.78867	5.846095	H	2.744625	13.1528	6.418782
C	7.558637	4.401467	10.21218	H	6.634884	10.68474	10.09575
C	3.929512	9.514233	6.149305	H	3.746325	7.737913	11.32048
C	6.279406	5.513334	8.048977	H	5.168709	9.710147	11.89282
C	4.436011	8.113731	5.985173	H	4.830594	9.465879	2.957732
C	2.215593	11.0822	6.787502	H	3.304231	10.41509	1.26617
C	8.173857	5.453709	9.538657	H	7.424135	4.864071	3.980994
C	5.979894	9.248715	8.626487	H	5.648395	1.081341	6.538956
C	3.050707	12.11399	6.361883	H	0.95199	9.509778	1.096369
C	5.996632	9.829253	9.893145	H	8.428638	2.607627	3.605925
C	4.392857	8.19006	10.57119	H	0.276077	7.688435	2.660057
C	5.186895	9.291867	10.8916	H	5.600129	6.765627	2.099411
N	5.52975	3.087807	6.127084	H	7.508655	0.652475	4.896241
C	3.81838	9.08318	2.872737	H	5.164116	5.487946	-0.00131
C	4.459917	5.394402	3.321786	H	2.87966	2.705739	2.35799
C	4.211893	7.433626	4.772726	H	3.762587	3.401408	0.1295
C	2.955426	9.620674	1.919161	Cu	6.592718	10.25735	4.939262
C	4.699811	6.123016	4.611699	N	8.237255	9.438365	5.54652
C	7.058021	3.997174	4.520772	C	9.334009	9.074221	5.637388
N	2.095388	7.580387	3.623349	C	10.71938	8.632104	5.718535
N	3.7144	4.279292	3.391754	Cl	6.781646	11.30349	2.947729
C	3.350589	8.061921	3.707958	H	10.76211	7.549724	5.867979
C	6.069006	1.875937	5.927087	H	11.2422	8.884976	4.791512
C	1.6576	9.123232	1.824744	H	11.22224	9.125868	6.554666



G°	-2404.781056
G° (acetonitrile)	-2405.386986

Cu	3.883587	-0.44267	1.244714	C	3.458561	-1.32905	-3.58488
Cl	5.979311	0.249053	1.454136	C	2.362927	-0.68472	-1.53841
N	2.469311	-0.99826	2.39784	C	1.131281	-0.32206	-0.76421
C	1.622259	-1.29306	3.132078	C	-2.92664	-3.29554	2.322187

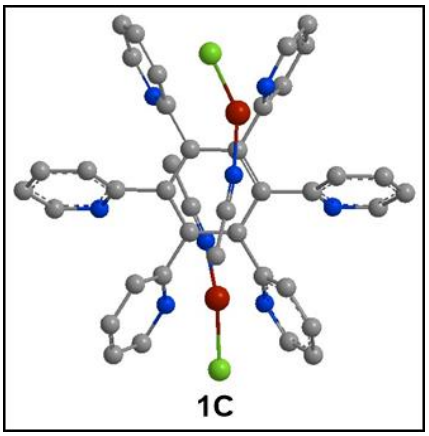
C	0.539645	-1.66573	4.029554	N	-0.18983	-3.01523	-2.16687
H	0.816097	-2.56409	4.589441	C	4.677175	-1.25	-2.9148
H	-0.37031	-1.86066	3.441489	C	-0.03251	-4.26436	-2.6228
H	0.354708	-0.85438	4.739525	C	1.223044	-4.93474	-0.70035
N	-3.5472	0.656951	0.886814	C	0.661022	-5.25892	-1.93341
N	2.013511	2.404287	-1.94892	H	-1.4966	3.364342	-0.74074
C	-1.07036	3.659127	0.211817	H	4.477258	3.950487	0.620577
C	-0.35462	2.729179	0.975537	H	-1.32161	1.114224	3.371079
C	0.966353	0.994035	-0.28595	H	2.759149	2.292179	1.341468
C	-0.16238	1.320173	0.486616	H	-5.59324	0.836424	0.991488
C	3.779086	3.53637	-0.09953	H	4.553272	4.627094	-1.80464
C	-2.29105	1.058568	2.890832	H	-3.42024	1.625493	4.636071
C	2.829231	2.602356	0.306003	H	2.925975	3.581603	-3.37665
C	-4.67663	0.92248	1.569079	H	-5.61928	1.475009	3.419115
C	3.828081	3.906034	-1.44212	H	0.483848	4.498866	3.588877
C	1.969737	2.050268	-0.65067	H	-1.78057	5.694025	0.130644
C	-3.46114	1.349246	3.586474	H	-0.75932	6.274316	2.355422
C	-2.36615	0.704547	1.539768	H	1.491053	-3.34536	0.742881
C	-1.13464	0.341845	0.765379	H	-4.47975	-3.93145	-0.62021
C	2.922265	3.316062	-2.32116	H	1.318945	-1.09428	-3.37004
N	0.187598	3.035531	2.167243	H	-2.76132	-2.2733	-1.3408
C	-4.67994	1.270174	2.916745	H	5.589889	-0.81663	-0.98916
C	0.030246	4.284684	2.623089	H	-4.55723	-4.60694	1.80525
C	-1.22768	4.954143	0.701866	H	3.41797	-1.60514	-4.63453
C	-0.66445	5.278808	1.934241	H	-2.93098	-3.5606	3.377795
N	3.543798	-0.63724	-0.8851	H	5.616669	-1.45466	-3.41695
N	-2.01771	-2.38389	1.950102	H	-0.48516	-4.47815	-3.58912
C	1.065725	-3.63977	-0.2102	H	1.775015	-5.67497	-0.12869
C	0.351226	-2.70935	-0.97451	H	0.755911	-6.25438	-2.35469
C	-0.96971	-0.97425	0.28713	Cu	-3.88805	0.461238	-1.24339
C	0.159011	-1.30038	-0.48548	Cl	-5.98357	-0.23113	-1.45069
C	-3.78204	-3.51695	0.100122	N	-2.47357	1.017182	-2.396
C	2.288244	-1.03856	-2.88953	C	-1.6265	1.311818	-3.13028
C	-2.83201	-2.58304	-0.30524	C	-0.54391	1.684279	-4.02786
C	4.673458	-0.90258	-1.56706	H	-0.35807	0.872192	-4.73675
C	-3.83185	-3.886	1.442853	H	-0.82093	2.581709	-4.58894
C	-1.97315	-2.03045	0.651713	H	0.365766	1.880535	-3.43978



G°	-2404.782813
G° (acetonitrile)	-2405.395011

Cu	3.492578	-1.10466	1.335172	C	-1.30325	-2.22079	0.605131
N	2.566509	0.061055	2.585123	C	-0.82	-3.05084	1.621849
C	2.077797	0.896134	3.225017	C	-1.27345	2.822982	0.699492
C	1.453466	1.972347	3.982745	C	-4.87888	-0.02576	1.198445
Cl	5.541749	-2.07599	1.63469	C	-1.44774	-4.27353	1.851245
H	2.222218	2.617262	4.418919	C	-0.63619	-0.91299	0.295742
H	0.846722	1.559341	4.794117	C	-1.26405	0.307433	0.619623
H	0.81593	2.563295	3.31109	C	-2.45342	3.248718	0.075291
N	-2.56342	0.067151	-2.58538	C	-5.057	0.324902	2.535327
C	-2.07413	0.902931	-3.2239	C	-2.96998	-3.74075	0.077638
C	-1.44919	1.980076	-3.9798	C	-0.6258	1.523665	0.321804
Cl	-5.53987	-2.06972	-1.63815	C	-2.68575	0.66958	2.674984
Cu	-3.48987	-1.10028	-1.33733	C	-2.53848	-4.62893	1.060439
H	-0.8111	2.569357	-3.30721	C	-3.93733	0.674414	3.287307
H	-0.8429	1.568088	-4.79202	C	-3.01723	4.463032	0.455095
H	-2.21758	2.626321	-4.41466	C	-1.21866	4.713658	2.010652
N	3.678078	-0.03008	-0.60526	C	-2.3873	5.217766	1.444042
N	2.369518	-2.56277	0.145398	H	-0.03738	-2.73789	-2.2126
C	2.59377	0.315162	-1.32501	H	5.706829	-0.34579	-0.56618
N	0.670585	3.547479	-1.65254	H	1.08699	-4.93179	-2.64137
C	1.30488	-2.22074	-0.609	H	2.917632	2.627387	0.691707
C	0.820874	-3.04898	-1.62684	H	6.05361	0.312053	-2.97149
C	1.278621	2.823187	-0.69538	H	3.839408	-3.94446	0.537141
C	4.882052	-0.02709	-1.19887	H	1.795183	0.942935	-3.22464
C	1.447756	-4.27174	-1.85817	H	3.057226	-5.57096	-1.21153
C	0.638734	-0.91297	-0.29756	H	4.037766	0.947844	-4.33391
C	1.26744	0.307534	-0.6195	H	3.93784	4.811463	0.021736
C	2.458927	3.24708	-0.07055	H	0.706616	5.274809	-2.78019
C	5.06035	0.325238	-2.53529	H	2.796694	6.171702	-1.76232
C	2.970708	-3.74258	-0.08409	H	0.038333	-2.74118	2.208242

C	0.630059	1.523735	-0.31972	H	-5.70382	-0.34311	0.565285
C	2.689313	0.6716	-2.6744	H	-1.08757	-4.93497	2.63354
C	2.538422	-4.62903	-1.06811	H	-2.91255	2.630568	-0.68796
C	3.940878	0.676462	-3.28677	H	-6.05028	0.311769	2.971465
C	3.023601	4.461582	-0.44845	H	-3.8387	-3.94114	-0.54405
C	1.225144	4.715989	-2.00352	H	-1.79147	0.939614	3.225607
C	2.394177	5.218343	-1.43617	H	-3.05793	-5.57073	1.202365
N	-3.67489	-0.02871	0.60487	H	-4.03408	0.944457	4.334812
N	-2.36796	-2.561	-0.14999	H	-3.9312	4.814321	-0.01458
C	-2.59039	0.314893	1.325108	H	-0.69977	5.270867	2.788229
N	-0.66493	3.545307	1.657842	H	-2.78914	6.170899	1.77169



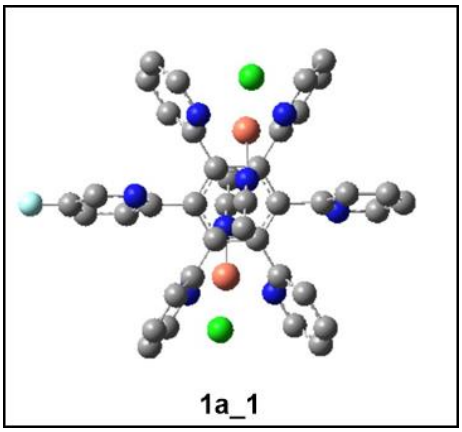
1C

G° -2404.772845

G° (acetonitrile) -2405.388802

Cu	1.960072	13.9971	11.77102	C	3.694116	16.88598	16.42949
N	0.923725	14.80138	13.16697	C	2.615203	17.67998	16.02075
C	0.213013	15.13017	14.02155	C	3.961093	11.82717	16.40002
C	-0.68619	15.52955	15.09594	C	3.524265	14.67547	20.04074
Cl	1.195154	12.47933	10.31201	C	2.391388	18.90505	16.64445
H	-1.16004	16.48408	14.85046	C	3.975206	15.58581	15.73221
H	-0.1279	15.6396	16.0303	C	3.797518	14.34568	16.37967
H	-1.46627	14.77445	15.2292	C	3.03983	10.85133	15.99399
N	7.084644	14.77191	17.49522	C	2.273223	14.14115	20.34463
C	7.634345	13.89117	16.98068	C	4.292972	18.45089	18.02765
C	8.286948	12.76749	16.32522	C	4.064276	13.1442	15.68752
Cl	6.191351	16.96562	20.49388	C	1.97608	13.73385	17.99972
Cu	5.868268	15.9153	18.47281	C	3.251967	19.30274	17.66437
H	7.603511	12.33058	15.58507	C	1.48295	13.66504	19.30092
H	9.203912	13.10028	15.82988	C	4.722636	10.483	18.1017
H	8.544606	12.00713	17.06819	C	2.980709	9.647477	16.692
N	3.971962	14.28431	11.31728	C	3.840783	9.453666	17.77117
N	5.644251	17.64585	14.15773	H	2.973071	16.77631	12.28526
C	4.956055	14.44937	12.22914	H	3.46726	14.07915	9.330325

N	6.079372	11.42558	13.99654	H	6.761811	19.36677	13.98678
C	4.605387	16.93381	13.69077	H	3.116016	11.70065	12.38381
C	3.804797	17.38055	12.63024	H	5.802327	14.4168	8.489474
C	4.877002	11.91274	13.63539	H	3.489558	18.97782	11.21676
C	4.293619	14.26376	10.0099	H	7.047127	14.75387	12.60692
C	5.913254	18.82113	13.57919	H	5.439334	20.30833	12.08837
C	4.356242	15.6189	14.37476	H	7.641222	14.75954	10.17283
C	4.561463	14.4171	13.67462	H	3.93426	9.633931	11.30453
C	4.078272	11.28872	12.66964	H	7.483421	9.941008	13.7242
C	5.596347	14.43689	9.554082	H	6.184328	8.711683	11.98645
C	4.096913	18.60731	12.03762	H	1.980297	17.34337	15.2081
C	4.456643	13.17853	14.3363	H	4.180147	15.08975	20.80289
C	6.287759	14.6224	11.84462	H	1.562904	19.53653	16.33629
C	5.17507	19.3477	12.51851	H	2.384342	11.03646	15.14973
C	6.611789	14.62335	10.49015	H	1.932748	14.10805	21.37426
C	4.541442	10.12473	12.0591	H	4.972026	18.68266	18.84418
C	6.508386	10.3041	13.40446	H	1.395966	13.35781	17.16317
C	5.783162	9.615751	12.43298	H	3.121836	20.24802	18.18065
N	4.001232	14.74142	18.78868	H	0.500093	13.24461	19.49418
N	4.512742	17.26939	17.42761	H	5.408798	10.37342	18.93918
C	3.24921	14.27543	17.77714	H	2.273175	8.877411	16.39867
N	4.78924	11.64409	17.44157	H	3.830626	8.532855	18.3453

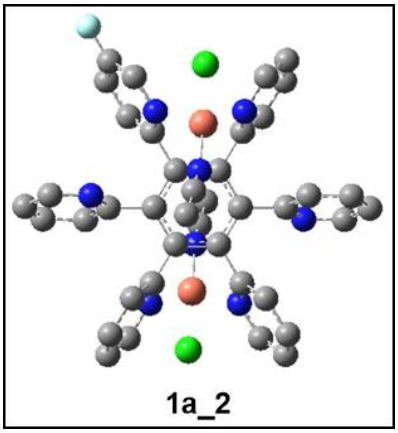


G° -2504.525139

G° (acetonitrile) -2504.623268

Cu	3.694378	-0.02648	-1.64647	C	-2.41255	1.452098	-0.76686
Cl	5.992561	-0.07054	-2.10377	C	1.165773	0.733627	0.313132
N	2.733015	0.050476	-3.33527	C	3.535684	3.00217	2.211192
C	2.504443	0.191052	-4.46336	C	-3.5588	2.842103	-2.36451
C	2.26797	0.377558	-5.88873	C	-0.8736	3.619346	0.890858
H	1.803081	1.350709	-6.07023	C	4.629714	2.965034	1.349461

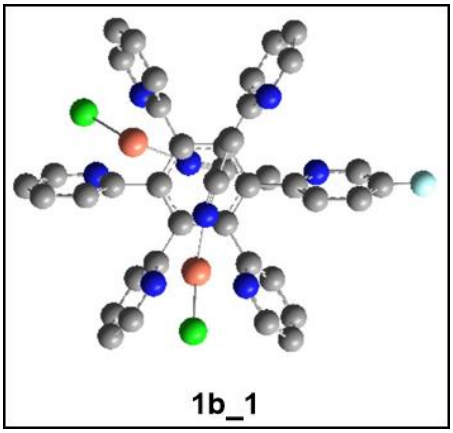
H	1.609788	-0.40616	-6.2743	C	-0.85847	5.011697	0.866123
H	3.21972	0.33576	-6.42667	C	0.751683	4.875785	-0.89837
N	-3.46162	-1.45845	0.085994	C	-0.02844	5.659243	-0.04774
N	3.462751	-1.45911	-0.06681	F	-0.02118	-6.95634	0.06551
N	-0.77018	-3.52591	0.84407	H	5.388531	-2.09578	-0.39397
C	0.044338	-2.89526	-0.01838	H	-1.52867	-2.22339	-2.56535
C	1.180097	-0.67516	0.31775	H	1.533109	-2.04674	2.632701
C	4.557489	-2.14641	0.304727	H	-5.38812	-2.07288	0.4482
C	0.01424	-1.39583	-0.00967	H	5.543087	-3.37817	1.764242
C	-2.40134	-2.23029	-1.9214	H	-3.55919	-3.54842	-3.17392
C	2.40986	-2.08936	1.995738	H	3.571721	-3.32357	3.327611
C	-4.55329	-2.17035	-0.24094	H	1.532817	-3.04919	-1.58032
C	4.637436	-2.83727	1.511027	H	-5.53267	-3.50555	-1.61209
C	-2.39158	-1.49286	-0.73197	H	1.507013	-5.56934	-1.5538
C	2.399611	-1.42962	0.761604	H	-1.44139	-5.35836	1.560619
C	-1.17538	-0.71186	-0.32994	H	-5.40663	2.091508	0.3903
C	-3.53368	-2.96866	-2.25587	H	1.526902	2.27182	2.530234
C	3.544055	-2.80342	2.374643	H	-1.54322	2.099501	-2.62629
C	0.884238	-3.5923	-0.90132	H	5.383117	2.067242	-0.48422
C	-4.6286	-2.94676	-1.39465	H	-5.5617	3.400451	-1.7514
C	0.878611	-4.98433	-0.89076	H	3.564587	3.592501	3.122374
C	-0.77753	-4.86086	0.857827	H	-3.5862	3.374703	-3.31059
C	0.028827	-5.61282	0.008649	H	-1.5097	3.078341	1.58347
N	3.454476	1.465083	-0.11266	H	5.536754	3.52181	1.559665
N	-3.47789	1.465843	0.059121	H	-1.48339	5.579142	1.549555
N	0.749773	3.538015	-0.88582	H	1.412135	5.342528	-1.62655
C	-0.05132	2.917996	-0.00345	H	0.016642	6.742109	-0.10311
C	-1.19099	0.697067	-0.32994	Cu	-3.70948	0.022333	1.628466
C	-4.57427	2.153932	-0.30586	Cl	-6.00961	0.048415	2.080349
C	-0.02415	1.417486	-0.00586	N	-2.75574	-0.05551	3.321626
C	2.399445	2.265638	1.886284	C	-2.53502	-0.19067	4.45195
C	-2.4225	2.128159	-1.99216	C	-2.309	-0.36966	5.879987
C	4.549577	2.175865	0.204808	H	-1.8435	-1.34087	6.070119
C	-4.65431	2.860107	-1.50321	H	-1.65549	0.417445	6.26661
C	2.385127	1.514327	0.705689	H	-3.26496	-0.32728	6.410378



G°	-2504.524602
G° (acetonitrile)	-2504.62265

Cu	3.692711	-0.03886	-1.64504	C	-2.41013	1.454211	-0.78201
Cl	5.992173	-0.09277	-2.10141	C	1.16374	0.735994	0.309405
N	2.742578	0.067865	-3.33934	C	3.533189	3.016073	2.194117
C	2.528159	0.239816	-4.46586	C	-3.54421	2.834681	-2.39704
C	2.311013	0.467722	-5.88827	C	-0.86968	3.62822	0.870543
H	1.827401	1.435865	-6.04615	C	4.623808	2.981777	1.328027
H	1.677364	-0.31726	-6.31058	C	-0.85346	5.020338	0.836794
H	3.272399	0.464551	-6.4105	C	0.752474	4.871846	-0.93036
N	-3.46996	-1.44259	0.104066	C	-0.02513	5.661446	-0.08308
N	3.459941	-1.4548	-0.0591	F	-5.73184	-3.64857	-1.60257
N	-0.77526	-3.50743	0.891915	H	5.385993	-2.09175	-0.38374
C	0.032158	-2.89396	0.010222	H	-1.54181	-2.26434	-2.5336
C	1.175878	-0.6729	0.322338	H	1.523272	-2.05009	2.633425
C	4.553541	-2.14361	0.313219	H	-5.41378	-2.05402	0.475281
C	0.007835	-1.39347	0.002882	H	5.535259	-3.37957	1.771526
C	-2.41225	-2.25337	-1.88718	H	-3.59577	-3.60237	-3.11271
C	2.402177	-2.09014	1.999368	H	3.559966	-3.32871	3.330433
C	-4.56531	-2.1537	-0.19723	H	1.497695	-3.06783	-1.56899
C	4.63036	-2.8376	1.517901	H	1.464946	-5.56766	-1.52051
C	-2.39881	-1.49251	-0.71203	H	-1.44533	-5.3062	1.639998
C	2.394725	-1.42742	0.766887	H	-0.04538	-6.71788	0.131684
C	-1.18058	-0.70964	-0.32215	H	-5.40833	2.11439	0.354654
C	-3.54196	-2.99836	-2.21335	H	1.528225	2.279465	2.522148
C	3.535024	-2.80573	2.378929	H	-1.53037	2.081827	-2.64267
C	0.856843	-3.60279	-0.87594	H	5.374084	2.083505	-0.50609
C	-4.61829	-2.94338	-1.33957	H	-5.54825	3.405097	-1.79859
C	0.838286	-4.99498	-0.84305	H	3.563029	3.608763	3.103743
C	-0.78001	-4.84519	0.9126	H	-3.5649	3.359362	-3.34768
C	0.002646	-5.63548	0.07055	H	-1.50417	3.092564	1.568912
N	3.450258	1.470926	-0.12439	H	5.528936	3.543626	1.532908
N	-3.47971	1.47947	0.038853	H	-1.47607	5.592546	1.518369
N	0.749419	3.534126	-0.90926	H	1.411859	5.333303	-1.66286
C	-0.05028	2.92031	-0.02115	H	0.020738	6.743906	-0.14521
C	-1.19263	0.699301	-0.33484	Cu	-3.713	0.087409	1.632898
C	-4.57231	2.168033	-0.33774	Cl	-6.01271	0.095882	2.063367
C	-0.02493	1.419807	-0.01412	N	-2.75391	-0.05751	3.31561

C	2.398635	2.274267	1.875281	C	-2.51988	-0.25576	4.433754
C	-2.41261	2.119527	-2.01316	C	-2.276	-0.51748	5.84593
C	4.542783	2.188598	0.18614	H	-1.82015	-1.50346	5.97304
C	-4.64392	2.863888	-1.54148	H	-1.60718	0.238528	6.266831
C	2.383374	1.519116	0.697139	H	-3.22374	-0.49444	6.391984

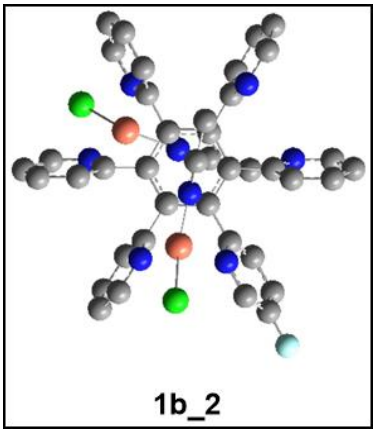


G° -2504.519099

G° (acetonitrile) -2504.616698

Cu	4.079368	3.284944	7.815448	C	5.997087	4.127711	5.435888
Cl	4.257292	1.279753	8.931771	C	5.386269	5.480956	5.668055
N	2.487764	4.113712	7.089037	C	7.603043	2.721777	4.318373
C	1.656585	4.532503	6.398641	C	1.286243	8.116372	2.699004
C	0.644358	5.071045	5.502455	C	5.014533	5.848879	2.117027
H	0.282205	4.279949	4.839559	C	7.078421	1.636187	5.016263
H	1.086067	5.873624	4.896837	C	4.767765	5.135363	0.946582
H	-0.19983	5.462737	6.077699	C	3.474077	3.608441	2.256373
N	4.727238	10.5183	5.747029	C	3.979135	3.988301	1.012592
N	5.692544	4.470275	8.682675	F	5.221114	9.820265	12.09592
N	4.408728	7.616313	9.372669	H	5.808514	3.069039	10.17837
C	5.163104	8.143966	8.393997	H	2.038385	8.912709	6.982171
C	5.546027	6.143354	6.902334	H	7.966741	6.830184	7.904556
C	6.318978	3.920638	9.73608	H	4.943649	12.55189	5.466259
C	5.070417	7.461237	7.058443	H	8.010477	3.89598	11.06364
C	2.651137	9.751284	6.672249	H	1.212721	11.2688	7.19511
C	7.522798	6.002072	8.447016	H	9.134041	5.804893	9.868177
C	4.2736	11.78421	5.839987	H	6.579158	9.660699	7.792313
C	7.549823	4.37429	10.2057	H	2.708852	13.13661	6.413881
C	3.9224	9.507075	6.146498	H	6.632605	10.72126	10.08015
C	6.276441	5.504613	8.048178	H	3.824924	7.736343	11.36314
C	4.437191	8.109357	5.982789	H	4.85058	9.44087	2.938604
C	2.197075	11.06232	6.786348	H	3.329942	10.39546	1.245082
C	8.167802	5.430944	9.541538	H	7.43596	4.853315	4.002356

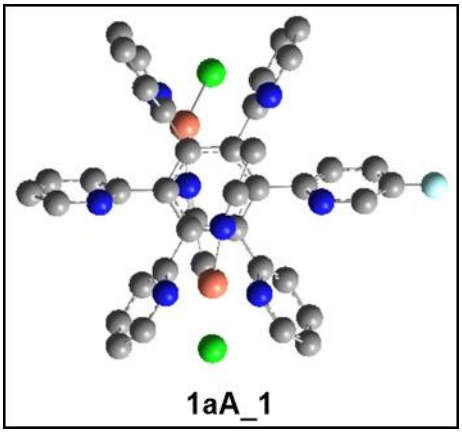
C	5.980035	9.264283	8.604188	H	5.599975	1.066555	6.511098
C	3.023126	12.10024	6.357784	H	0.967655	9.514188	1.087899
C	6.015214	9.855391	9.865102	H	8.424206	2.590082	3.619593
C	4.439803	8.177839	10.58279	H	0.276878	7.710268	2.664764
C	5.22742	9.292126	10.85838	H	5.626113	6.744775	2.103848
N	5.504581	3.077904	6.115912	H	7.470884	0.633432	4.883187
C	3.834412	9.067976	2.858476	H	5.187596	5.468968	0.002077
C	4.461974	5.389182	3.320658	H	2.856645	2.717387	2.351622
C	4.215336	7.429178	4.77001	H	3.760811	3.39939	0.127616
C	2.974572	9.608758	1.903799	Cu	6.58096	10.27706	4.935258
C	4.70123	6.117725	4.610795	N	8.230398	9.472828	5.549927
C	7.056744	3.98528	4.531209	C	9.332781	9.12762	5.646932
N	2.097246	7.589463	3.624632	C	10.72643	8.714737	5.738992
N	3.703127	4.283	3.388217	Cl	6.767352	11.33191	2.950235
C	3.357632	8.058286	3.702604	H	10.79192	7.629428	5.855078
C	6.033652	1.862513	5.910462	H	11.25894	9.008695	4.829782
C	1.671202	9.124864	1.816768	H	11.20305	9.193031	6.599145



G°	-2504.51741
G° (acetonitrile)	-2504.615586

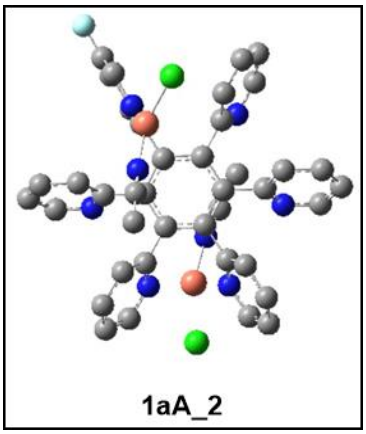
Cu	4.076117	3.30782	7.828223	C	5.999535	4.132678	5.447287
Cl	4.24259	1.304453	8.950834	C	5.392848	5.488559	5.674299
N	2.487023	4.133486	7.094644	C	7.598402	2.716385	4.332859
C	1.651635	4.549742	6.407923	C	1.302857	8.109383	2.686848
C	0.633788	5.085319	5.516272	C	5.006711	5.848795	2.119435
H	0.260656	4.290293	4.864229	C	7.074803	1.636375	5.040178
H	1.074416	5.879773	4.899579	C	4.756948	5.129866	0.953023
H	-0.20277	5.487062	6.095693	C	3.481435	3.599352	2.276174
N	4.739501	10.5291	5.727558	C	3.97607	3.978092	1.027834
N	5.688775	4.490032	8.695676	F	2.659792	13.37177	6.42501

N	4.386185	7.664248	9.356041	H	5.79367	3.095658	10.19855
C	5.174601	8.164524	8.390467	H	2.066498	8.934752	7.009992
C	5.555016	6.154744	6.90651	H	7.975278	6.835752	7.9125
C	6.309324	3.94276	9.753762	H	4.943637	12.57891	5.429705
C	5.084003	7.474423	7.057399	H	7.997086	3.916889	11.08607
C	2.676992	9.76882	6.684341	H	1.243492	11.31251	7.21561
C	7.527107	6.011574	8.457293	H	9.13248	5.814877	9.885141
C	4.298264	11.79662	5.815243	H	6.638725	9.635544	7.796134
C	7.541005	4.392952	10.22441	H	6.686168	10.71175	10.05535
C	3.94192	9.519373	6.14282	H	3.767976	7.808941	11.31492
C	6.279823	5.517831	8.057061	H	5.210005	9.773469	11.8634
C	4.452704	8.120754	5.979975	H	4.852083	9.466662	2.953275
C	2.217261	11.07692	6.800194	H	3.332603	10.41649	1.257775
C	8.165852	5.443291	9.556923	H	7.434337	4.846027	4.003316
C	6.017066	9.264252	8.603262	H	5.600536	1.079392	6.544304
C	3.052174	12.09066	6.350635	H	0.979876	9.513087	1.081625
C	6.039861	9.860033	9.862876	H	8.416303	2.578277	3.631462
C	4.419159	8.245278	10.56032	H	0.29742	7.694346	2.645223
C	5.224402	9.342684	10.86747	H	5.612181	6.748654	2.09877
N	5.507614	3.088099	6.135725	H	7.465125	0.632133	4.912095
C	3.84053	9.083489	2.865424	H	5.168557	5.462849	0.004684
C	4.465206	5.389827	3.328464	H	2.870133	2.704883	2.378539
C	4.226938	7.43706	4.769851	H	3.755735	3.384932	0.146204
C	2.981188	9.622089	1.909283	Cu	6.602147	10.29146	4.895606
C	4.708716	6.123415	4.614917	N	8.215516	9.417158	5.47782
C	7.055569	3.982328	4.539537	C	9.297367	9.017975	5.595333
N	2.113641	7.585043	3.614255	C	10.66529	8.532263	5.714132
N	3.713931	4.279052	3.404182	Cl	6.703637	11.47485	2.983813
C	3.369497	8.064422	3.701567	H	10.66987	7.449233	5.86498
C	6.03386	1.870378	5.936749	H	11.22187	8.767895	4.802378
C	1.68312	9.126084	1.811966	H	11.15963	9.011048	6.563975



G°	-2504.533556
G° (acetonitrile)	-2504.622633

Cu	3.486396	-1.10369	1.341545	C	-1.30031	-2.22194	0.608057
N	2.567839	0.075429	2.580565	C	-0.81784	-3.05024	1.626506
C	2.083038	0.912243	3.221231	C	-1.27198	2.821493	0.699844
C	1.463887	1.989964	3.981154	C	-4.87625	-0.03545	1.191692
Cl	5.540081	-2.0666	1.634964	C	-1.45163	-4.26857	1.862991
H	2.235569	2.633713	4.41392	C	-0.63358	-0.91446	0.296118
H	0.860101	1.578019	4.795231	C	-1.26164	0.306203	0.620511
H	0.823902	2.581446	3.312217	C	-2.45312	3.24517	0.076551
N	-2.55452	0.064029	-2.5883	C	-5.05858	0.313301	2.528591
C	-2.0763	0.903151	-3.23081	C	-2.97594	-3.73608	0.090949
C	-1.46661	1.984428	-3.99351	C	-0.62381	1.522342	0.322438
Cl	-5.5282	-2.06955	-1.65234	C	-2.68871	0.666692	2.673719
Cu	-3.47455	-1.10974	-1.34402	C	-2.54719	-4.62126	1.077606
H	-0.8347	2.584991	-3.32613	C	-3.94191	0.667447	3.282987
H	-0.85657	1.576313	-4.80482	C	-3.01727	4.459944	0.454572
H	-2.24374	2.618996	-4.42999	C	-1.217	4.714896	2.007358
N	3.676671	-0.03591	-0.61234	C	-2.38666	5.2172	1.441032
N	2.371314	-2.56129	0.150032	F	2.890555	6.384102	-1.8025
C	2.593046	0.31412	-1.33056	H	-0.02705	-2.742	-2.21654
N	0.669315	3.560503	-1.6351	H	5.703168	-0.3633	-0.57577
C	1.308772	-2.22126	-0.60829	H	1.107035	-4.93098	-2.64412
C	0.830585	-3.05022	-1.62827	H	2.937214	2.608849	0.67533
C	1.281288	2.821817	-0.6922	H	6.050677	0.294995	-2.98179
C	4.879682	-0.03945	-1.20762	H	3.847233	-3.93532	0.542818
C	1.462842	-4.27047	-1.85907	H	1.79498	0.948396	-3.22854
C	0.6402	-0.91399	-0.29934	H	3.076443	-5.56353	-1.21067
C	1.267478	0.306729	-0.62358	H	4.036707	0.945956	-4.33995
C	2.470649	3.236637	-0.07535	H	3.960826	4.815045	0.008917
C	5.058238	0.313512	-2.54401	H	0.712253	5.319754	-2.74865
C	2.978638	-3.7378	-0.07983	H	0.043402	-2.74179	2.209269
C	0.631174	1.522741	-0.32092	H	-5.69811	-0.35674	0.556529
C	2.68861	0.67297	-2.6793	H	-1.09295	-4.92843	2.647293
C	2.552948	-4.62429	-1.06672	H	-2.91301	2.625402	-0.68508
C	3.93968	0.673108	-3.29321	H	-6.05254	0.295138	2.963013
C	3.042575	4.451256	-0.43951	H	-3.84791	-3.93328	-0.5272
C	1.215007	4.730437	-1.9859	H	-1.79647	0.938633	3.226732
C	2.389712	5.199557	-1.40957	H	-3.07212	-5.5589	1.226679
N	-3.67133	-0.03141	0.600354	H	-4.04198	0.936582	4.330412
N	-2.36696	-2.56148	-0.1444	H	-3.93205	4.809673	-0.01466
C	-2.58947	0.313734	1.323703	H	-0.69756	5.273963	2.783203
N	-0.66225	3.54663	1.655375	H	-2.78845	6.170826	1.767163

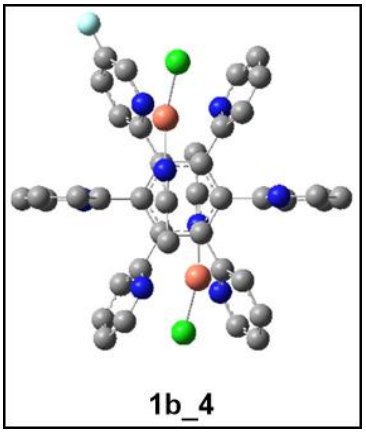


1aA_2

G°	-2504.532625
G° (acetonitrile)	-2504.621851

Cu	3.47645	-1.09974	1.327853	C	-1.29839	-2.21135	0.616669
N	2.594783	0.140264	2.527232	C	-0.82111	-3.04754	1.630794
C	2.06488	0.882177	3.243696	C	-1.25783	2.831852	0.724652
C	1.365225	1.848317	4.08009	C	-4.86326	-0.02111	1.236379
Cl	5.540925	-2.03147	1.624361	C	-1.45079	-4.27125	1.8499
H	2.08403	2.467792	4.624436	C	-0.62877	-0.90358	0.312388
H	0.733662	1.329633	4.807126	C	-1.2524	0.316225	0.6454
H	0.741951	2.484913	3.437207	C	-2.41277	3.286487	0.075324
N	-2.52813	0.137194	-2.51632	C	-5.04063	0.337357	2.571526
C	-2.05066	0.908126	-3.23919	C	-2.96395	-3.7269	0.071985
C	-1.40216	1.893658	-4.09312	C	-0.6176	1.531356	0.336465
Cl	-5.50553	-2.03299	-1.67483	C	-2.66978	0.691136	2.704057
Cu	-3.46445	-1.07538	-1.32721	C	-2.53793	-4.62113	1.051819
H	-0.75654	2.528456	-3.47161	C	-3.92064	0.696498	3.318396
H	-0.80019	1.39145	-4.85624	C	-2.97218	4.499564	0.466317
H	-2.1512	2.513556	-4.5946	C	-1.21758	4.690232	2.080346
N	3.669698	-0.03139	-0.6517	C	-2.36175	5.222837	1.490445
N	2.37367	-2.54696	0.157659	F	6.2356	0.33539	-3.13337
C	2.578731	0.326832	-1.35464	H	-0.03793	-2.74736	-2.19339
N	0.678564	3.520334	-1.71701	H	5.713085	-0.36076	-0.63793
C	1.306922	-2.21267	-0.59861	H	1.085509	-4.94564	-2.6014
C	0.82176	-3.05204	-1.60643	H	2.854348	2.693876	0.727808
C	1.263803	2.831399	-0.72004	H	3.845395	-3.92436	0.559602
C	4.87067	-0.03159	-1.24196	H	1.772946	0.984472	-3.24367
C	1.447819	-4.27739	-1.82594	H	3.058819	-5.56952	-1.16864
C	0.639355	-0.90383	-0.29577	H	4.028638	0.989968	-4.37063
C	1.26028	0.315677	-0.63592	H	3.869706	4.875549	0.034877
C	2.415274	3.288016	-0.06585	H	0.731219	5.219399	-2.88681
C	5.014591	0.340487	-2.57441	H	2.771398	6.172037	-1.82176
C	2.974535	-3.72974	-0.06081	H	0.034536	-2.74227	2.22345

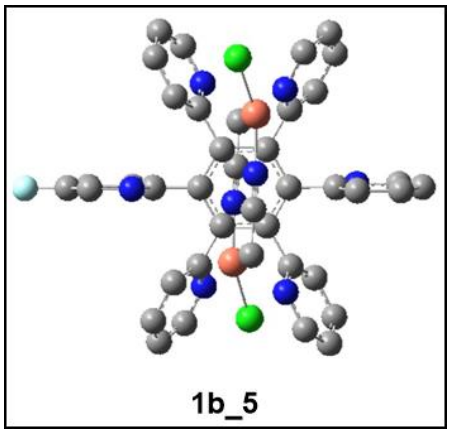
C	0.623679	1.531061	-0.33042	H	-5.68901	-0.34214	0.60592
C	2.667238	0.70048	-2.70071	H	-1.09506	-4.93764	2.630018
C	2.539903	-4.62639	-1.0342	H	-2.85573	2.690027	-0.71431
C	3.910174	0.71018	-3.32939	H	-6.03302	0.323934	3.009688
C	2.976736	4.500371	-0.45614	H	-3.82973	-3.92278	-0.55531
C	1.229508	4.687896	-2.07841	H	-1.77599	0.96879	3.251437
C	2.370973	5.221732	-1.48433	H	-3.05886	-5.56326	1.1859
N	-3.66095	-0.02372	0.641259	H	-4.0163	0.974195	4.364011
N	-2.35968	-2.54656	-0.14605	H	-3.86754	4.873875	-0.02103
C	-2.5757	0.326685	1.356654	H	-0.71547	5.222826	2.885641
N	-0.66821	3.522559	1.717416	H	-2.76078	6.173719	1.827982



G°	-2504.527445
G° (acetonitrile)	-2504.613444

Cu	3.486396	-1.10369	1.341545	C	-1.30031	-2.22194	0.608057
N	2.567839	0.075429	2.580565	C	-0.81784	-3.05024	1.626506
C	2.083038	0.912243	3.221231	C	-1.27198	2.821493	0.699844
C	1.463887	1.989964	3.981154	C	-4.87625	-0.03545	1.191692
Cl	5.540081	-2.0666	1.634964	C	-1.45163	-4.26857	1.862991
H	2.235569	2.633713	4.41392	C	-0.63358	-0.91446	0.296118
H	0.860101	1.578019	4.795231	C	-1.26164	0.306203	0.620511
H	0.823902	2.581446	3.312217	C	-2.45312	3.24517	0.076551
N	-2.55452	0.064029	-2.5883	C	-5.05858	0.313301	2.528591
C	-2.0763	0.903151	-3.23081	C	-2.97594	-3.73608	0.090949
C	-1.46661	1.984428	-3.99351	C	-0.62381	1.522342	0.322438
Cl	-5.5282	-2.06955	-1.65234	C	-2.68871	0.666692	2.673719
Cu	-3.47455	-1.10974	-1.34402	C	-2.54719	-4.62126	1.077606
H	-0.8347	2.584991	-3.32613	C	-3.94191	0.667447	3.282987
H	-0.85657	1.576313	-4.80482	C	-3.01727	4.459944	0.454572
H	-2.24374	2.618996	-4.42999	C	-1.217	4.714896	2.007358
N	3.676671	-0.03591	-0.61234	C	-2.38666	5.2172	1.441032
N	2.371314	-2.56129	0.150032	F	2.890555	6.384102	-1.8025
C	2.593046	0.31412	-1.33056	H	-0.02705	-2.742	-2.21654
N	0.669315	3.560503	-1.6351	H	5.703168	-0.3633	-0.57577

C	1.308772	-2.22126	-0.60829	H	1.107035	-4.93098	-2.64412
C	0.830585	-3.05022	-1.62827	H	2.937214	2.608849	0.67533
C	1.281288	2.821817	-0.6922	H	6.050677	0.294995	-2.98179
C	4.879682	-0.03945	-1.20762	H	3.847233	-3.93532	0.542818
C	1.462842	-4.27047	-1.85907	H	1.79498	0.948396	-3.22854
C	0.6402	-0.91399	-0.29934	H	3.076443	-5.56353	-1.21067
C	1.267478	0.306729	-0.62358	H	4.036707	0.945956	-4.33995
C	2.470649	3.236637	-0.07535	H	3.960826	4.815045	0.008917
C	5.058238	0.313512	-2.54401	H	0.712253	5.319754	-2.74865
C	2.978638	-3.7378	-0.07983	H	0.043402	-2.74179	2.209269
C	0.631174	1.522741	-0.32092	H	-5.69811	-0.35674	0.556529
C	2.68861	0.67297	-2.6793	H	-1.09295	-4.92843	2.647293
C	2.552948	-4.62429	-1.06672	H	-2.91301	2.625402	-0.68508
C	3.93968	0.673108	-3.29321	H	-6.05254	0.295138	2.963013
C	3.042575	4.451256	-0.43951	H	-3.84791	-3.93328	-0.5272
C	1.215007	4.730437	-1.9859	H	-1.79647	0.938633	3.226732
C	2.389712	5.199557	-1.40957	H	-3.07212	-5.5589	1.226679
N	-3.67133	-0.03141	0.600354	H	-4.04198	0.936582	4.330412
N	-2.36696	-2.56148	-0.1444	H	-3.93205	4.809673	-0.01466
C	-2.58947	0.313734	1.323703	H	-0.69756	5.273963	2.783203
N	-0.66225	3.54663	1.655375	H	-2.78845	6.170826	1.767163

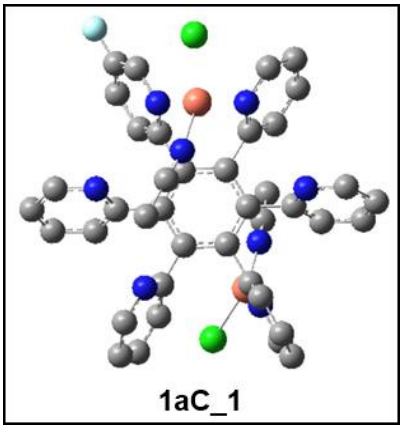


G° -2504.527967

G° (acetonitrile) -2504.614692

Cu	3.47645	-1.09974	1.327853	C	-1.29839	-2.21135	0.616669
N	2.594783	0.140264	2.527232	C	-0.82111	-3.04754	1.630794
C	2.06488	0.882177	3.243696	C	-1.25783	2.831852	0.724652
C	1.365225	1.848317	4.08009	C	-4.86326	-0.02111	1.236379
Cl	5.540925	-2.03147	1.624361	C	-1.45079	-4.27125	1.8499
H	2.08403	2.467792	4.624436	C	-0.62877	-0.90358	0.312388
H	0.733662	1.329633	4.807126	C	-1.2524	0.316225	0.6454
H	0.741951	2.484913	3.437207	C	-2.41277	3.286487	0.075324
N	-2.52813	0.137194	-2.51632	C	-5.04063	0.337357	2.571526

C	-2.05066	0.908126	-3.23919	C	-2.96395	-3.7269	0.071985
C	-1.40216	1.893658	-4.09312	C	-0.6176	1.531356	0.336465
Cl	-5.50553	-2.03299	-1.67483	C	-2.66978	0.691136	2.704057
Cu	-3.46445	-1.07538	-1.32721	C	-2.53793	-4.62113	1.051819
H	-0.75654	2.528456	-3.47161	C	-3.92064	0.696498	3.318396
H	-0.80019	1.39145	-4.85624	C	-2.97218	4.499564	0.466317
H	-2.1512	2.513556	-4.5946	C	-1.21758	4.690232	2.080346
N	3.669698	-0.03139	-0.6517	C	-2.36175	5.222837	1.490445
N	2.37367	-2.54696	0.157659	F	6.2356	0.33539	-3.13337
C	2.578731	0.326832	-1.35464	H	-0.03793	-2.74736	-2.19339
N	0.678564	3.520334	-1.71701	H	5.713085	-0.36076	-0.63793
C	1.306922	-2.21267	-0.59861	H	1.085509	-4.94564	-2.6014
C	0.82176	-3.05204	-1.60643	H	2.854348	2.693876	0.727808
C	1.263803	2.831399	-0.72004	H	3.845395	-3.92436	0.559602
C	4.87067	-0.03159	-1.24196	H	1.772946	0.984472	-3.24367
C	1.447819	-4.27739	-1.82594	H	3.058819	-5.56952	-1.16864
C	0.639355	-0.90383	-0.29577	H	4.028638	0.989968	-4.37063
C	1.26028	0.315677	-0.63592	H	3.869706	4.875549	0.034877
C	2.415274	3.288016	-0.06585	H	0.731219	5.219399	-2.88681
C	5.014591	0.340487	-2.57441	H	2.771398	6.172037	-1.82176
C	2.974535	-3.72974	-0.06081	H	0.034536	-2.74227	2.22345
C	0.623679	1.531061	-0.33042	H	-5.68901	-0.34214	0.60592
C	2.667238	0.70048	-2.70071	H	-1.09506	-4.93764	2.630018
C	2.539903	-4.62639	-1.0342	H	-2.85573	2.690027	-0.71431
C	3.910174	0.71018	-3.32939	H	-6.03302	0.323934	3.009688
C	2.976736	4.500371	-0.45614	H	-3.82973	-3.92278	-0.55531
C	1.229508	4.687896	-2.07841	H	-1.77599	0.96879	3.251437
C	2.370973	5.221732	-1.48433	H	-3.05886	-5.56326	1.1859
N	-3.66095	-0.02372	0.641259	H	-4.0163	0.974195	4.364011
N	-2.35968	-2.54656	-0.14605	H	-3.86754	4.873875	-0.02103
C	-2.5757	0.326685	1.356654	H	-0.71547	5.222826	2.885641
N	-0.66821	3.522559	1.717416	H	-2.76078	6.173719	1.827982

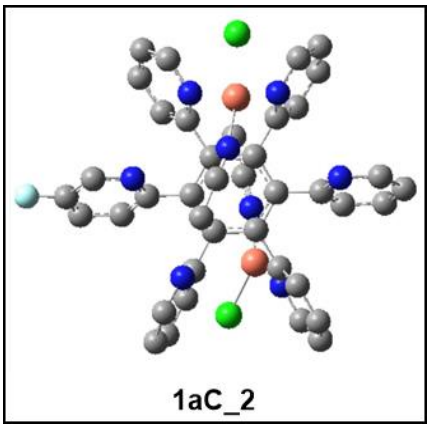


1aC_1

G°	-2504.518761
G° (acetonitrile)	-2504.616721

Cu	1.947463	14.08073	11.87213	C	3.740863	16.83264	16.53595
N	0.651567	15.13239	12.85096	C	2.617721	17.59378	16.19114
C	-0.3322	15.54403	13.30545	C	4.070098	11.77881	16.47725
C	-1.58748	16.03206	13.85979	C	3.797329	14.63702	20.14335
Cl	1.060967	12.26562	10.86422	C	2.39778	18.81349	16.82676
H	-1.82437	17.01542	13.44424	C	4.015859	15.53937	15.82445
H	-1.51272	16.11536	14.94751	C	3.88009	14.29568	16.47471
H	-2.39521	15.33778	13.61034	C	3.142445	10.79965	16.09468
N	7.214859	14.76554	17.44201	C	2.572559	14.07548	20.48683
C	7.750936	13.874	16.93178	C	4.388326	18.41496	18.09766
C	8.385083	12.73639	16.28273	C	4.138323	13.10031	15.76927
Cl	6.42378	16.95251	20.4671	C	2.149853	13.6578	18.18603
Cu	6.04023	15.92258	18.44864	C	3.3055	19.23735	17.79406
H	7.688099	12.29956	15.55515	C	1.722145	13.58013	19.50881
H	9.300349	13.05387	15.77437	C	4.894186	10.43053	18.146
H	8.641877	11.98174	17.03174	C	3.113296	9.591703	16.78758
N	3.914587	14.31363	11.39507	C	4.008545	9.397472	17.83768
N	5.672772	17.58124	14.19045	F	2.207715	14.02222	21.78001
C	4.918835	14.42921	12.29379	H	2.870831	16.81081	12.47334
N	6.128438	11.42102	14.00919	H	3.377949	14.1674	9.407126
C	4.588593	16.90407	13.77757	H	6.821847	19.27683	13.97969
C	3.737293	17.38852	12.77509	H	3.108068	11.64692	12.49021
C	4.906347	11.88774	13.68773	H	5.704426	14.42794	8.538965
C	4.217208	14.30437	10.08156	H	3.379479	19.01784	11.40836
C	5.936357	18.75974	13.61584	H	7.023711	14.65538	12.64025
C	4.353774	15.58311	14.45677	H	5.411106	20.28441	12.18114
C	4.553283	14.38609	13.74618	H	7.581165	14.6793	10.19773
C	4.087903	11.25523	12.74463	H	3.93019	9.602739	11.37953
C	5.516578	14.43812	9.606971	H	7.548696	9.962008	13.68685
C	4.02509	18.61784	12.18516	H	6.217224	8.717071	11.98521
C	4.486244	13.14391	14.40597	H	1.938108	17.22804	15.42875
C	6.249077	14.56277	11.88787	H	4.467085	15.06679	20.88499
C	5.148825	19.32314	12.61111	H	1.533552	19.41984	16.57069
C	6.552768	14.57408	10.52945	H	2.458839	10.986	15.27323
C	4.553442	10.10183	12.11545	H	5.10416	18.66403	18.87659
C	6.558135	10.30963	13.39895	H	1.524216	13.28139	17.38391
C	5.8148	9.612735	12.44742	H	3.178425	20.17886	18.31796
N	4.195185	14.70077	18.86743	H	0.763156	13.15278	19.78177
N	4.60591	17.23976	17.48455	H	5.607131	10.32044	18.96076
C	3.400296	14.21887	17.89579	H	2.401098	8.819037	16.51299

N	4.932514	11.59577	17.49077	H	4.021953	8.473768	18.40708



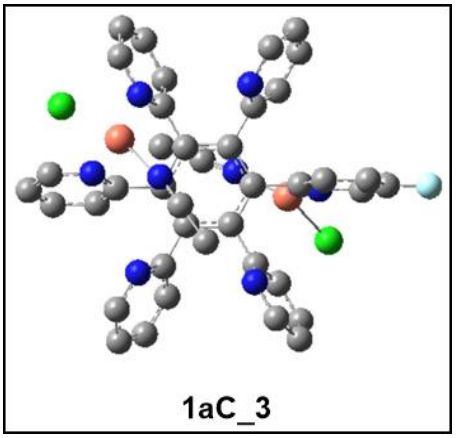
1aC_2

G° -2504.519112

G° (acetonitrile) -2504.616698

Cu	1.958421	13.99597	11.80288	C	3.697436	16.87995	16.43044
N	0.91231	14.82529	13.17777	C	2.622801	17.67947	16.02122
C	0.194419	15.16494	14.02204	C	3.956266	11.82197	16.40066
C	-0.70918	15.5769	15.08797	C	3.510454	14.66494	20.03995
Cl	1.195599	12.42226	10.40121	C	2.402735	18.90399	16.64762
H	-1.18743	16.52496	14.82646	C	3.975642	15.57964	15.73235
H	-0.15289	15.7047	16.02131	C	3.796289	14.33963	16.37976
H	-1.4857	14.82013	15.23204	C	3.049786	10.83887	15.9763
N	7.085967	14.76709	17.49351	C	2.254866	14.13813	20.33791
C	7.651561	13.90499	16.96486	C	4.299248	18.43823	18.03386
C	8.322381	12.80349	16.2903	C	4.067275	13.13793	15.68966
Cl	6.179396	16.94053	20.50465	C	1.963019	13.73902	17.99087
Cu	5.865161	15.89453	18.48105	C	3.262636	19.29549	17.67049
H	7.630706	12.342	15.57287	C	1.464714	13.6704	19.29019
H	9.210005	13.16759	15.76451	C	4.693302	10.48678	18.12817
H	8.632261	12.05451	17.02495	C	2.976288	9.632486	16.66756
N	3.960681	14.29035	11.32444	C	3.819266	9.469035	17.75733
N	5.659511	17.62831	14.1445	F	3.79423	8.325292	18.46545
C	4.952934	14.44423	12.22939	H	2.953127	16.78588	12.31055
N	6.084483	11.41058	14.02734	H	3.440006	14.1011	9.339348
C	4.608003	16.92648	13.69095	H	6.787085	19.34167	13.96236
C	3.794791	17.38265	12.6442	H	3.154242	11.70258	12.35504
C	4.892219	11.90549	13.64258	H	5.769684	14.42896	8.483253
C	4.271996	14.27589	10.01451	H	3.470595	18.98741	11.24093
C	5.928363	18.80376	13.566	H	7.048384	14.73559	12.59265
C	4.358027	15.61176	14.37559	H	5.443008	20.29989	12.08807
C	4.565622	14.4096	13.67665	H	7.623616	14.75052	10.15395
C	4.109292	11.28722	12.66013	H	3.982674	9.633996	11.29173
C	5.572122	14.44371	9.549521	H	7.485557	9.918781	13.78049

C	4.087223	18.60922	12.0513	H	6.214414	8.6988	12.01588
C	4.464737	13.17129	14.33937	H	1.987762	17.34749	15.2068
C	6.282531	14.61159	11.83562	H	4.165802	15.07446	20.80505
C	5.178039	19.33966	12.51865	H	1.577441	19.53955	16.33935
C	6.595998	14.61838	10.47868	H	2.410854	11.01589	15.11801
C	4.578392	10.12106	12.0578	H	1.91045	14.10478	21.36619
C	6.519215	10.2879	13.44188	H	4.977428	18.6649	18.85257
C	5.809655	9.604816	12.4551	H	1.382586	13.37156	17.15066
N	3.992898	14.72953	18.78988	H	3.135293	20.23993	18.18896
N	4.515322	17.25743	17.43128	H	0.478043	13.25701	19.4791
C	3.241253	14.27106	17.77471	H	5.348733	10.35683	18.98585
N	4.759312	11.64121	17.46219	H	2.290263	8.842849	16.3803



1aC_3

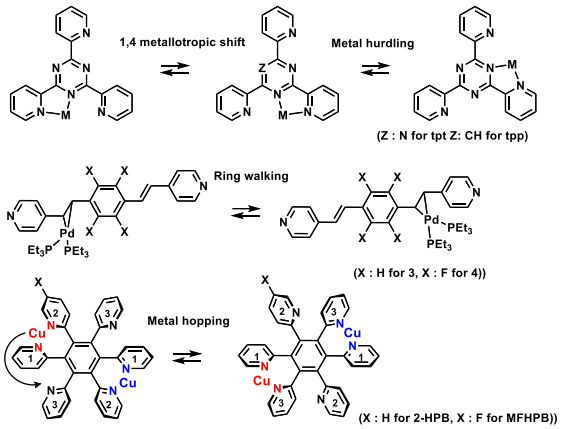
G° -2504.517679

G° (acetonitrile) -2504.615187

Cu	1.947463	14.08073	11.87213	C	3.740863	16.83264	16.53595
N	0.651567	15.13239	12.85096	C	2.617721	17.59378	16.19114
C	-0.3322	15.54403	13.30545	C	4.070098	11.77881	16.47725
C	-1.58748	16.03206	13.85979	C	3.797329	14.63702	20.14335
Cl	1.060967	12.26562	10.86422	C	2.39778	18.81349	16.82676
H	-1.82437	17.01542	13.44424	C	4.015859	15.53937	15.82445
H	-1.51272	16.11536	14.94751	C	3.88009	14.29568	16.47471
H	-2.39521	15.33778	13.61034	C	3.142445	10.79965	16.09468
N	7.214859	14.76554	17.44201	C	2.572559	14.07548	20.48683
C	7.750936	13.874	16.93178	C	4.388326	18.41496	18.09766
C	8.385083	12.73639	16.28273	C	4.138323	13.10031	15.76927
Cl	6.42378	16.95251	20.4671	C	2.149853	13.6578	18.18603
Cu	6.04023	15.92258	18.44864	C	3.3055	19.23735	17.79406
H	7.688099	12.29956	15.55515	C	1.722145	13.58013	19.50881
H	9.300349	13.05387	15.77437	C	4.894186	10.43053	18.146
H	8.641877	11.98174	17.03174	C	3.113296	9.591703	16.78758
N	3.914587	14.31363	11.39507	C	4.008545	9.397472	17.83768
N	5.672772	17.58124	14.19045	F	2.207715	14.02222	21.78001

C	4.918835	14.42921	12.29379	H	2.870831	16.81081	12.47334
N	6.128438	11.42102	14.00919	H	3.377949	14.1674	9.407126
C	4.588593	16.90407	13.77757	H	6.821847	19.27683	13.97969
C	3.737293	17.38852	12.77509	H	3.108068	11.64692	12.49021
C	4.906347	11.88774	13.68773	H	5.704426	14.42794	8.538965
C	4.217208	14.30437	10.08156	H	3.379479	19.01784	11.40836
C	5.936357	18.75974	13.61584	H	7.023711	14.65538	12.64025
C	4.353774	15.58311	14.45677	H	5.411106	20.28441	12.18114
C	4.553283	14.38609	13.74618	H	7.581165	14.6793	10.19773
C	4.087903	11.25523	12.74463	H	3.93019	9.602739	11.37953
C	5.516578	14.43812	9.606971	H	7.548696	9.962008	13.68685
C	4.02509	18.61784	12.18516	H	6.217224	8.717071	11.98521
C	4.486244	13.14391	14.40597	H	1.938108	17.22804	15.42875
C	6.249077	14.56277	11.88787	H	4.467085	15.06679	20.88499
C	5.148825	19.32314	12.61111	H	1.533552	19.41984	16.57069
C	6.552768	14.57408	10.52945	H	2.458839	10.986	15.27323
C	4.553442	10.10183	12.11545	H	5.10416	18.66403	18.87659
C	6.558135	10.30963	13.39895	H	1.524216	13.28139	17.38391
C	5.8148	9.612735	12.44742	H	3.178425	20.17886	18.31796
N	4.195185	14.70077	18.86743	H	0.763156	13.15278	19.78177
N	4.60591	17.23976	17.48455	H	5.607131	10.32044	18.96076
C	3.400296	14.21887	17.89579	H	2.401098	8.819037	16.51299
N	4.932514	11.59577	17.49077	H	4.021953	8.473768	18.40708

7. Other Dynamic Processes



Complex	Motion	$\Delta G^{\ddagger}$ (kcal/mol)	reference
$[Pt(C_6F_4CF_3\text{-}p)_2(tpt)]$	1,4-shift	24.6 ± 0.1	11
$[Pt(C_6F_4CF_3\text{-}p)_2(tpt)]$	hurdling	22.1	11
$[Pd(C_6F_4CF_3\text{-}p)_2(tpt)]$	1,4-shift	17.2 ± 0.1	11
$[Pd(C_6F_4CF_3\text{-}p)_2(tpt)]$	hurdling	17.6	11
$[Pt(C_6F_4CF_3\text{-}p)_2(tpp)]$	1,4-shift	28.2	11
$[Pt(C_6F_4CF_3\text{-}p)_2(tpp)]$	hurdling	27	11
$[Pd(C_6F_4CF_3\text{-}p)_2(tpp)]$	1,4-shift	16.5	11
3	ring-walking	15.2 ± 0.5	12
4	ring-walking	15.9 ± 0.4	12
$[Cu_2(\mathbf{2\text{-}HPB})(MeCN)_2Cl_2]$	hopping	13.4 ± 0.1	This work
$[Cu_2(\mathbf{MFHPB})(MeCN)_2Cl_2]$	hopping	12.8	This work

Table S3. Type of motions and $\Delta G^{\ddagger}$ values for other fluxional coordination systems.

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