Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information for:

Macrocyclic Complexes Based on $[N\cdots I\cdots N]^+$ Halogen Bond

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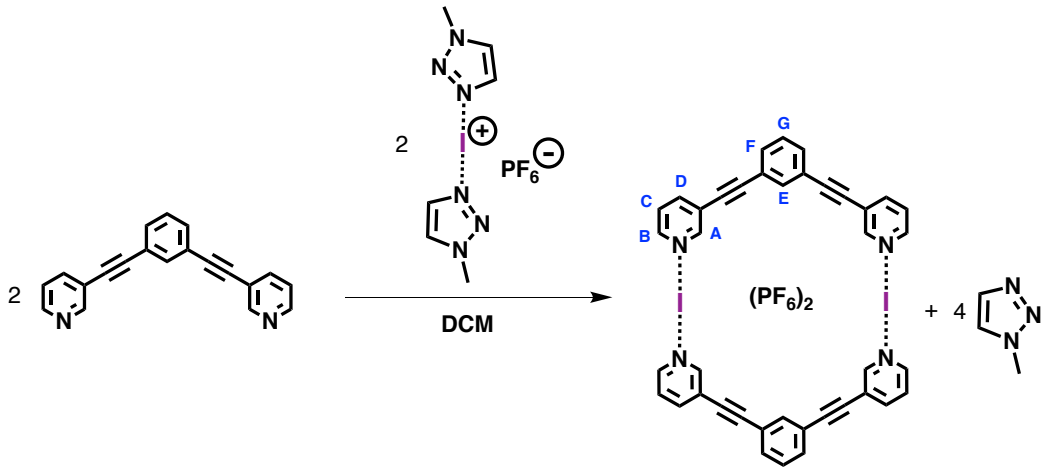
1. General Experimental Section

All reagents and solvents were purchased from commercial suppliers and used without further purification. Ligands **L1-L3** and iodonium complex *bis*(1-methyl-1H-1,2,3-triazole)iodine(I) hexafluorophosphate ([I(*mtz*)$_2$]PF_6) were prepared according to literature procedures.[1–4] ^{1}H and ^{13}C NMR spectra, and the ^{1}H-^{15}N NMR correlation were recorded at 298 K on a Bruker Avance III 500 MHz instrument in CD_2Cl_2. Signals in the ^{1}H-NMR spectra of the complexes were assigned with the aid of two-dimensional NMR experiments (COSY HMQC and ^{1}H-^{15}N HMBC). Chemical shifts are reported on the δ scale in ppm using the residual solvent signal as internal standard, or for ^{1}H-^{15}N NMR spectroscopy, to an external d_3-$MeNO_2$ standard. Abbreviations of coupling patterns are as follows: br, broad; s, singlet; d, doublet; t, triplet; m, multiplet. Coupling constants (*J*) are expressed in Hz.

2. Synthetic and Spectroscopic Data

Synthesis of complex **1**



To a solution of [I(*mtz*)$_2$]PF$_6$ (21.4 mg, 0.049 mmol, 1.0 eq.) in dichloromethane (2 mL), a solution of **L1** (13.7 mg, 0.049mmol, 1 eq.) in dichloromethane (1 mL) was added. The reaction mixture was stirred for 5 mins and a white solid was precipitated from the colorless solution, which was filtered and washed with Et$_2$O. The product was dried under reduced pressure to obtain complex **1** (21.4 mg, 79.0%). **^{1}H NMR** (500 MHz, CD$_3$CN): δ 8.81 (s, 4H, H_A), 8.51 (d, J = 5.5 Hz, 4H, H_B), 8.15 (d, J = 8.4 Hz, 4H, H_D), 7.73 (s, 2H, H_E), 7.58-7.47 (m, 8H, H_C and H_F), 7.43 (t, J = 7.6 Hz, 2H, H_G); **^{13}C NMR** (125 MHz, CD$_3$CN): δ 150.8, 148.3, 143.6, 134.3, 132.9, 129.3, 127.3, 123.3, 121.6, 94.1, 53.4; **^{1}H-^{15}N HMBC NMR** (500 MHz, CD$_3$CN): δ -173.3; **^{1}H 2D DOSY NMR** (500 MHz, CD$_3$CN) of complex **1**: Recorded diffusion coefficient for assigned peaks 1.33e^{-9} m^{2}s^{-1}, Calculated hydrodynamic radius 4.9 Å; HRMS (ESI+) calcd for $C_{40}H_{24}F_6I_2N_4P$ $[M - PF_6]^+$ 958.9732, found 958.9719.

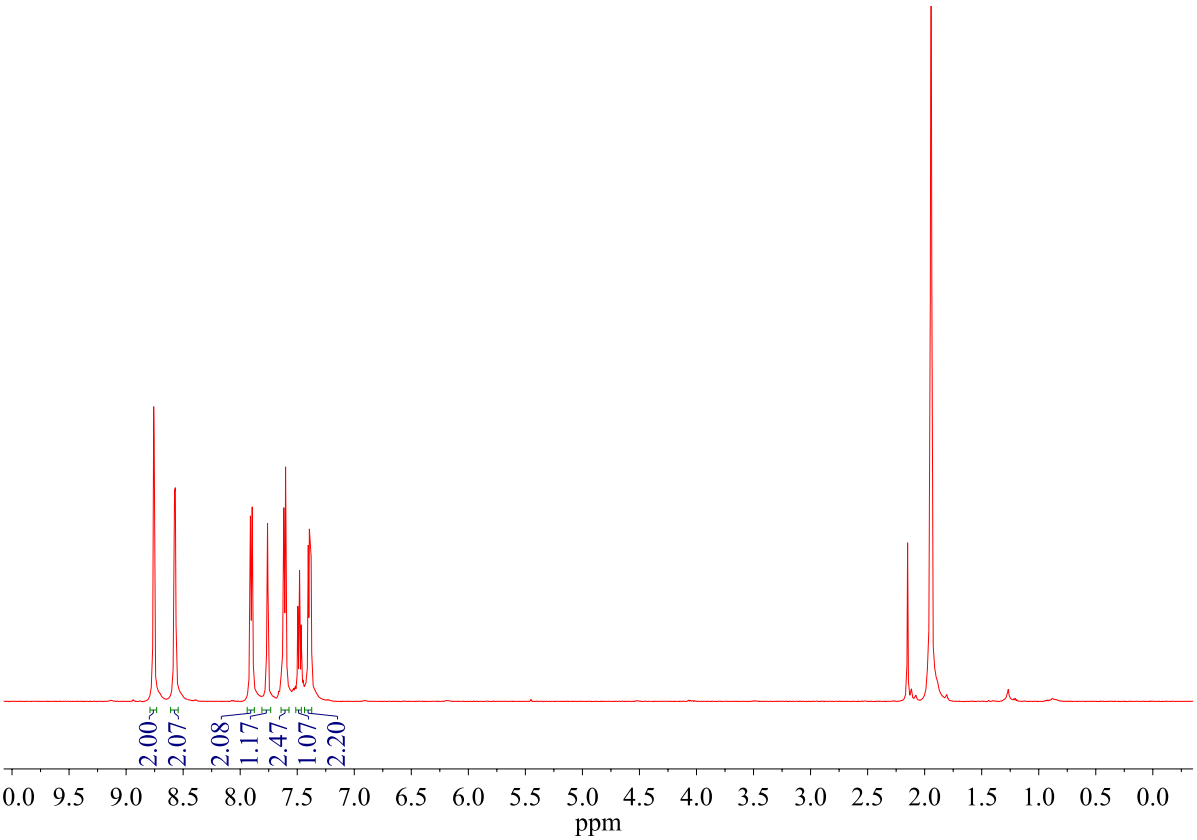


Figure S1. The ^{1}H NMR spectrum of **L1** (CD_3CN, 500 MHz, 25 °C).

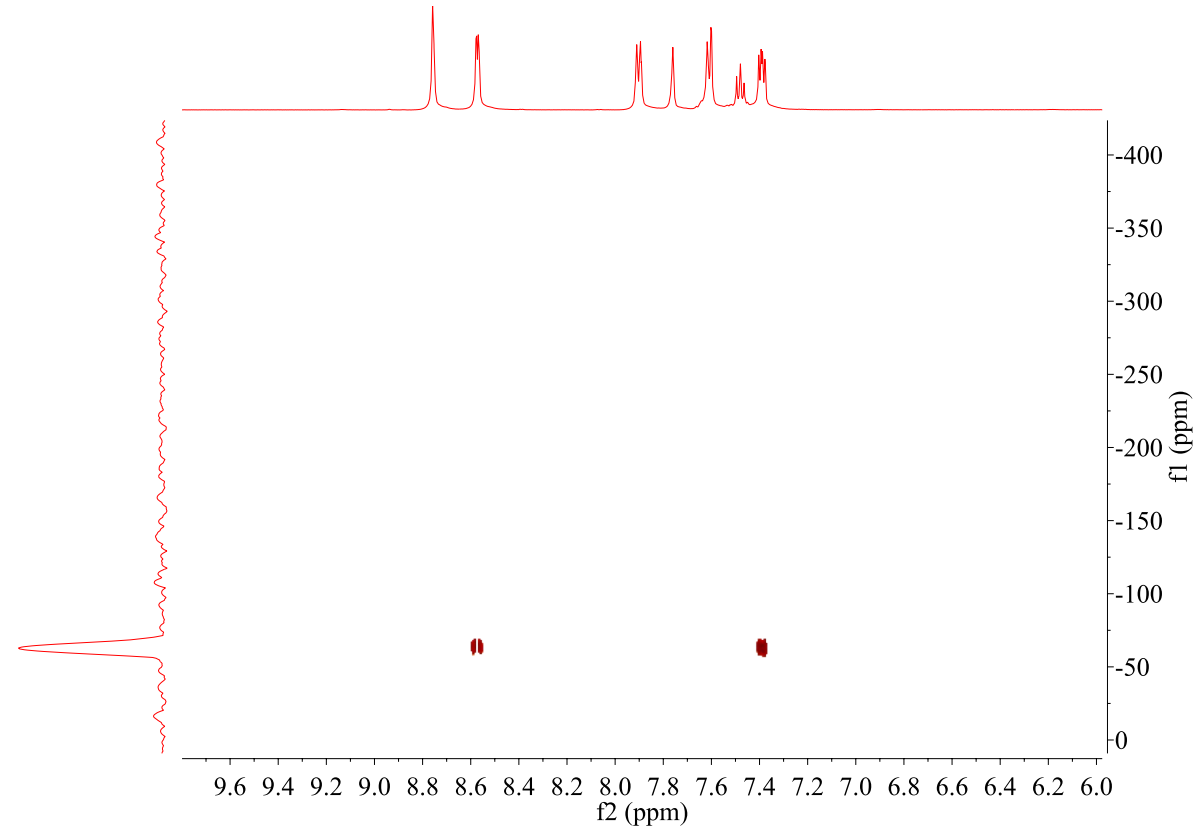


Figure S2. The ^{1}H-^{15}N-HMBC spectrum of **L1** (CD_3CN, 500 MHz, 25 °C).

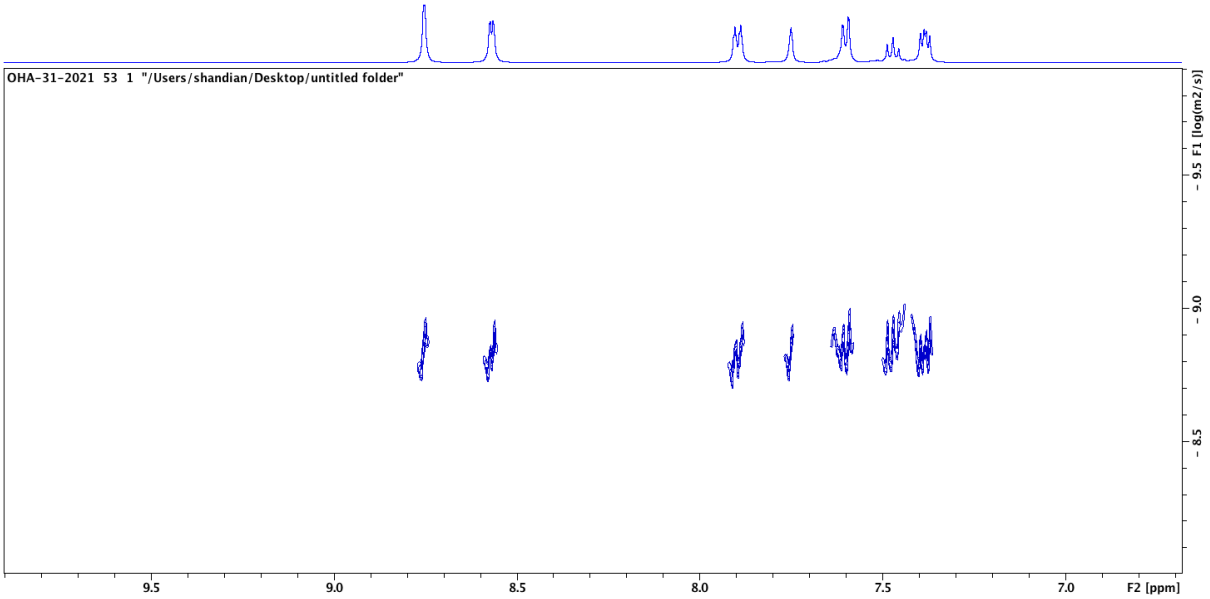


Figure S3. The ^{1}H DOSY spectrum of **L1** (CD_3CN, 500 MHz, 25 °C).

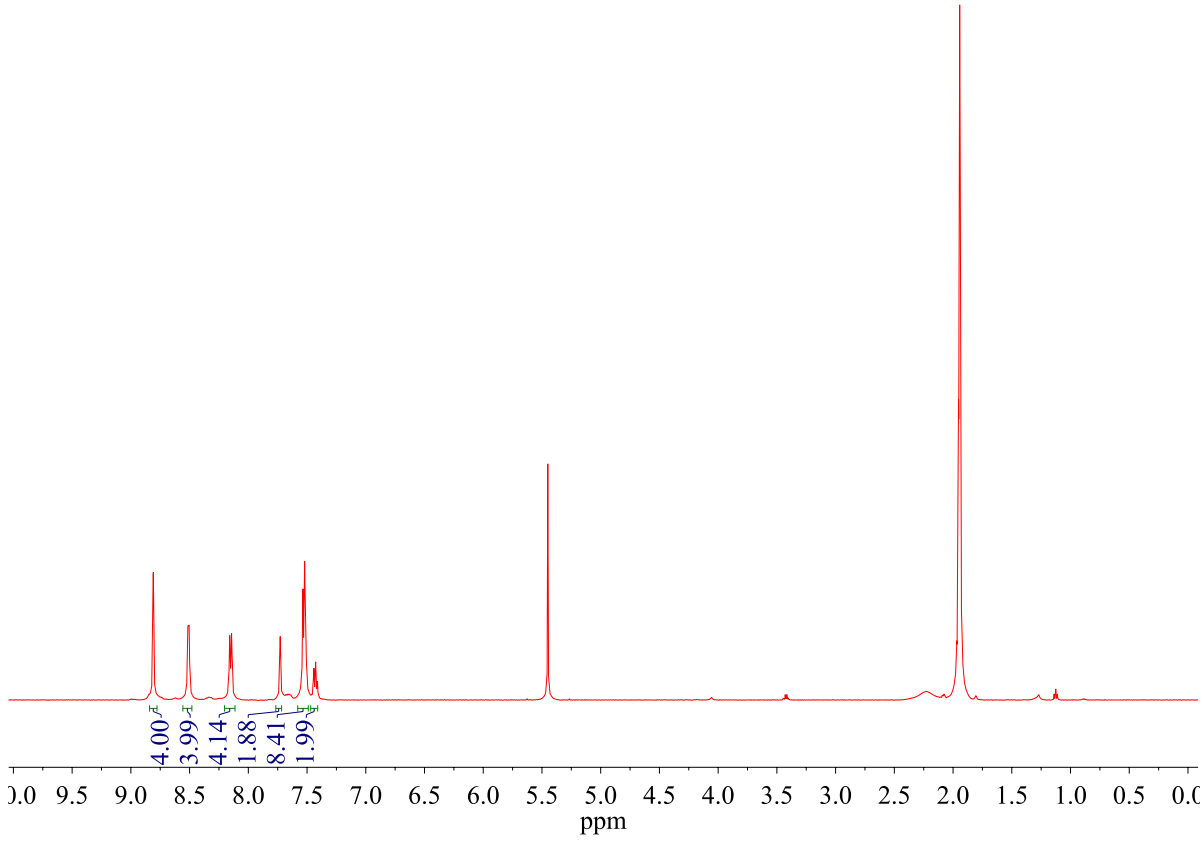


Figure S4. The ^{1}H NMR spectrum of complex **1** (CD_3CN, 500 MHz, 25 °C).

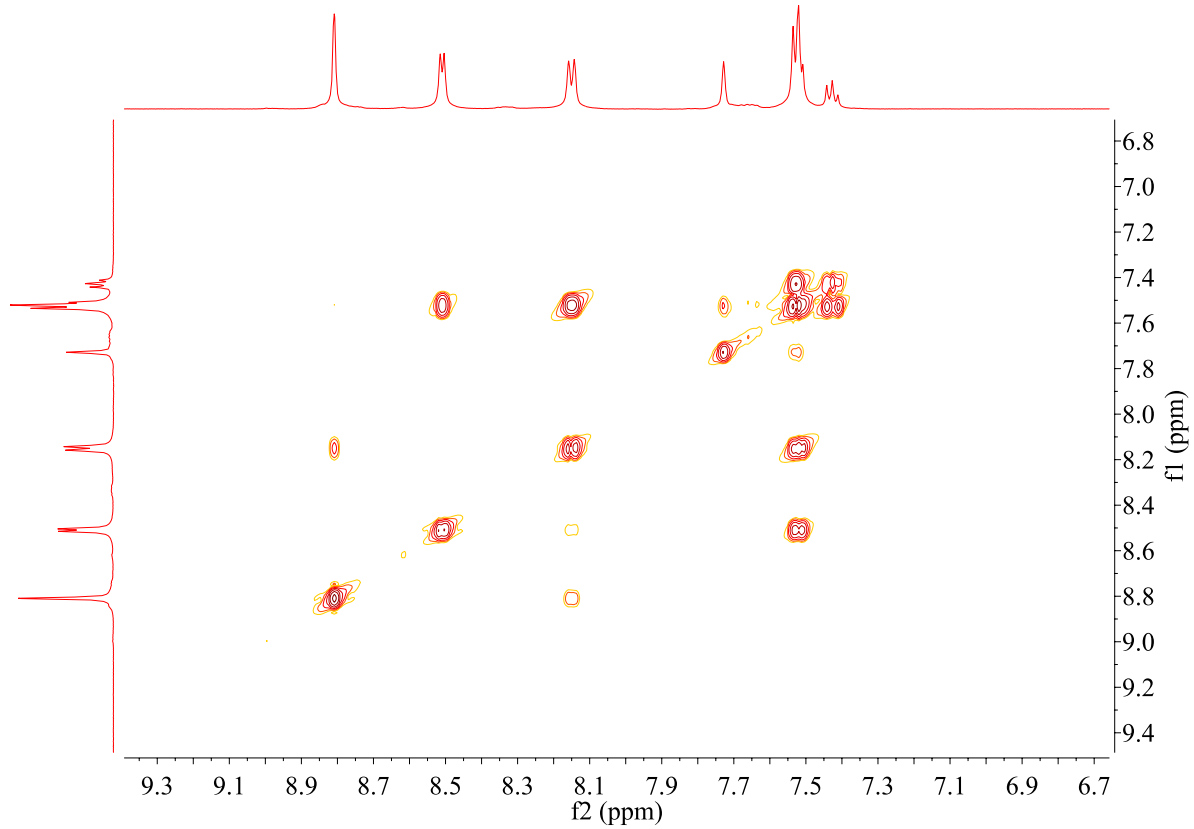


Figure S5. The H-H COSY NMR spectrum of complex **1** (CD_3CN, 500 MHz, 25 °C).

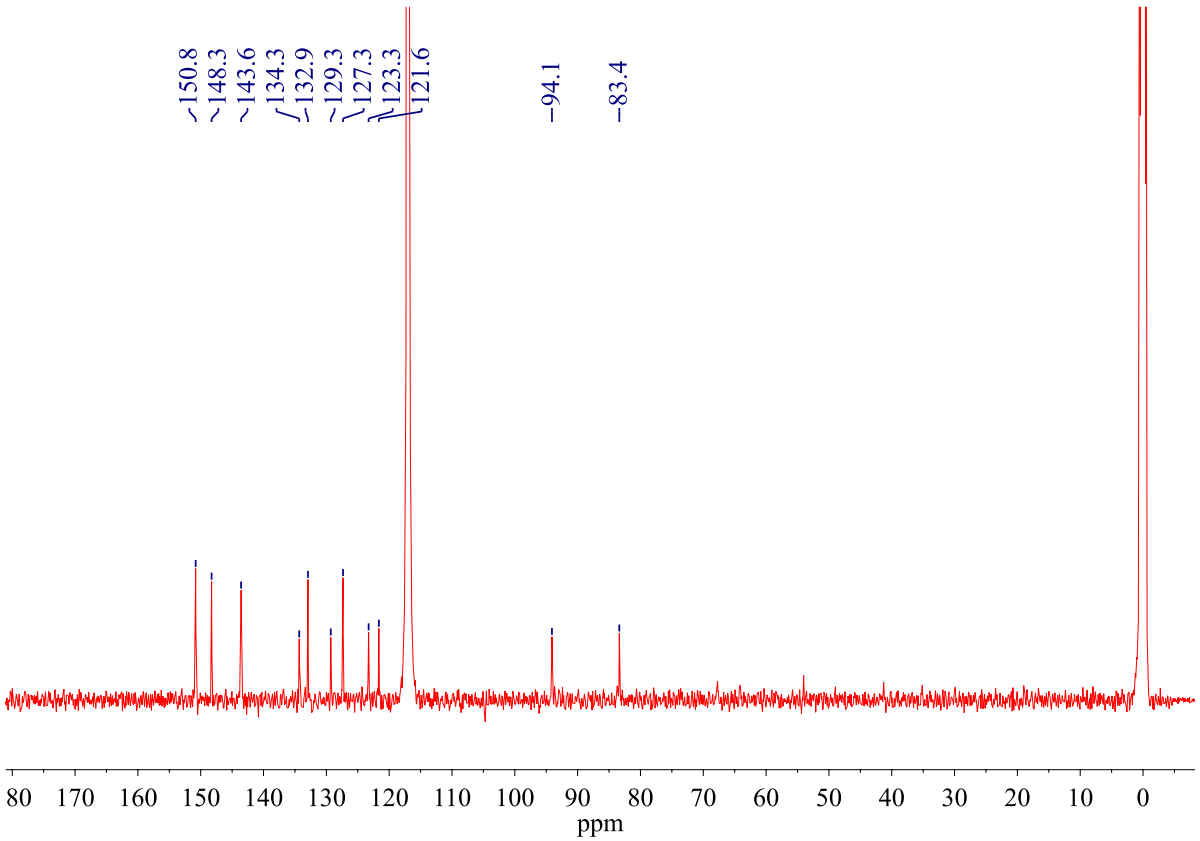


Figure S6. The ^{13}C NMR spectrum of complex **1** (CD_3CN, 125 MHz, 25 °C).

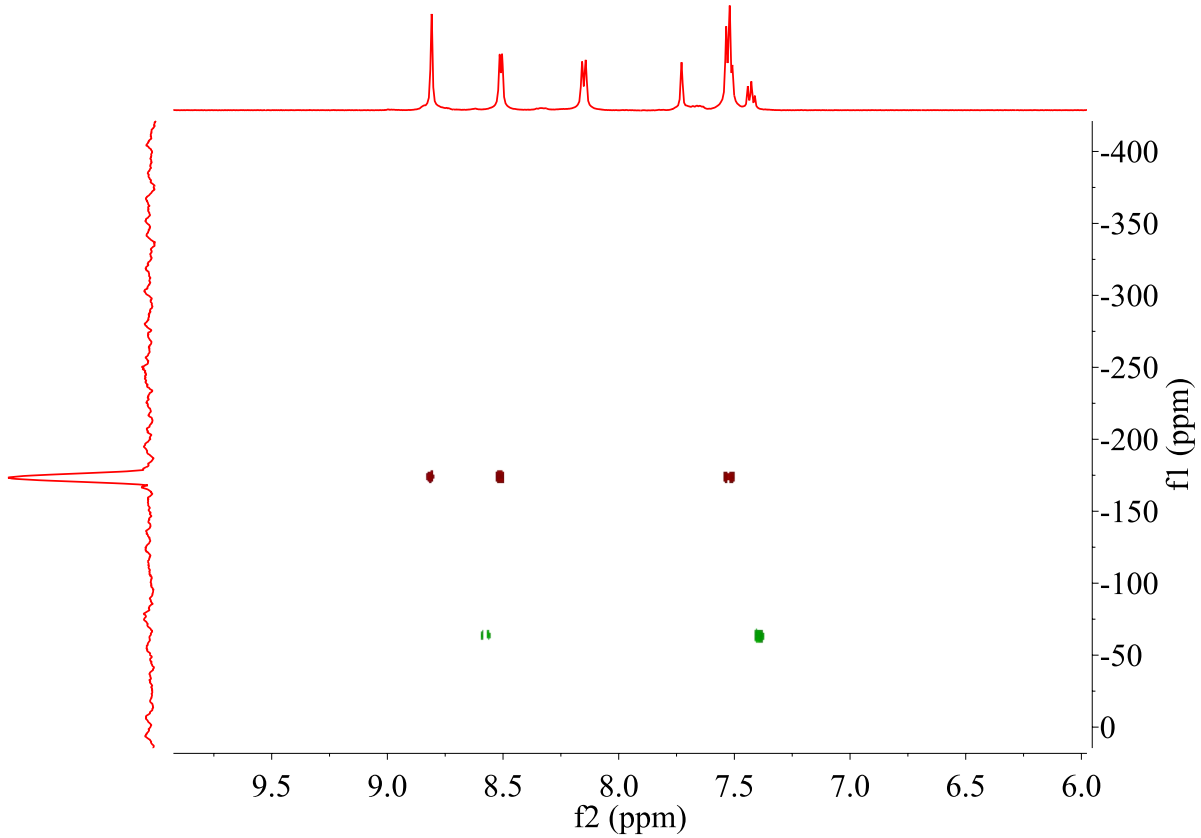


Figure S7. The stacked ^{1}H-^{15}N-HMBC spectra of complex **1** (red) and ligand **L1** (green) (CD_3CN, 500 MHz, 25 °C).

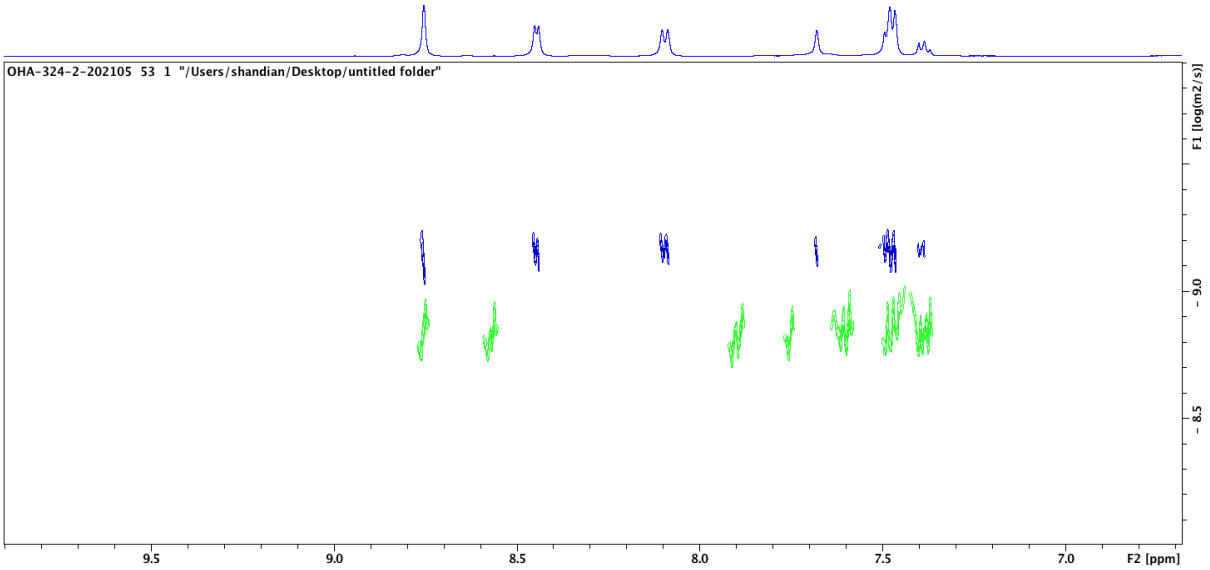
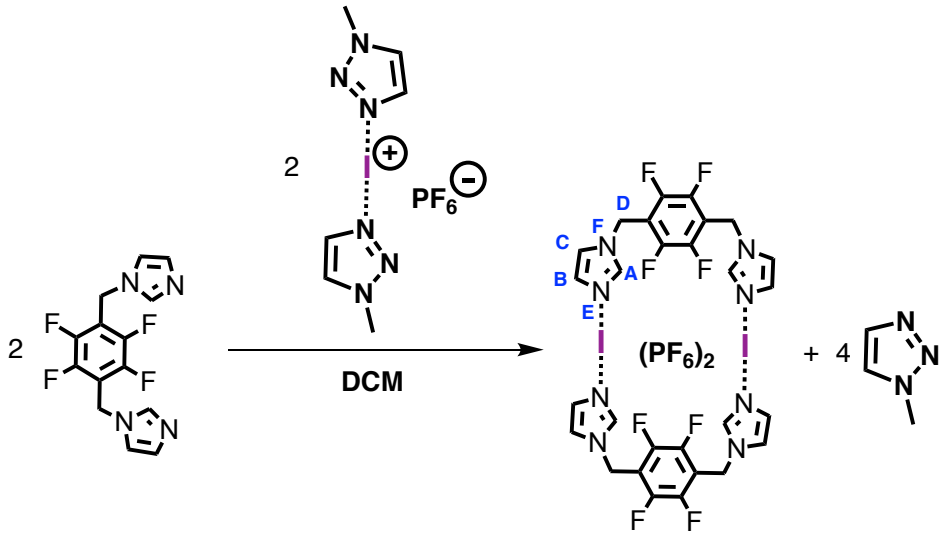


Figure S8. The stacked ^{1}H DOSY spectra of complex **1** (blue) and ligand **L1** (green) (CD_3CN, 500 MHz, 25 °C).

Synthesis of complex **2**



To a solution of [I(*mtz*)$_2$]PF$_6$ (22.4 mg, 0.051 mmol, 1.0 eq.) in dichloromethane (2 mL), a solution of **L2** (15.9 mg, 0.051 mmol, 1 eq.) in dichloromethane (1 mL) was added. The reaction mixture was stirred for 5 mins and a white solid was precipitated from the colorless solution, which was filtered and washed with Et$_2$O. The product was dried under reduced pressure to obtain complex **2** (25.9 mg, 87%). **^{1}H NMR** (500 MHz, CD$_3$CN): δ 7.87 (s, 4H, H_A), 7.31 (s, 4H, H_B or H_C), 7.19 (s, 4H, H_C or H_B), 5.39 (s, 4H, H_D); **^{13}C NMR** (125 MHz, CD$_3$CN): δ 144.8 (CF), 138.2, 127.4, 122.8, 114.5, 39.2; **^{1}H-^{15}N HMBC NMR** (500 MHz, CD$_3$CN): δ -216.1 (N_E), -204.5 (N_F); **^{1}H 2D DOSY NMR** (500 MHz, CD$_3$CN) of complex **2**: Recorded diffusion coefficient for assigned peaks 1.33e^{-9} m^{2}s^{-1}, Calculated hydrodynamic radius 4.9 Å; HRMS (ESI+) calcd for C$_{28}$H$_{20}$F$_{14}$I$_2$N$_8$P [M – PF$_6$]$^+$ 1018.9403, found 1018.9424.

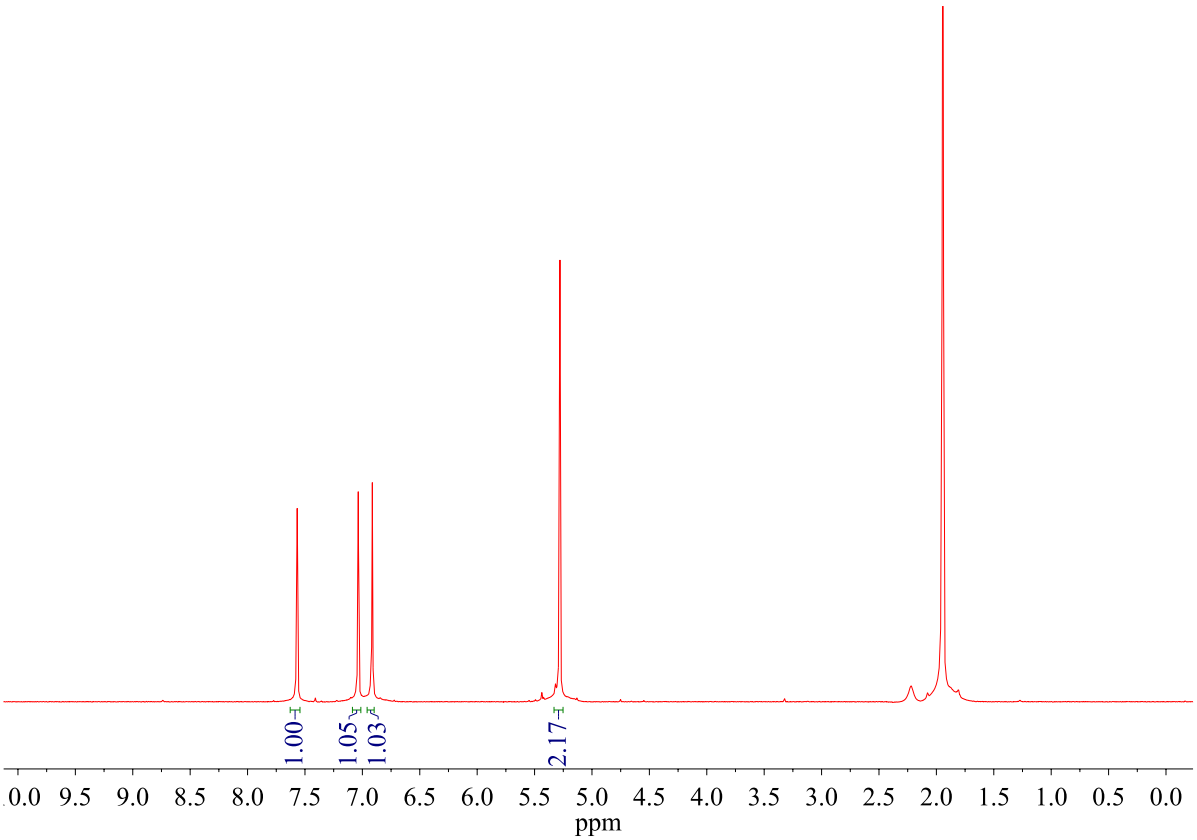


Figure S9. The ^{1}H NMR spectrum of **L2** (CD_3CN, 500 MHz, 25 °C).

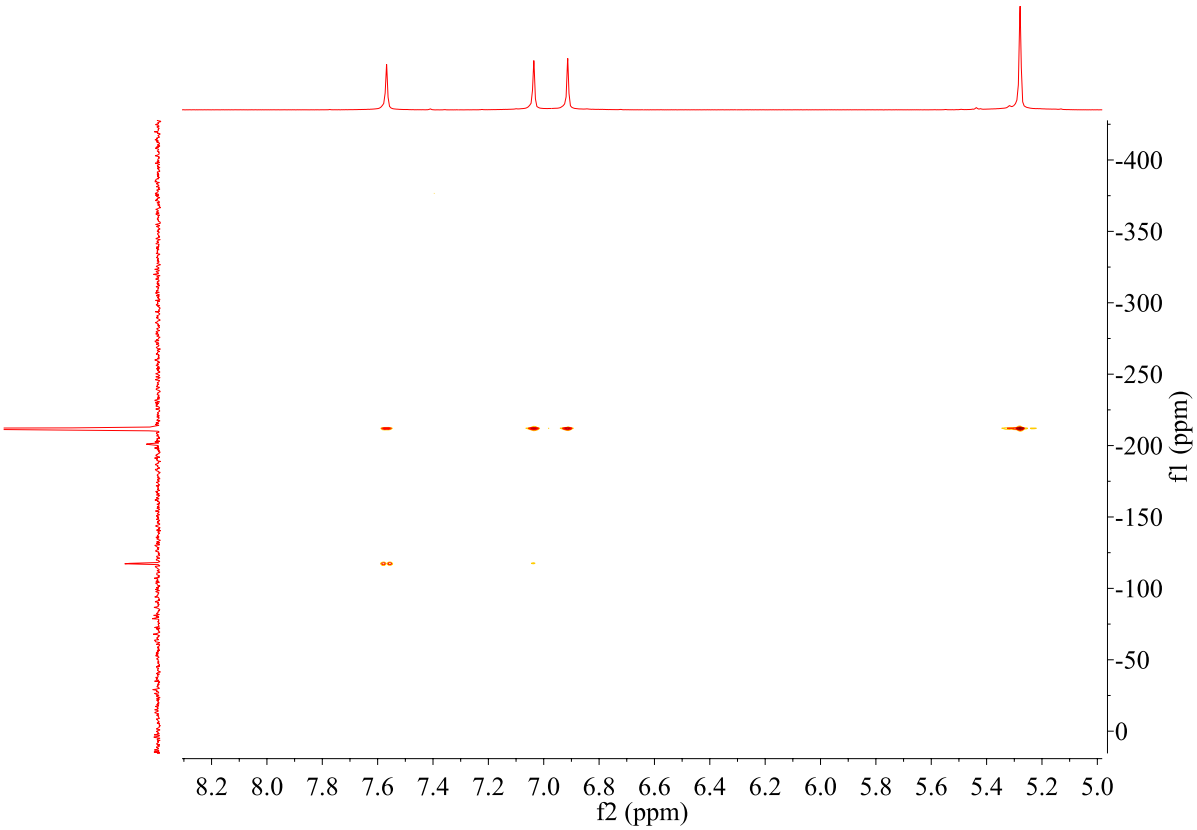


Figure S10. The ^{1}H-^{15}N-HMBC spectrum of **L2** (CD_3CN, 500 MHz, 25 °C).

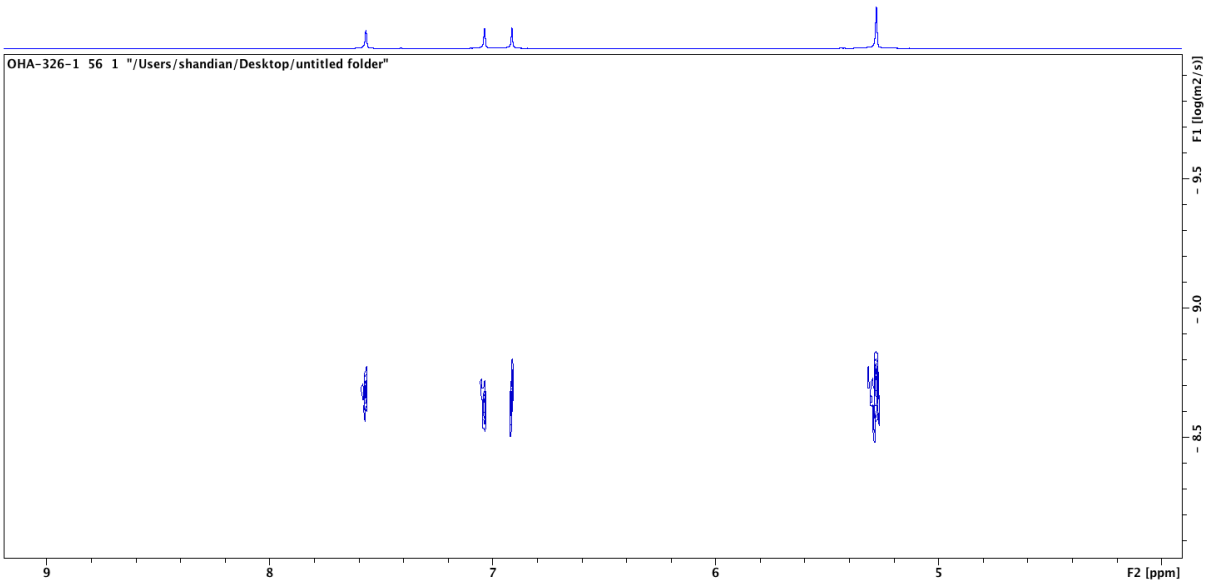


Figure S11. The ^{1}H DOSY spectrum of **L2** (CD_3CN, 500 MHz, 25 °C).

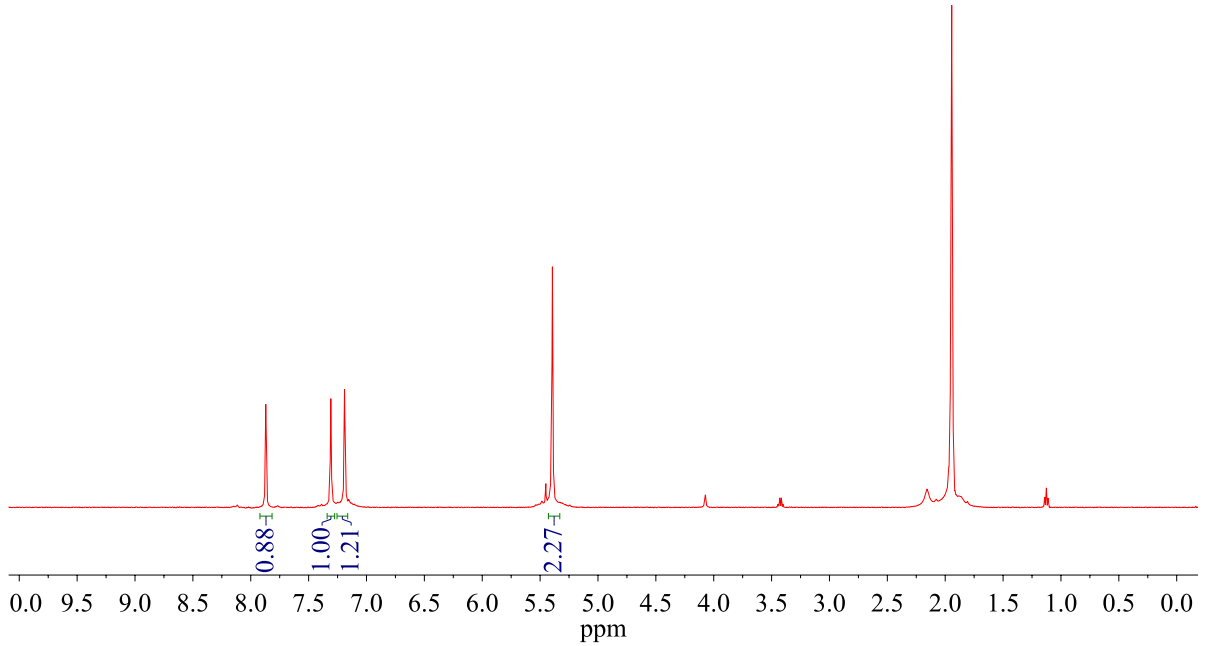


Figure S12. The ^{1}H NMR spectrum of complex **2** (CD_3CN, 500 MHz, 25 °C).

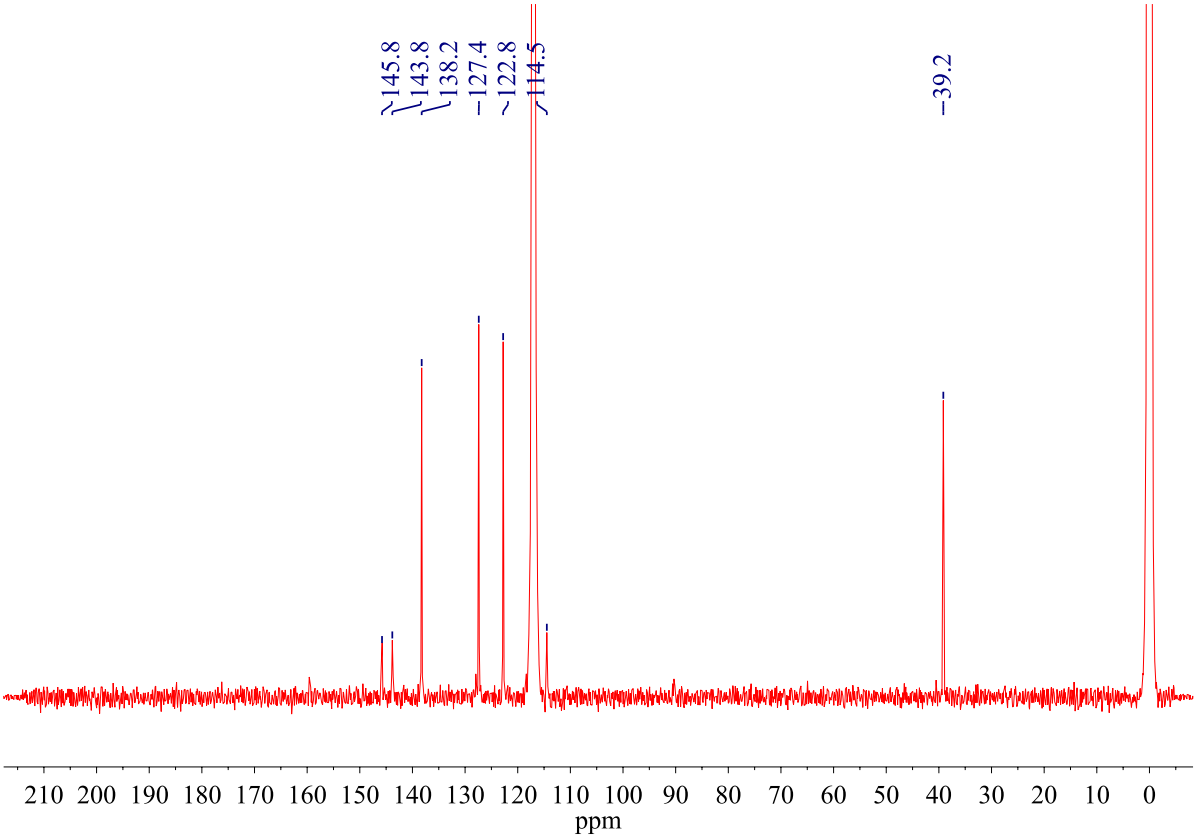


Figure S13. The ^{13}C NMR spectrum of complex **2** (CD_3CN, 125 MHz, 25 °C).

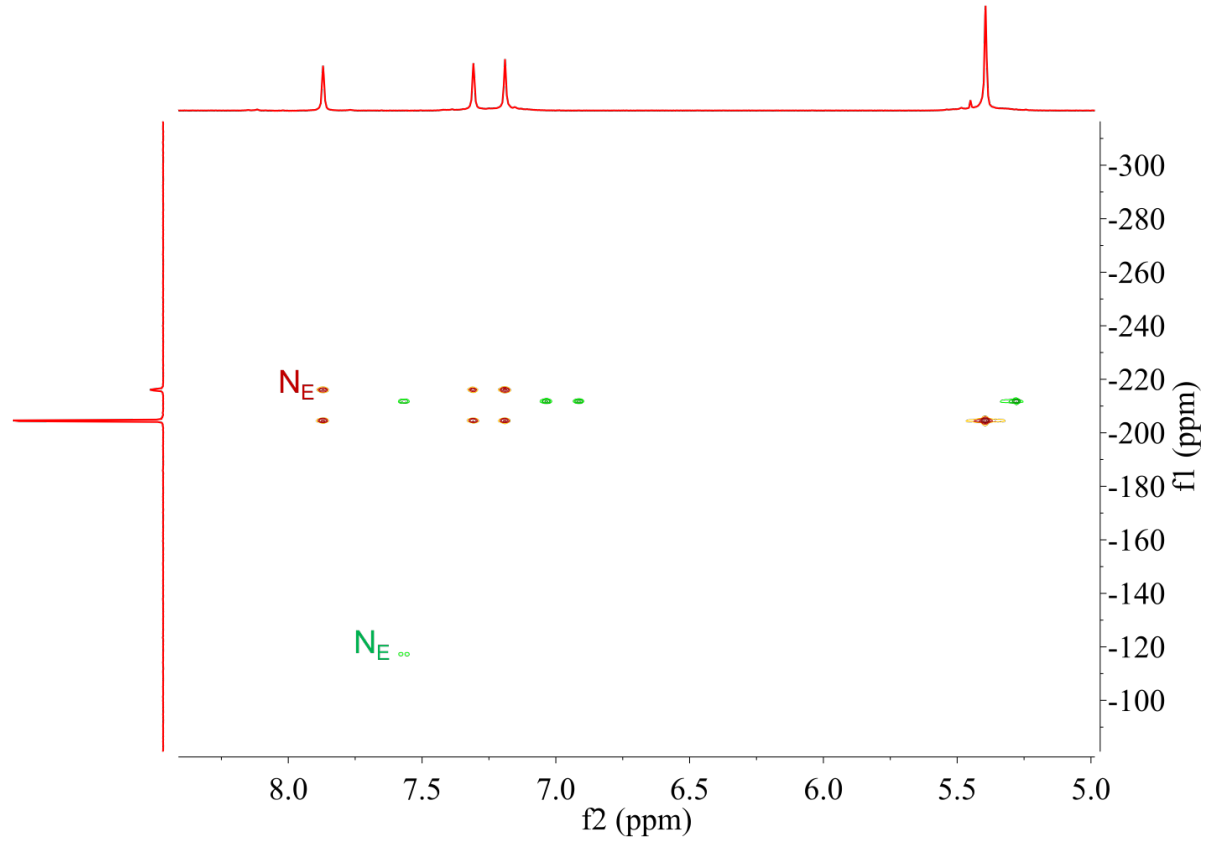


Figure S14. The stacked ^{1}H-^{15}N-HMBC spectra of complex **2** and ligand **L2** (CD_3CN, 500 MHz, 25 °C).

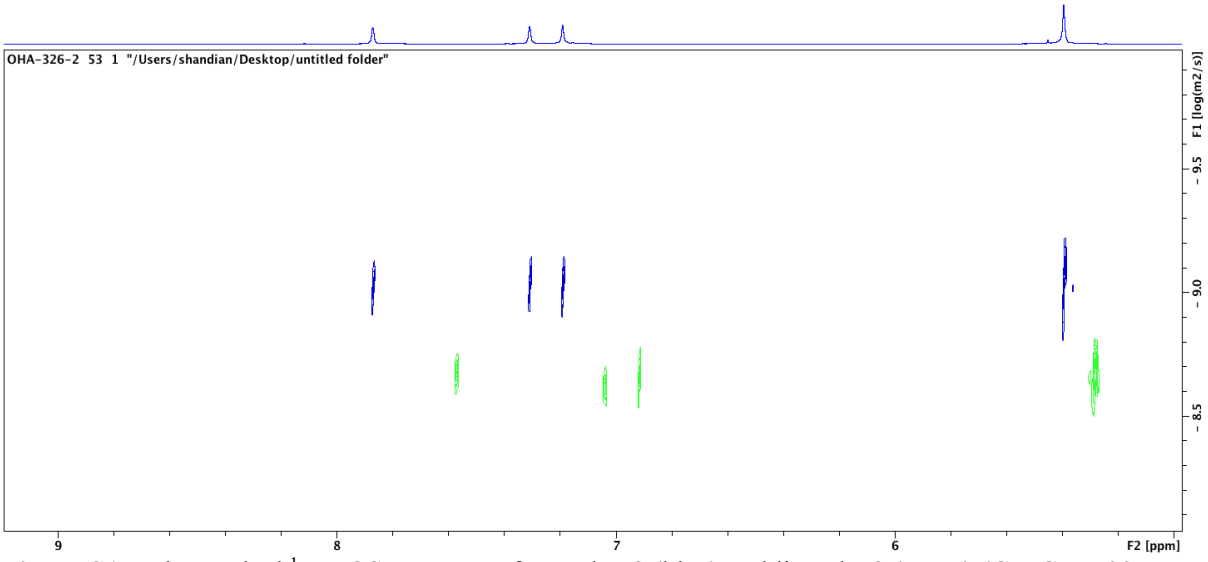


Figure S15. The stacked ^{1}H DOSY spectra of complex **2** (blue) and ligand **L2** (green) (CD_3CN, 500 MHz, 25 °C).

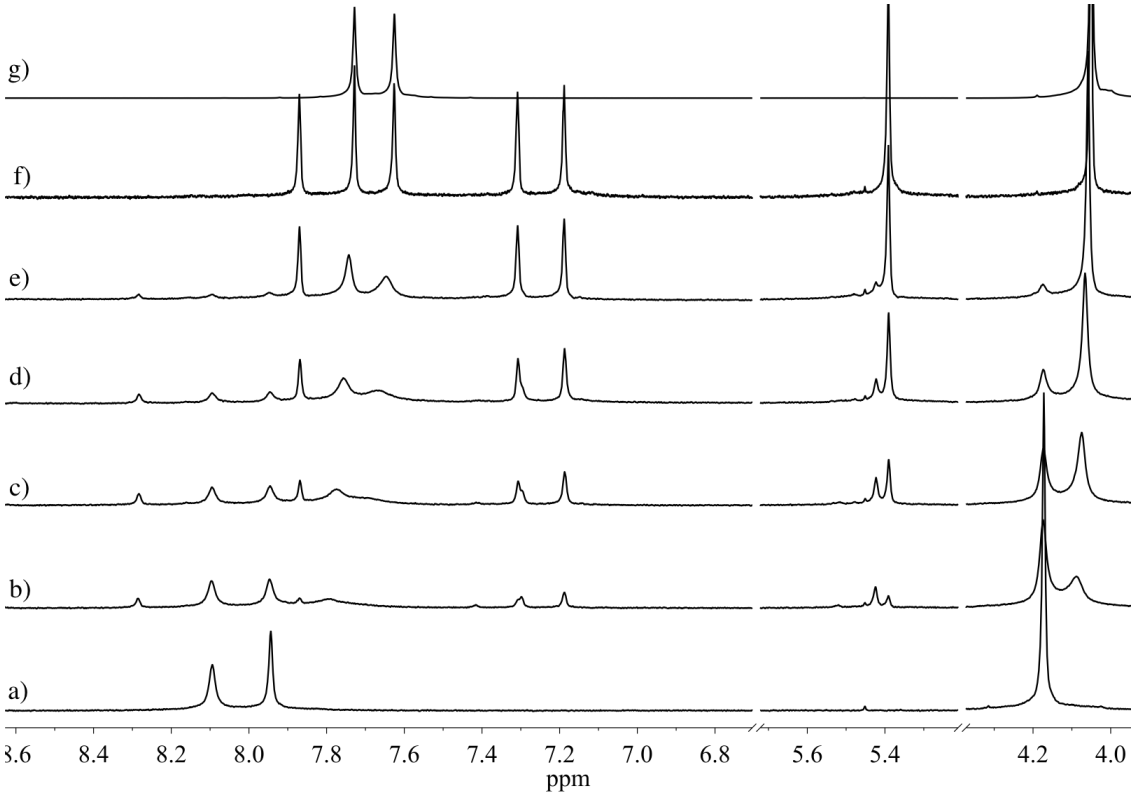
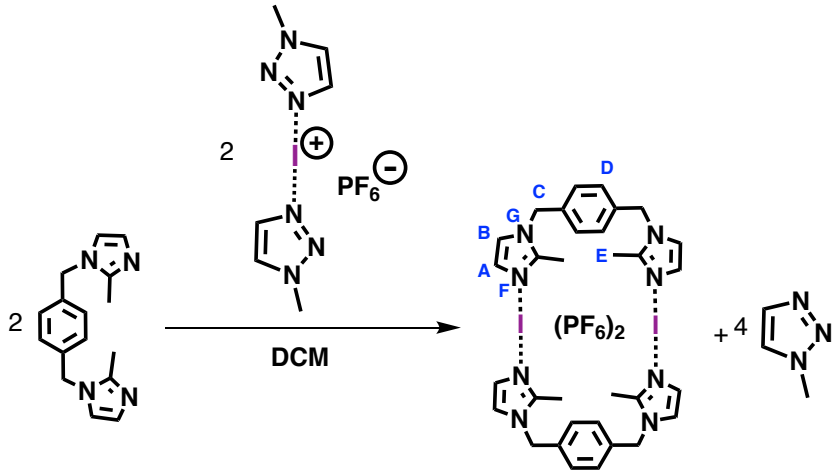


Figure S16. Selected ^{1}H NMR spectra (500 MHz, CD_3CN, 25 °C) of pure [I(*mtz*)$_2$]PF_6 (a) and [I(*mtz*)$_2$]PF_6 in the presence of 0.2 (b), 0.4 (c), 0.6 (d), 0.8 (e) and 1.0 (f) equivalents of **L2** and 1-methyl-1H-1,2,3-triazole (g), showing the self-assembly of macrocycle **2** from the ligand exchange between **L2** and iodine(I) complex [I(*mtz*)$_2$]PF_6.

Synthesis of complex **3**



To a solution of [I(*mtz*)$_2$]PF$_6$ (12.7 mg, 0.029 mmol, 1.0 eq.) in dichloromethane (2 mL), a solution of **L3** (7.7 mg, 0.029 mmol, 1 eq.) in dichloromethane (1 mL) was added. The reaction mixture was stirred for 5 mins and a white solid was precipitated from the colorless solution, which was filtered and washed with Et_2O.

^{1}H 2D DOSY NMR (500 MHz, CD_3CN) of reaction **3**: Recorded diffusion coefficient for assigned peaks 1.78e^{-9} and 1.93e^{-9} m^{2}s^{-1}, Calculated hydrodynamic radius 3.7 and 3.4 Å;

HRMS (ESI+) calcd for $C_{32}H_{36}F_6I_2N_8P$ $[M - PF_6]^+$ 931.0794, found 931.0797.

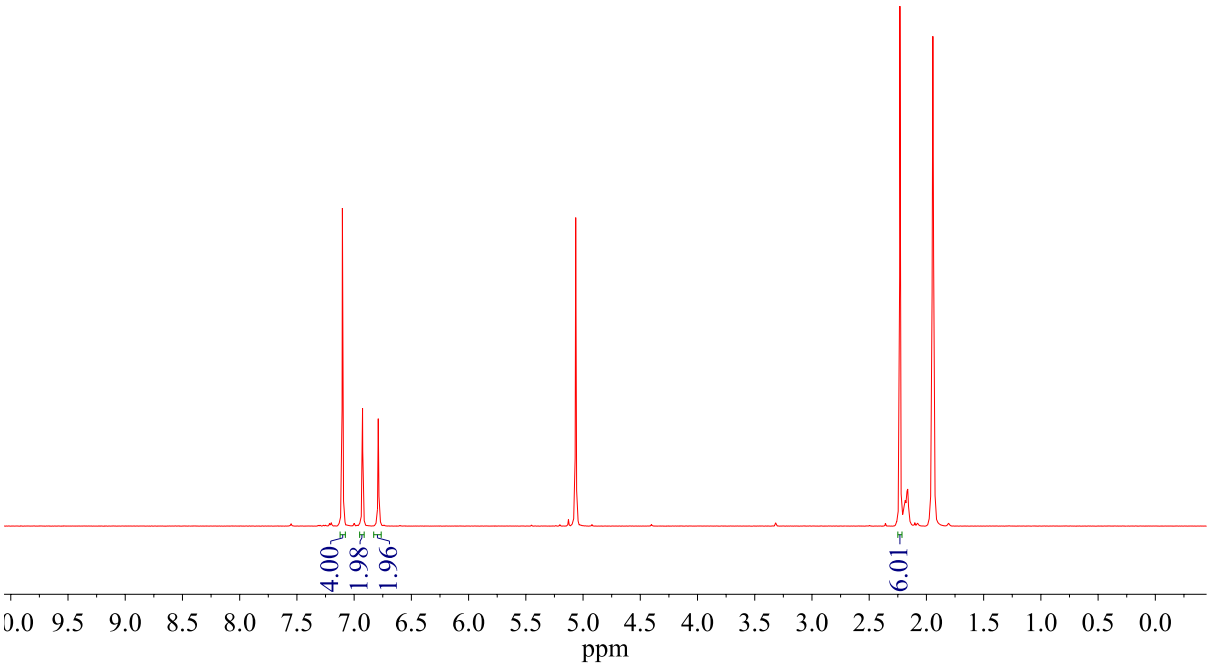


Figure S17. The ^{1}H NMR spectrum of **L3** (CD_3CN, 500 MHz, 25 °C).

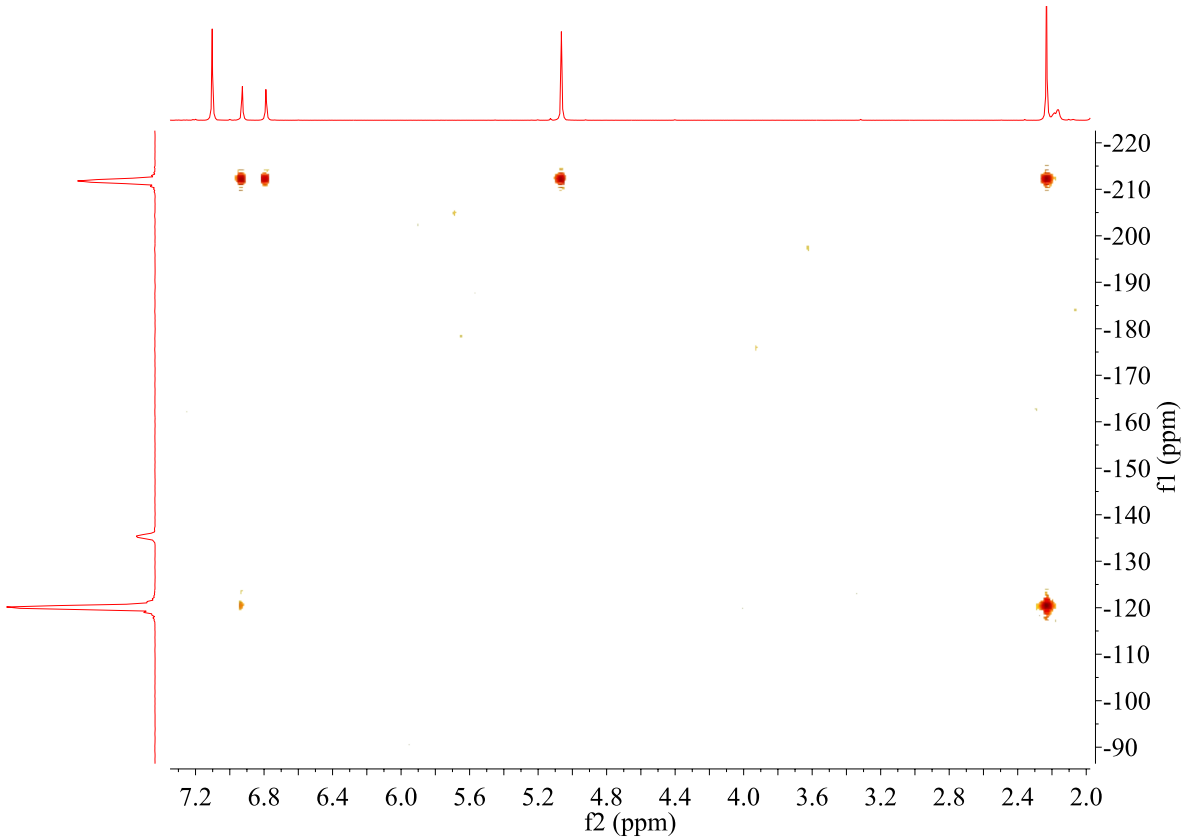


Figure S18. The ^{1}H-^{15}N-HMBC spectrum of **L3** (CD_3CN, 500 MHz, 25 °C).

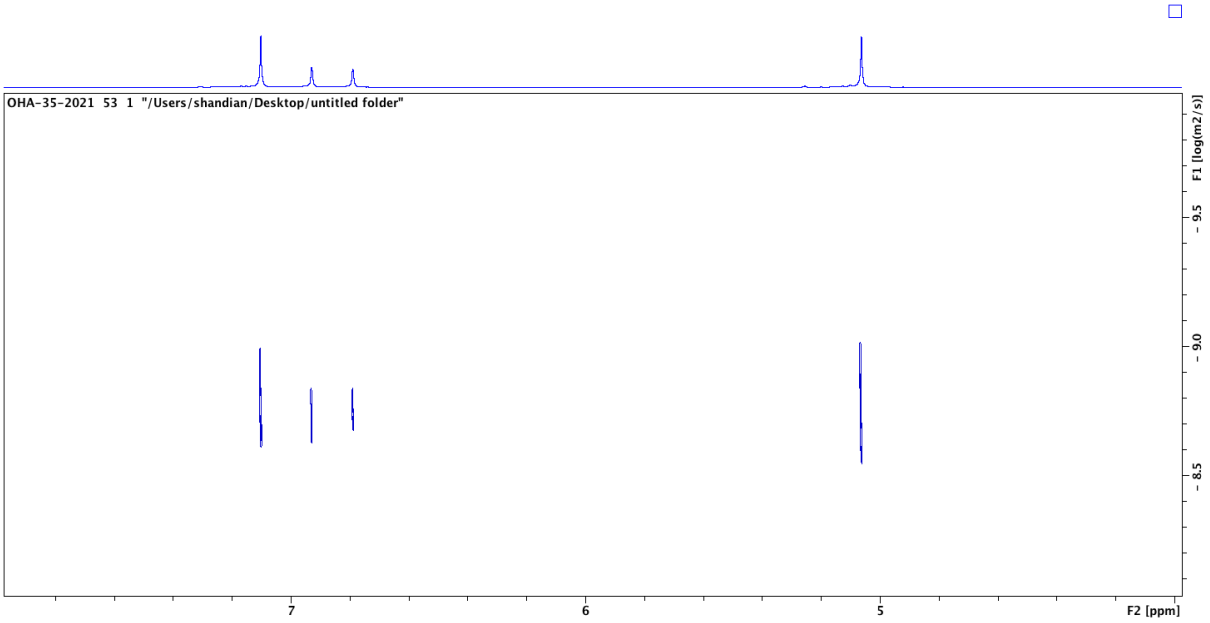


Figure S19. The ^{1}H DOSY spectrum of **L3** (CD_3CN, 500 MHz, 25 °C).

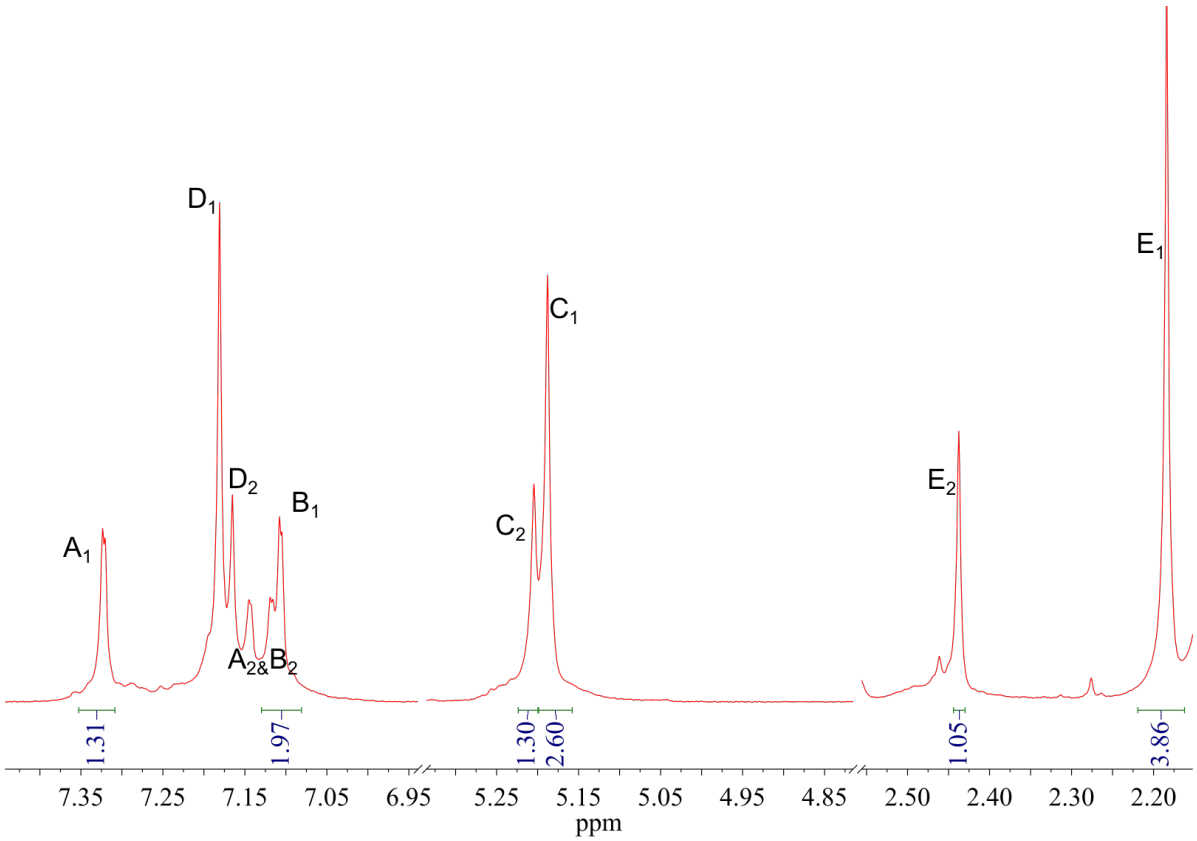


Figure S20. The ^{1}H NMR spectrum of reaction **3** (CD_3CN, 500 MHz, 25 °C).

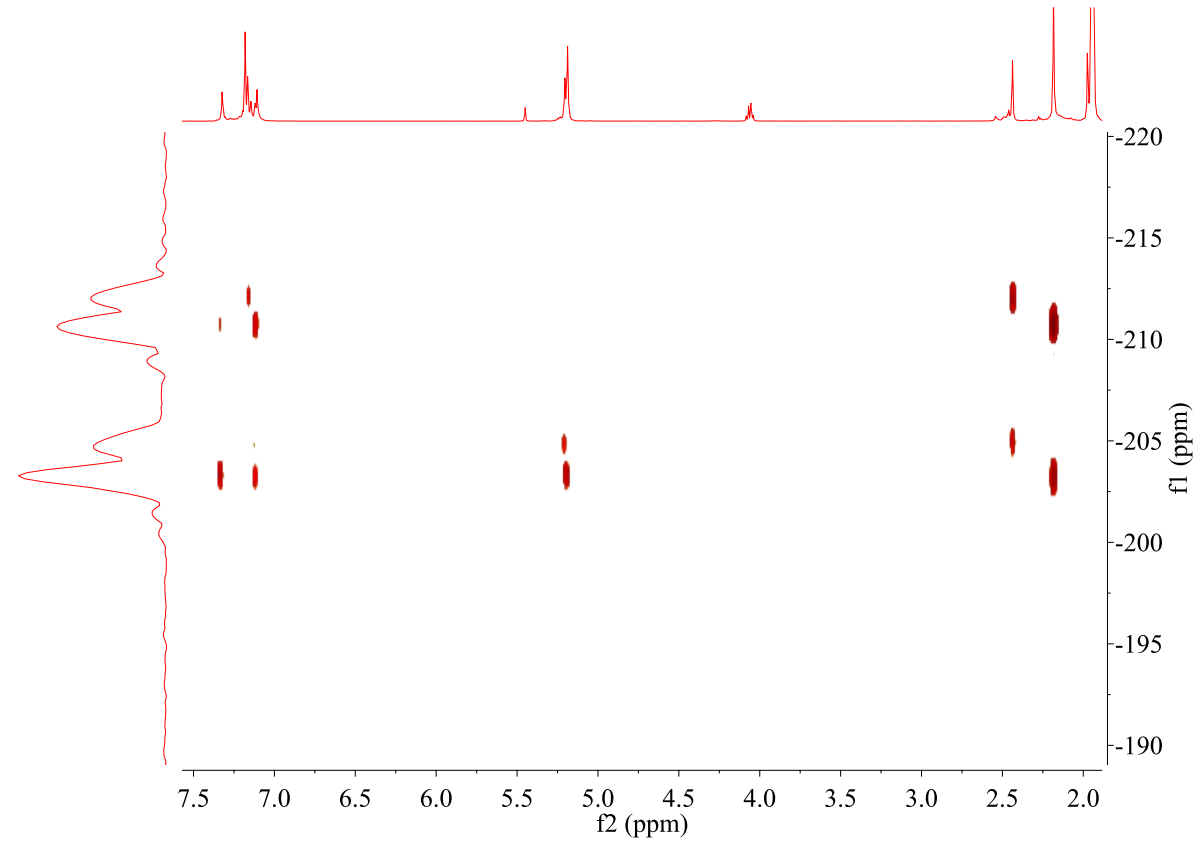


Figure S21. The ^{1}H-^{15}N-HMBC spectrum of reaction **3** (CD_3CN, 500 MHz, 25 °C).

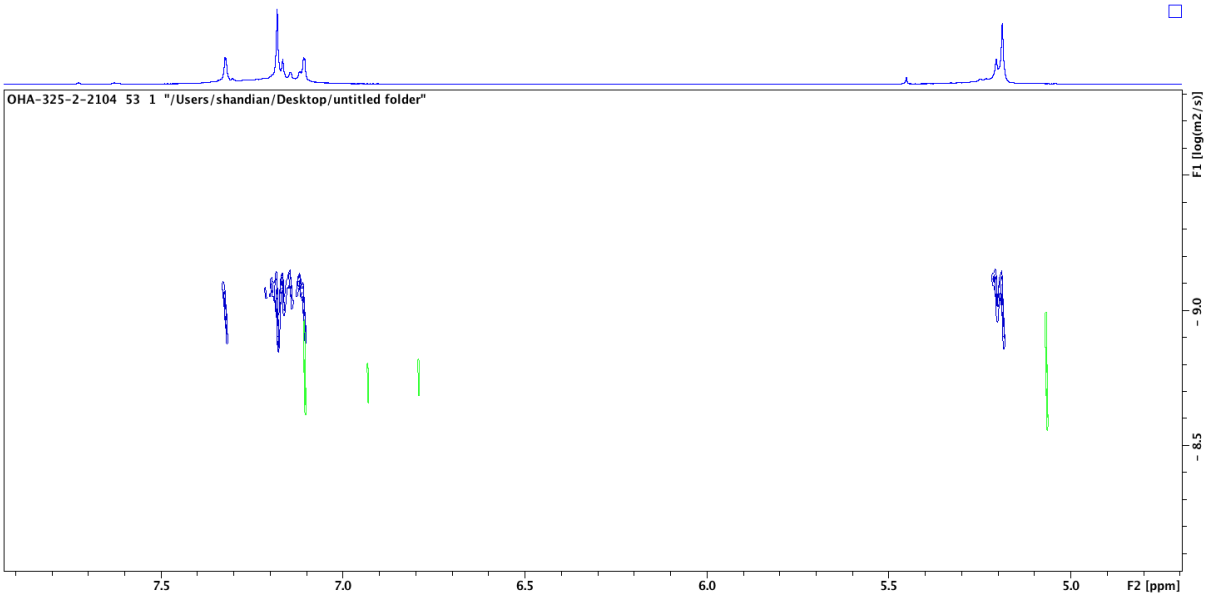
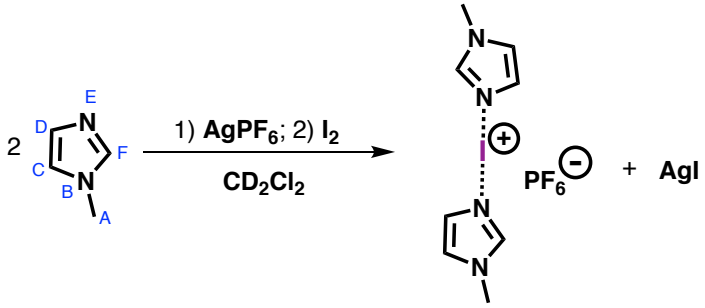


Figure S22. The stacked ^{1}H 2D DOSY spectra of reaction **3** (blue) and ligand **L3** (green) (CD_3CN, 500 MHz, 25 °C).

Synthesis of [I(1-methylimidazole)$_2$]PF$_6$



To a solution of silver hexafluorophosphate (5.7 mg, 0.023 mmol, 1.0 eq) in CD_2Cl_2 (1.0 mL), a solution of 1-methylimidazole (3.7 mg, 0.045 mmol, 2.0 eq) in CD_2Cl_2 (0.8 mL) was added. After the solution was stirred for 3 mins at room temperature, the elementary I_2 (5.7 mg, 0.023 mmol, 1.0 eq) in CD_2Cl_2 (0.2 mL) was added. The mixture was centrifuged for 5 mins and was filtered, then the solution of [I(1-methylimidazole)$_2$]PF$_6$ (96%, determined by ^{1}H NMR integration of the crude reaction mixture) was stored in an 4 mL vial in fridge. **^{1}H NMR** (500 MHz, CD_2Cl_2): δ 7.87 (s, 2H, H_F), 7.15 (s, 2H, H_D), 6.97 (s, 2H, H_C), 3.83 (s, 6H, H_A); **^{13}C NMR** (125 MHz, CD_2Cl_2): δ 138.6, 128.2, 122.7, 35.0; **^{1}H-^{15}N HMBC NMR** (500 MHz, CD_3CN): δ -217.0 (N_E), -212.5 (N_B). **NMR characterization for 1-methylimidazole**: **^{1}H NMR** (500 MHz, CD_2Cl_2): δ 7.40 (s, 1H, H_F), 6.98 (s, 1H, H_C), 6.91 (s, 1H, H_D), 3.68 (s, 3H, H_A); **^{1}H-^{15}N HMBC NMR** (500 MHz, CD_3CN): δ -221.3 (N_B), -122.7 (N_E).

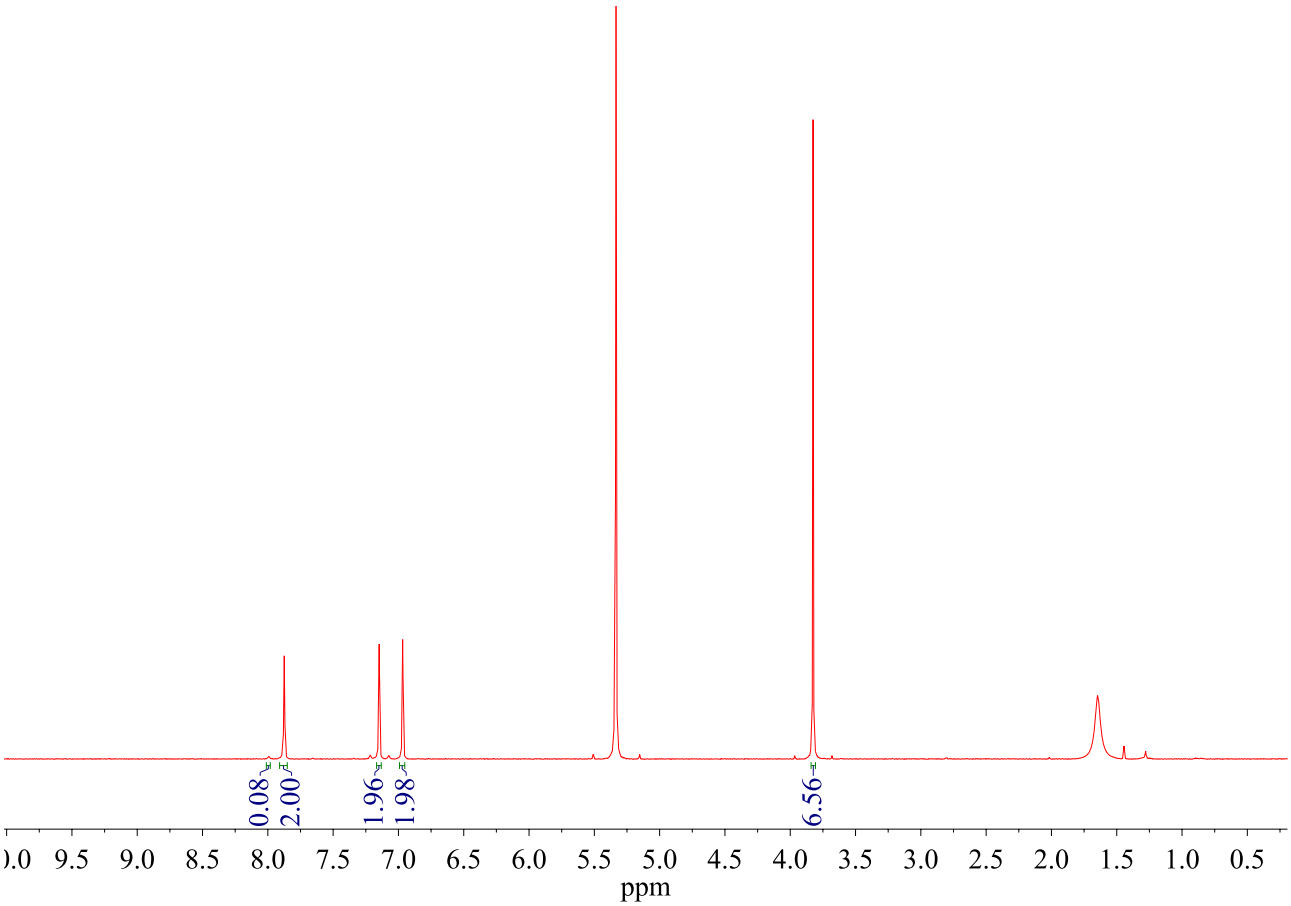


Figure S23. ^{1}H NMR spectrum of [I(1-methylimidazole)$_2$]PF$_6$ (CD_2Cl_2, 500 MHz, 25 °C).

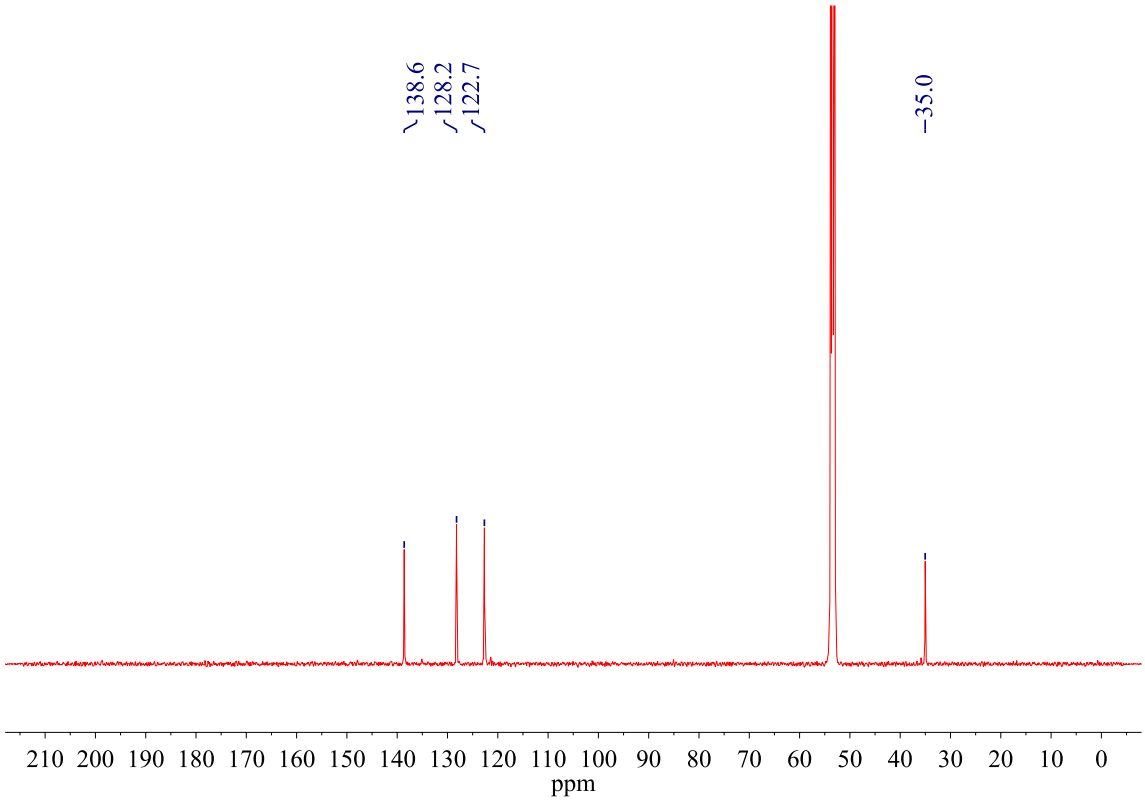


Figure S24. The ^{13}C NMR spectrum of [I(1-methylimidazole)$_2$]PF$_6$ (CD_2Cl_2, 125 MHz, 25 °C).

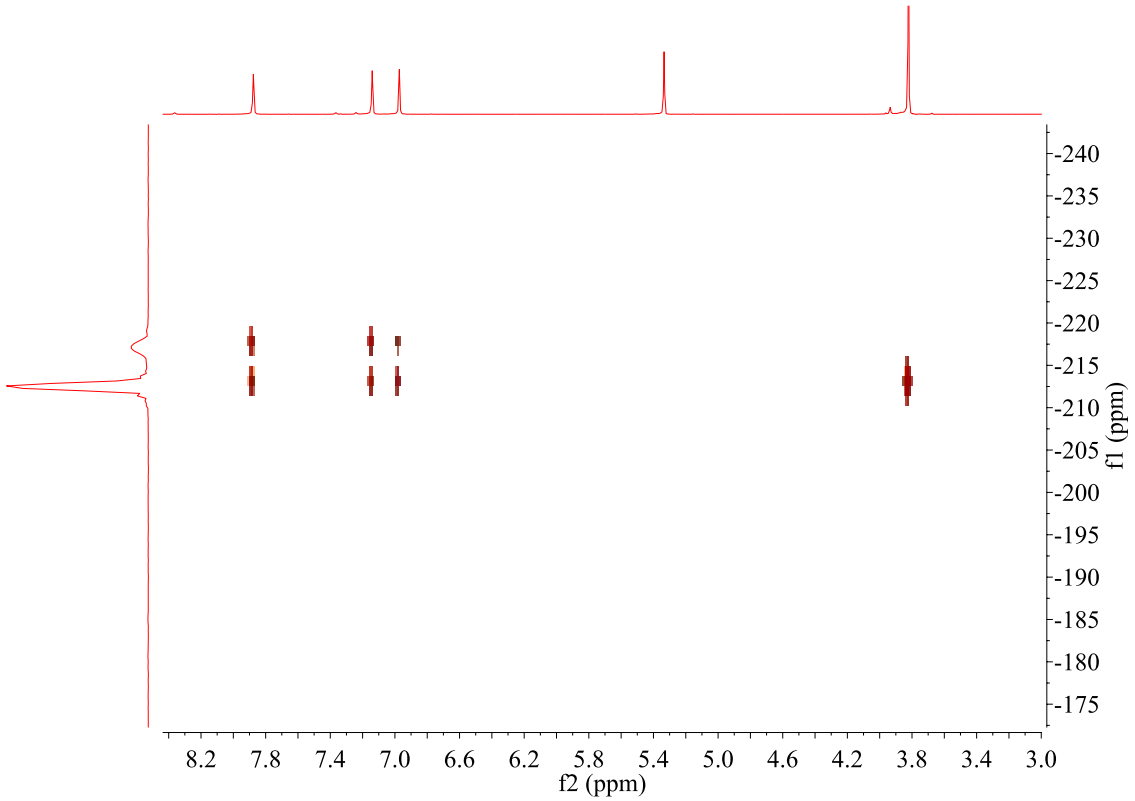


Figure S25. The ^{1}H-^{15}N-HMBC spectrum of $[I(1\text{-methylimidazole})_2]PF_6$ (CD_2Cl_2, 500 MHz, 25 °C).

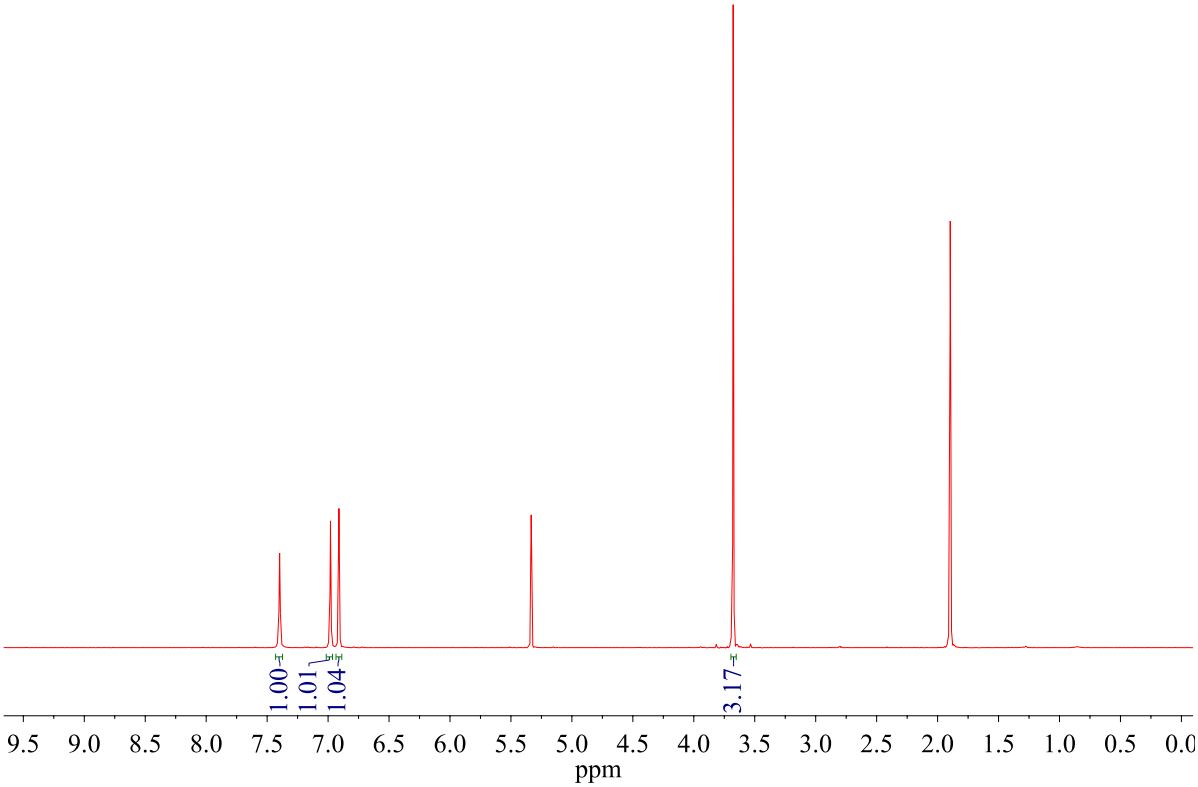


Figure S26. ^{1}H NMR spectrum of 1-methylimidazole (CD_2Cl_2, 500 MHz, 25 °C).

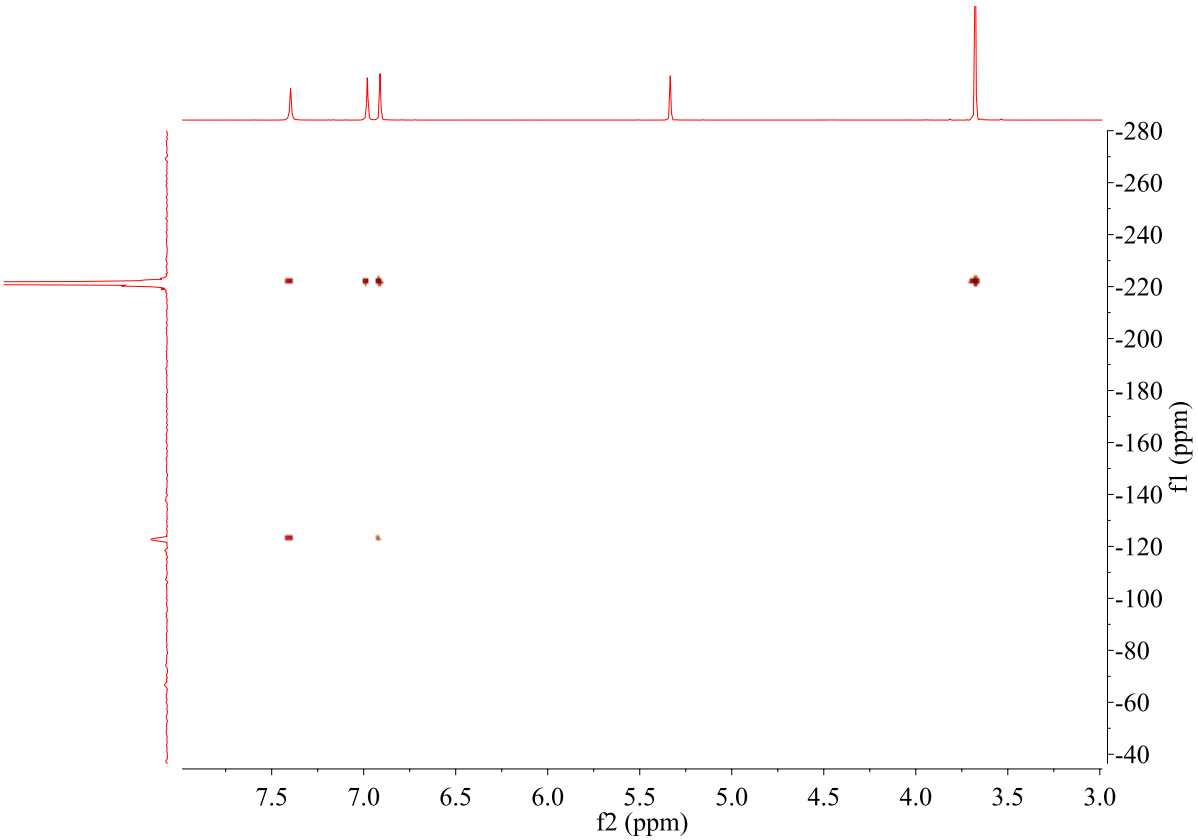


Figure S27. The ^{1}H-^{15}N-HMBC spectrum of 1-methylimidazole (CD_2Cl_2, 500 MHz, 25 °C).

Table S1. The diffusion coefficient ($m^2 \cdot s^{-1}$) and calculated dynamic radius (in parentheses) of ligands **L1-L3** and complexes **1-3**.

X	1	2	3
Ligand **LX**	15.0×10^{-10} (4.23 Å)	17.70×10^{-10} (3.59 Å)	17.9×10^{-10} (3.55 Å)
Complex **X**	6.95×10^{-10} (9.13 Å)	9.25×10^{-10} (6.86 Å)	1.026×10^{-10} (6.19 Å); 8.15×10^{-10} (7.79 Å)

3. Ion Mobility Mass Spectrometry (ESI-QTOF, ESI-IMMS)

Ion mobility mass spectrometry experiments were performed with Agilent 6560 IM-QTOF-MS instrument, which was equipped with a dual ESI ion source. The samples used for analyses were dissolved in MeCN (1 mg/ml, ~1 mM) and then diluted in MeCN (~50 μM). Samples were injected by direct infusion with syringe pump using flow rates from 5 to 9 μl/min.

The parameters were optimized to get maximum abundance of the ions under study. Following ion source parameters were used: Drying gas temperature 150 ºC, drying gas flow 2 l/min, nebulizer pressure 20 psi, fragmentor voltage 350 V, capillary voltage of 5000 V and nozzle voltage 2000 V. Nitrogen from N_2 generator was used as drying gas. Mass spectra were externally calibrated by ESI Tuning mix (Agilent Technologies). The charge states and composition of the ions were determined by comparison of experimental and theoretical isotopic distributions, which was calculated on basis of natural abundances of elements. The compositions of the ions were finally verified by comparing experimental *m/z* values with the theoretical ones. MS/MS (CID) experiments were performed for isolated selected ions. N_2 (99.9999%) was used collision gas and activation (lab frame) voltage (CE) was 10V. Mass spectra was recorded and analysed using Mass Hunter B.08.00 software package (Acquisition and Qualitative Analysis).

In IM-TOF experiments, either N_2 (99.999%) or He (99.9996%) from gas cylinders were used as drift gas. When N_2 was used as a drift gas, the drift tube entrance and exit voltages were set as 1574V and 224V, respectively. As a trap filling time 5000 μs and trap release time 350 μs were used. For He drift gas 875 V and 224 V were used as the drift tube entrance and exit voltages. Before introduction of samples, ES tuning mix (Agilent technologies) was measured as a reference for CCS values and to ensure stabile conditions for CCS determination.[1] For stepped-field measurements, the drift tube entrance voltage was varied in N_2 measurements from 1074 V to 1674 V with 100 V increments and in He measurements from 563 V to 875 V with 52 V increments. Data was analyzed using MassHunter IM-MS Browser (Version B08.00, Agilent Technologies, USA).

Theoretical $^{TMLJ}CCS_{He}$ values were calculated with IMoS.[2] Theoretical CCS values were obtained using the trajectory method (with Lennard Jones 4-6-12 parameters) with diffuse scattering in He gas. The number of rotations was 3 with 300000 gas molecules per rotations. Calculations were carried out using experimental parameters (gas, temperature and pressure) and coordinates for calculations were obtained from DFT-calculated structures optimized at M06-2X/def2-TZVP level of theory using Gaussian 16 program (see details below, 4. Computational Studies). This theoretical method for CCS calculation and drift gas was chosen to get the best fit for experimental data. Other tested methods were project approximation, elastic/diffuse hard sphere scattering, and diatomic trajectory method. All methods were also tested using N_2 as a drift gas.

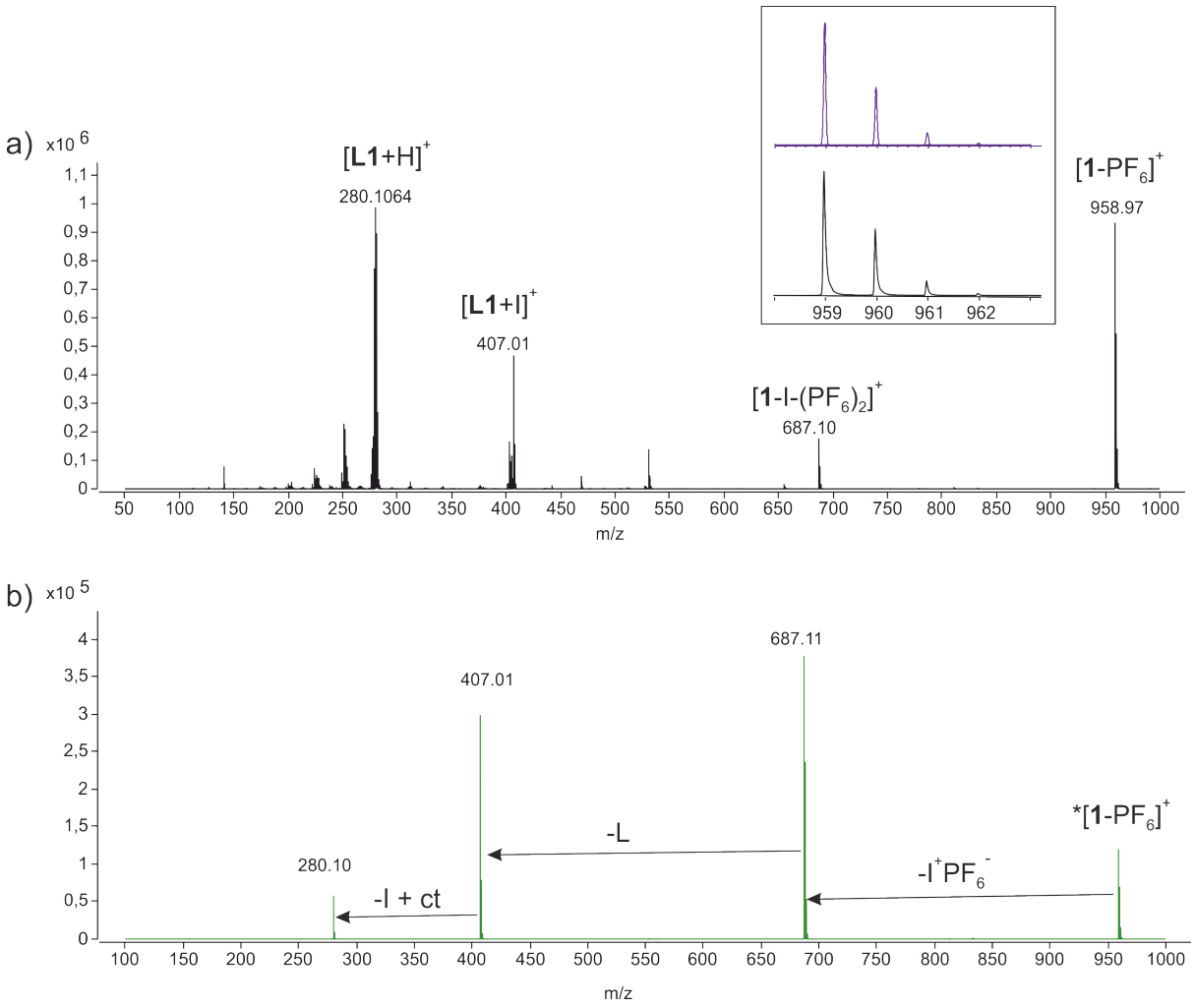


Figure S28. ESI-TOF mass spectra measured from iodine(I) complex **1** in MeCN. a) Profile mass spectrum. Inset show comparison between theoretical and experimental isotopic distributions for ion [**1**-PF_6]$^+$ at *m/z* 958.97; b) MS/MS for ion [**1**-PF_6]$^+$ at *m/z* 958.97 (isolated ion marked with asterisk).

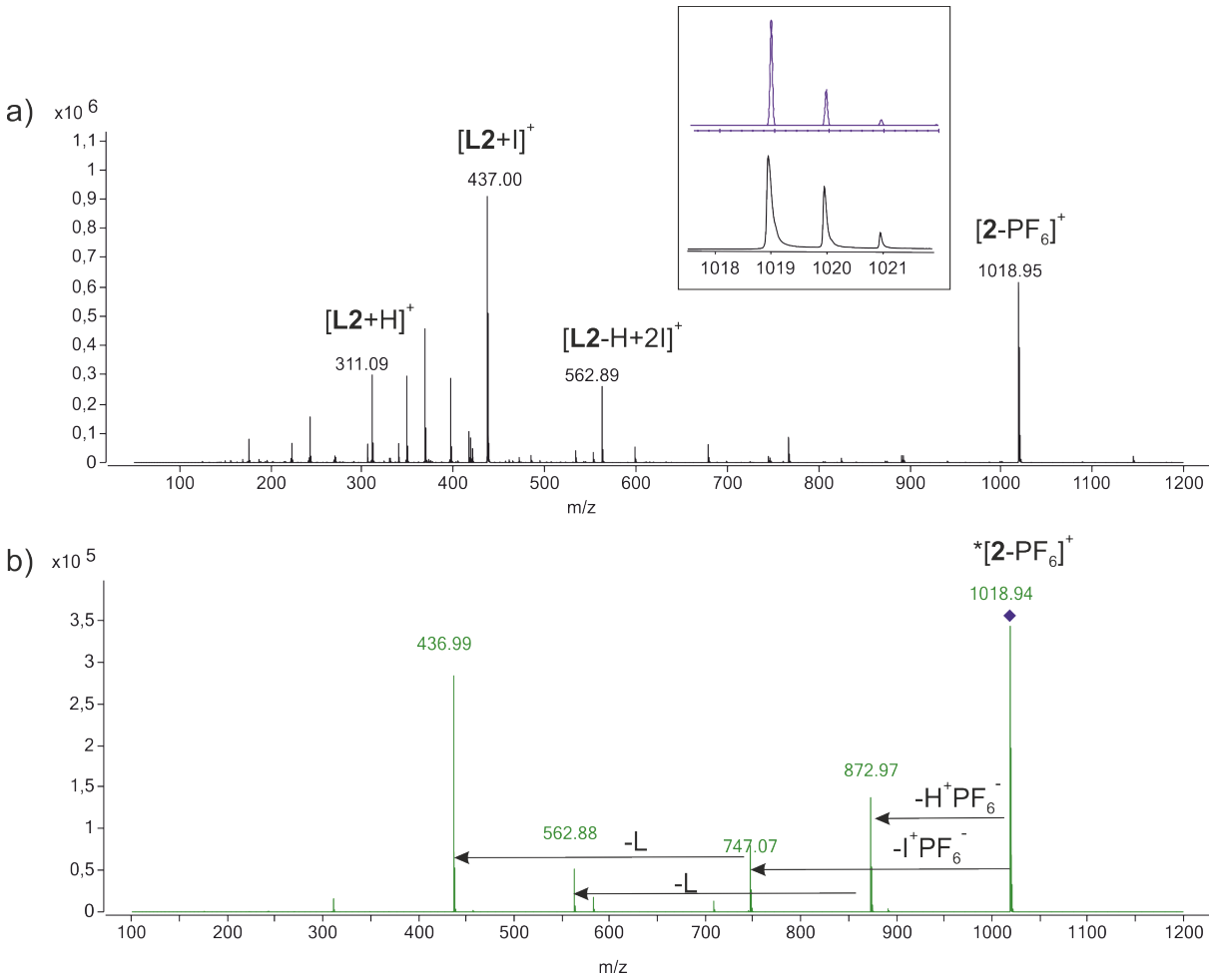


Figure S29. ESI-TOF mass spectra measured from iodine(I) complex **2** in MeCN. a) Profile mass spectrum. Inset shows comparison between theoretical and experimental isotopic distributions for ion [**2**-PF_6]$^+$ at *m/z* 1018.94; b) MS/MS for ion [**2**-PF_6]$^+$ at *m/z* 1018.94 (isolated ion marked with asterisk).

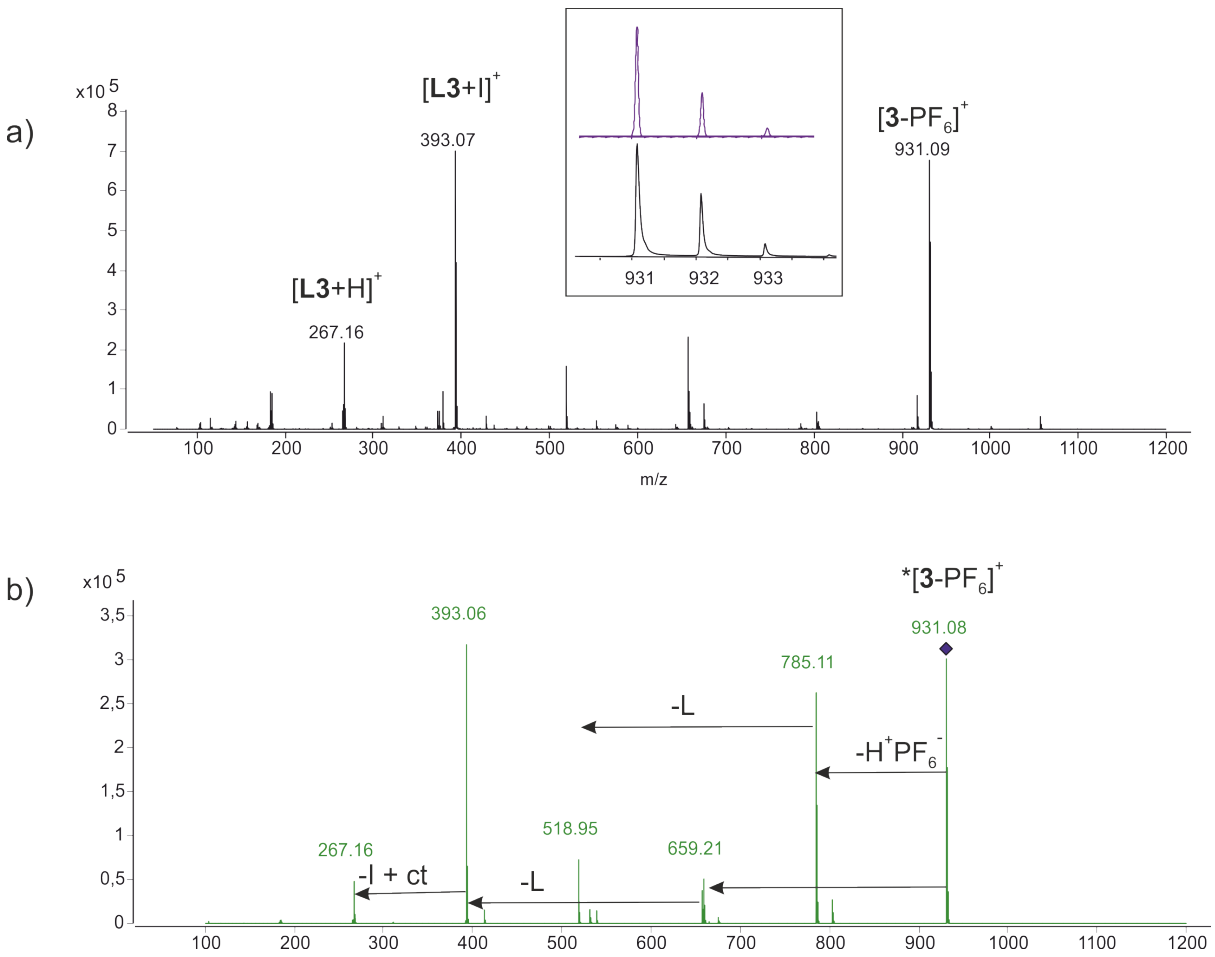


Figure S30. ESI-TOF mass spectra measured from iodonium complex **3** in MeCN. a) Profile mass spectrum. Inset shows comparison between theoretical and experimental isotopic distributions for ion [**3**-PF_6]$^+$ at *m/z* 1018.94; b) MS/MS for ion [**3**-PF_6]$^+$ at *m/z* 931.08 (isolated ion marked with asterisk).

Table S2. Ions observed, their formulas, charge states and comparison to theoretical values.

sample	ion	formula	Charge state	m/z_{theor}	m/z_{exp}	absolute mass accuracy (mDa)
Complex **1**	[**L1**+H]$^+$	$C_{20}H_{12}N_2$+H$^+$	1	281.1073	281.1079	-0.6
	[**L1**+I]$^+$	$C_{20}H_{12}N_2$+I	1	407.0040	407.0053	-1.3
	[**1**-I-$(PF_6)_2$]$^+$	$C_{40}H_{24}N_4$+I	1	687.1040	687.1039	0.1
	[**1**-PF_6]$^+$	$C_{40}H_{24}N_4I_2PF_6$	1	958.9727	958.9733	-0.6
Complex **2**	[**L2**+H]$^+$	$C_{14}H_{10}N_4F_4$+H$^+$	1	311.0914	311.0938	-2.4
	[**L2**+I]$^+$	$C_{14}H_{10}N_4F_4$+I$^+$	1	436.9881	436.9903	-2.2
	[**2**-PF_6]$^+$	$C_{28}H_{20}N_8F_{14}PI_2^+$	1	1018.9409	1018.9405	0.4
	[**2**-H-$(PF_6)_2$]$^+$	$C_{28}H_{19}N_8F_8I_2^+$	1	562.8853	562.8842	1.1
Complex **3**	[**L3**+H]$^+$	$C_{16}H_{18}N_4$+H$^+$	1	267.1604	267.1615	-1.1
	[**L3**+I]$^+$	$C_{16}H_{18}N_4$+I$^+$	1	393,0571	393,0590	-1,9
	[**3**-PF_6]$^+$	$C_{32}H_{36}N_8F_6PI_2^+$	1	931,0789	931,0845	-5.6

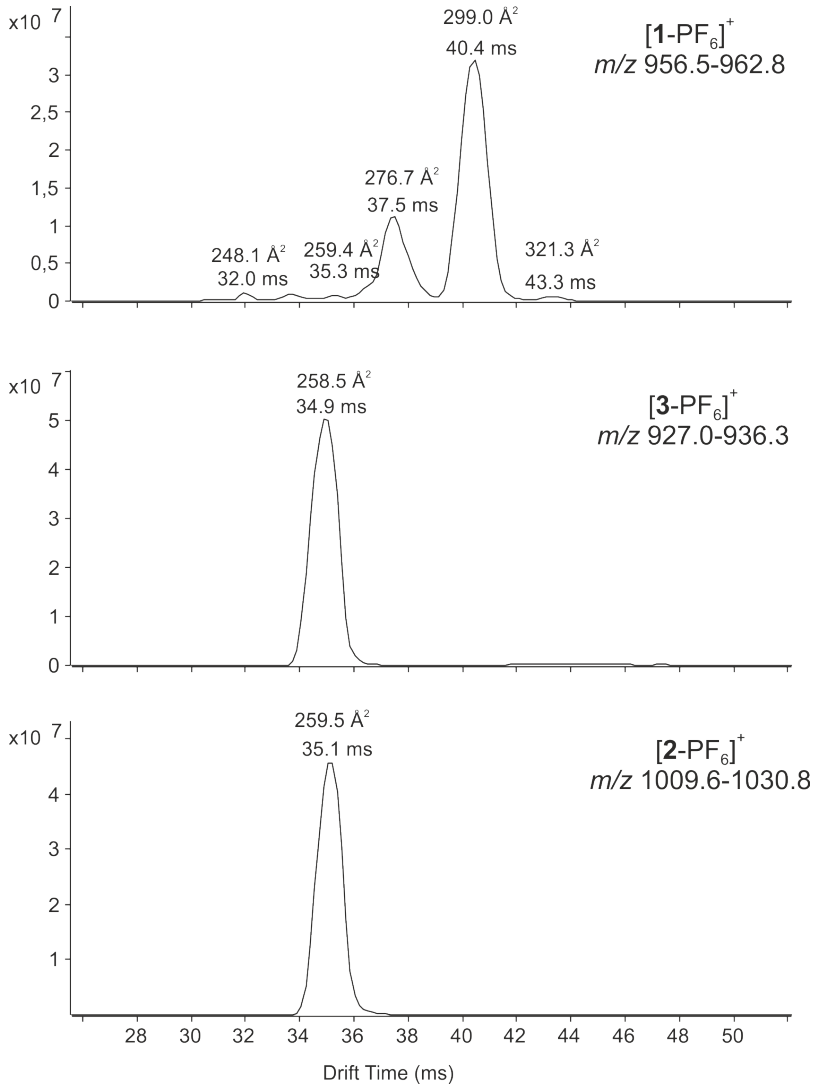


Figure S31. Comparison on arrival time distributions (ATD) for ions [**1**-PF_6]$^+$, [**2**-PF_6]$^+$ and [**3**-PF_6]$^+$. ATDs measured in N_2 drift gas and extracted $^{DT}CCS_{N2}$ values and drift times are indicated in figure.

Table S3. Experimental ^{DT}CCS values using N_2 and He as drift gas, theoretical $^{TMLJ}CCS_{He}$ (trajectory method with Lennard Jones 4-6-12 potential) and their comparison.

sample	ion	formula	Charge state	$^{DT}CCS_{N2}$ (Å^2)	$^{DT}CCS_{He}$ (Å2)	$^{TMLJ}CCS_{He}$ (Å^2 /%)		Model
Complex **1**	[**L1**+H]$^+$	$C_{20}H_{12}N_2$+H$^+$	1	194.8	114.9			
	[**L1**+I]$^+$	$C_{20}H_{12}N_2$+I	1	203.9	126.2			
	[**1**-I-$(PF_6)_2$]$^+$	$C_{40}H_{24}N_4$+I	1	301.5	215.7			
	[**1**-PF_6]$^+$	$C_{40}H_{24}N_4I2PF_6$	1	321.3	237.8	231.8	-2.5	PF_6 out
				299	219.3	228.8	4.3	PF_6 in
				276.7	199.1			
				259.4	196.6			
				248.1	na			
Complex **2**	[**L2**+H]$^+$	$C_{14}H_{10}N_4F_4$+H$^+$	1	170.7	97.4			
	[**L2**+I]$^+$	$C_{14}H_{10}N_4F_4$+I$^+$	1	179.8	104.9			
	[**2**-PF_6]$^+$	$C_{28}H_{20}N_8F_{14}PI_2^+$	1	259.5	184.4	180.9	-1.9	
	[**L2**-H+2I]$^+$	$C_{28}H19N_8F_8I_2^+$	1	193.7	114			
Complex **3**	[**L3**+H]$^+$	$C_{16}H_{18}N_4$+H$^+$	1	174.4	108.6			
	[**L3**+I]$^+$	$C_{16}H_{18}N_4$+I$^+$	1	189.7	112.1			
	[**3**-PF_6]$^+$	$C_{32}H_{36}N_8F_6PI_2^+$	1	258.5	182.3	185.3	1.6	**3b** up-down-up-down
						184.3	1.1	**3a** up-up-down-down

4. Computational Studies

4.1 General

The energetic features of the adducts analyzed in this work were calculated at the M06-2X[5]/def2-TZVP[6] level of theory using the crystallographic coordinates of the corresponding Ag complexes as starting points for the optimizations, replacing the Ag ions by I. For iodine, the inner shell electrons are modelled by ECPs (ECP-60 scheme),[7] which also accounts for scalar relativistic effects. The GAUSSIAN-16 program has been used for the geometry optimizations and energetic calculations.[8]

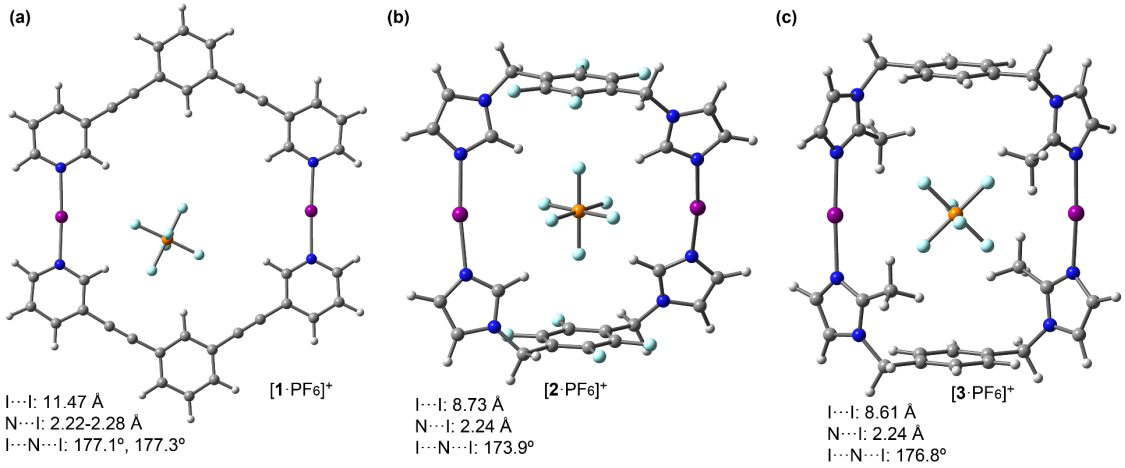


Figure S32. Optimized geometries of compounds [**1**–PF_6]$^+$ (a), [**2**–PF_6]$^+$ (b) and [**3**–PF_6]$^+$ (c) at the M06-2X/def2-TZVP level of theory.

4.2 X-ray coordinates

Complex 1

1	-5.958142	-6.083171	-0.001441
6	-5.971301	-5.001602	-0.001148
7	-5.987332	-2.256929	-0.000375
6	-4.762970	-4.298125	-0.000729
6	-7.167482	-4.307729	-0.001172
6	-7.144468	-2.925545	-0.000781
6	-4.825126	-2.906772	-0.000339
1	-8.115244	-4.826707	-0.001493
1	-8.049221	-2.332399	-0.000791
1	-3.924898	-2.306547	0.000009
6	-3.504546	-4.961775	-0.000701
6	-2.447803	-5.537922	-0.000702
6	-1.206463	-6.244648	-0.000679
6	1.200808	-7.643026	-0.000665
6	-1.201087	-7.643024	-0.001150
6	-0.000136	-5.547154	-0.000200
6	1.206189	-6.244648	-0.000190
6	-0.000139	-8.332348	-0.001142
1	-2.141010	-8.177766	-0.001523
1	-0.000135	-4.466076	0.000167
1	-0.000141	-9.413686	-0.001508
1	2.140732	-8.177768	-0.000658

6	2.447531	-5.537927	0.000326
6	3.504322	-4.961868	0.000718
6	4.762770	-4.298258	0.000875
6	7.144325	-2.925778	0.001221
6	5.971070	-5.001784	0.001325
6	4.824984	-2.906903	0.000603
7	5.987221	-2.257109	0.000778
6	7.167277	-4.307962	0.001498
1	5.957866	-6.083352	0.001536
1	3.924781	-2.306639	0.000235
1	8.115017	-4.826981	0.001851
1	8.049106	-2.332675	0.001355
1	-5.957894	6.083359	0.002214
6	-5.971106	5.001792	0.001833
7	-5.987274	2.257119	0.000865
6	-4.762810	4.298256	0.000832
6	-7.167321	4.307976	0.002335
6	-7.144377	2.925791	0.001839
6	-4.825035	2.906905	0.000361
1	-8.115058	4.827000	0.003113
1	-8.049159	2.332689	0.002207
1	-3.924838	2.306636	-0.000446
6	-3.504354	4.961846	0.000298
6	-2.447573	5.537924	-0.000122
6	-1.206220	6.244626	-0.000496
6	1.201075	7.642965	-0.001245
6	-1.200820	7.643002	-0.001066
6	0.000097	5.547112	-0.000305
6	1.206432	6.244587	-0.000676
6	0.000138	8.332307	-0.001439
1	-2.140736	8.177758	-0.001225
1	0.000079	4.466034	0.000139
1	0.000153	9.413645	-0.001880
1	2.141008	8.177691	-0.001527
6	2.447765	5.537849	-0.000456
6	3.504559	4.961792	-0.000316
6	4.762983	4.298138	-0.000500
6	7.144493	2.925580	-0.000784
6	5.971306	5.001625	-0.001071
6	4.825151	2.906782	-0.000082
7	5.987369	2.256949	-0.000230
6	7.167491	4.307763	-0.001211
1	5.958137	6.083193	-0.001395
1	3.924929	2.306547	0.000391
1	8.115248	4.826750	-0.001647
1	8.049254	2.332446	-0.000871
53	5.993619	-0.000079	0.000326
53	-5.993571	0.000095	0.000197

Complex 2

6	0.000000	5.603958	-1.408650
6	0.095364	5.602829	1.408390
6	-1.159654	5.614065	-0.649692
6	1.211295	5.587937	-0.733616
6	1.255015	5.595789	0.649441
6	-1.116052	5.605132	0.733349
53	0.000000	-0.000000	3.902561
6	-0.069331	5.592141	-2.913614
1	-0.771437	6.344795	-3.267138
1	0.907610	5.809419	-3.339415
6	0.164566	5.589683	2.913341
1	0.879097	6.330567	3.266841
1	-0.808604	5.823047	3.339250
7	0.605522	4.288816	3.419589
6	-0.106112	3.153439	3.372617
7	0.607007	2.159363	3.862769
6	1.823356	2.668324	4.243547
1	2.586644	2.051839	4.685109
6	1.831747	3.998744	3.966660
1	2.585980	4.753562	4.105139
7	-0.531866	4.298847	-3.419978
6	0.160171	3.151454	-3.372164
7	-0.569612	2.169584	-3.862446
6	-1.776782	2.699224	-4.244193
1	-2.550364	2.095828	-4.685933
6	-1.762541	4.029672	-3.967661

1	-2.503670	4.797283	-4.106601
6	-0.095364	-5.602829	1.408390
6	-0.000000	-5.603958	-1.408650
6	-1.255015	-5.595789	0.649441
6	1.116052	-5.605132	0.733349
6	1.159654	-5.614065	-0.649692
6	-1.211295	-5.587937	-0.733616
53	-0.000000	0.000000	-3.901803
6	-0.164566	-5.589683	2.913341
1	-0.879097	-6.330567	3.266841
1	0.808604	-5.823047	3.339250
6	0.069331	-5.592141	-2.913614
1	0.771437	-6.344795	-3.267138
1	-0.907610	-5.809419	-3.339415
7	0.531866	-4.298847	-3.419978
6	-0.160171	-3.151454	-3.372164
7	0.569612	-2.169584	-3.862446
6	1.776782	-2.699224	-4.244193
1	2.550364	-2.095828	-4.685933
6	1.762541	-4.029672	-3.967661
1	2.503670	-4.797283	-4.106601
7	-0.605522	-4.288816	3.419589
6	0.106112	-3.153439	3.372617
7	-0.607007	-2.159363	3.862769
6	-1.823356	-2.668324	4.243547
1	-2.586644	-2.051839	4.685109
6	-1.831747	-3.998744	3.966660
1	-2.585980	-4.753562	4.105139
9	2.431799	5.585192	1.266000
9	2.349785	5.554685	-1.417244
9	-2.254876	5.588647	1.417048
9	-2.336444	5.621207	-1.266302
9	-2.431799	-5.585192	1.266000
9	-2.349785	-5.554685	-1.417244
9	2.336444	-5.621207	-1.266302
9	2.254876	-5.588647	1.417048
1	1.164505	3.065475	-2.988644
1	-1.164505	-3.065475	-2.988644
1	-1.112007	3.084664	2.989699
1	1.112007	-3.084664	2.989699

Complex 3a

6	1.344686	-0.378593	5.529437
6	-1.344686	0.378593	5.529437
6	0.992786	0.966664	5.533831
6	0.342031	-1.341831	5.535690
6	-0.992786	-0.966664	5.533831
6	-0.342031	1.341831	5.535690
1	1.763950	1.728657	5.537024
1	0.603485	-2.393558	5.546436
1	-0.603485	2.393558	5.546436
53	-4.025520	0.000083	-0.000008
1	-1.763950	-1.728657	5.537024
6	2.800578	-0.782067	5.514479
1	3.326592	-0.376742	6.378252
1	2.901327	-1.866740	5.548487
6	-2.800578	0.782067	5.514479
1	-3.326592	0.376742	6.378252
1	-2.901327	1.866740	5.548487
7	-3.494774	0.280104	4.328197
6	-3.260534	0.673598	3.062082
7	-4.017221	-0.044106	2.243969
6	-4.756131	-0.919856	3.002464
1	-5.458391	-1.604530	2.560111
6	-4.434942	-0.724280	4.305090
1	-4.794623	-1.188548	5.206655
7	3.494774	-0.280104	4.328197
6	3.260534	-0.673598	3.062082
7	4.017221	0.044106	2.243969
6	4.756131	0.919856	3.002464
1	5.458391	1.604530	2.560111
6	4.434942	0.724280	4.305090
1	4.794623	1.188548	5.206655
6	-1.344747	-0.378382	-5.529350
6	1.344747	0.378382	-5.529350
6	-0.992638	0.966820	-5.533705

6	-0.342241	-1.341777	-5.535585
6	0.992638	-0.966820	-5.533705
6	0.342241	1.341777	-5.535585
1	-1.763680	1.728936	-5.536920
1	-0.603852	-2.393465	-5.546353
1	0.603852	2.393465	-5.546353
53	4.025520	-0.000083	-0.000008
1	1.763680	-1.728936	-5.536920
6	-2.800699	-0.781631	-5.514518
1	-3.326579	-0.376149	-6.378299
1	-2.901596	-1.866285	-5.548660
6	2.800699	0.781631	-5.514518
1	3.326579	0.376149	-6.378299
1	2.901596	1.866285	-5.548660
7	3.494915	0.279684	-4.328229
6	3.260866	0.673313	-3.062120
7	4.017571	-0.044396	-2.244018
6	4.756245	-0.920337	-3.002509
1	5.458485	-1.605041	-2.560172
6	4.434942	-0.724832	-4.305122
1	4.794472	-1.189226	-5.206681
7	-3.494915	-0.279684	-4.328229
6	-3.260866	-0.673313	-3.062120
7	-4.017571	0.044396	-2.244018
6	-4.756245	0.920337	-3.002509
1	-5.458485	1.605041	-2.560172
6	-4.434942	0.724832	-4.305122
1	-4.794472	1.189226	-5.206681
6	2.298996	1.736515	-2.678246
1	2.384998	2.593110	-3.347108
1	2.502699	2.068559	-1.663508
1	1.272636	1.369042	-2.733293
6	-2.298996	-1.736515	-2.678246
1	-1.272636	-1.369042	-2.733293
1	-2.384998	-2.593110	-3.347108
1	-2.502699	-2.068559	-1.663508
6	-2.298519	1.736685	2.678253
1	-2.501521	2.068069	1.663162
1	-1.272156	1.369380	2.734303
1	-2.385135	2.593692	3.346517
6	2.298519	-1.736685	2.678253
1	1.272156	-1.369380	2.734303
1	2.385135	-2.593692	3.346517
1	2.501521	-2.068069	1.663162

Complex 3b

7	0.380591	2.211872	3.923923
7	0.287139	4.337572	3.484582
6	1.454583	4.127009	4.181424
1	2.124575	4.932344	4.426745
6	0.845205	4.919446	0.692629
1	1.632661	4.400306	1.227383
6	1.504262	2.799791	4.453621
1	2.244482	2.233188	4.990819
6	-1.158561	6.235791	0.694317
1	-1.950506	6.747337	1.228488
6	-0.157425	5.579584	1.397624
6	-0.154839	5.603852	2.909538
1	0.524299	6.371291	3.281913
1	-1.149243	5.839903	3.289591
6	-1.633326	2.978870	2.628454
1	-1.478826	2.994752	1.547838
1	-2.326476	3.781753	2.879385
1	-2.083883	2.030043	2.908162
6	-0.344106	3.156604	3.341959
7	0.380591	2.211872	-3.923923
7	-0.380591	-2.211872	-3.923923
7	-0.380591	-2.211872	3.923923
7	0.287139	4.337572	-3.484582
7	-0.287139	-4.337572	-3.484582
7	-0.287139	-4.337572	3.484582
6	1.454583	4.127009	-4.181424
6	-1.454583	-4.127009	-4.181424
6	-1.454583	-4.127009	4.181424
1	2.124575	4.932344	-4.426745
1	-2.124575	-4.932344	4.426745

1	-2.124575	-4.932344	-4.426745
6	0.845205	4.919446	-0.692629
6	-0.845205	-4.919446	-0.692629
6	-0.845205	-4.919446	0.692629
1	1.632661	4.400306	-1.227383
1	-1.632661	-4.400306	1.227383
1	-1.632661	-4.400306	-1.227383
6	1.504262	2.799791	-4.453621
6	-1.504262	-2.799791	-4.453621
6	-1.504262	-2.799791	4.453621
1	-2.244482	-2.233188	4.990819
1	-2.244482	-2.233188	-4.990819
1	2.244482	2.233188	-4.990819
6	-1.158561	6.235791	-0.694317
6	1.158561	-6.235791	0.694317
6	1.158561	-6.235791	-0.694317
1	-1.950506	6.747337	-1.228488
1	1.950506	-6.747337	-1.228488
1	1.950506	-6.747337	1.228488
6	-0.157425	5.579584	-1.397624
6	0.157425	-5.579584	-1.397624
6	0.157425	-5.579584	1.397624
6	-0.154839	5.603852	-2.909538
6	0.154839	-5.603852	-2.909538
6	0.154839	-5.603852	2.909538
1	-0.524299	-6.371291	3.281913
1	-0.524299	-6.371291	-3.281913
1	0.524299	6.371291	-3.281913
1	1.149243	-5.839903	3.289591
1	1.149243	-5.839903	-3.289591
1	-1.149243	5.839903	-3.289591
6	1.633326	-2.978870	2.628454
6	1.633326	-2.978870	-2.628454
6	-1.633326	2.978870	-2.628454
1	1.478826	-2.994752	1.547838
1	1.478826	-2.994752	-1.547838
1	-1.478826	2.994752	-1.547838
1	2.326476	-3.781753	2.879385
1	2.326476	-3.781753	-2.879385
1	-2.326476	3.781753	-2.879385
1	2.083883	-2.030043	2.908162
1	2.083883	-2.030043	-2.908162
1	-2.083883	2.030043	-2.908162
6	0.344106	-3.156604	3.341959
6	0.344106	-3.156604	-3.341959
6	-0.344106	3.156604	-3.341959
53	-0.000000	0.000000	3.936872
53	-0.000000	0.000000	-3.936872

[**1**-PF_6]$^+$

1	-6.690376	5.175614	0.000000
6	-6.484382	4.113761	0.000000
7	-5.930873	1.430640	0.000000
6	-5.162054	3.672009	0.000000
6	-7.514526	3.189430	0.000000
6	-7.202937	1.846328	0.000000
6	-4.918005	2.295130	0.000000
1	-8.549446	3.499473	0.000000
1	-7.961882	1.075675	0.000000
1	-3.901144	1.911891	0.000000
6	-4.064245	4.570741	0.000000
6	-3.101876	5.289725	0.000000
6	-1.928961	6.098848	0.000000
6	0.363344	7.668075	0.000000
6	-2.028068	7.492963	0.000000
6	-0.679438	5.480714	0.000000
6	0.466410	6.273253	0.000000
6	-0.882586	8.270930	0.000000
1	-3.006913	7.953130	0.000000
1	-0.607834	4.399272	0.000000
1	-0.960966	9.349559	0.000000
1	1.264587	8.266030	0.000000
6	1.754497	5.663910	0.000000
6	2.848836	5.165443	0.000000
6	4.150968	4.605636	0.000000
6	6.649696	3.469203	0.000000

6	5.287879	5.419084	0.000000
6	4.336005	3.222223	0.000000
7	5.560172	2.695157	0.000000
6	6.545354	4.845320	0.000000
1	5.166867	6.493825	0.000000
1	3.491160	2.542936	0.000000
1	7.440095	5.450837	0.000000
1	7.604553	2.961040	0.000000
1	-4.852994	-6.824186	0.000000
6	-4.979888	-5.750077	0.000000
7	-5.267947	-3.025104	0.000000
6	-3.850762	-4.928360	0.000000
6	-6.241118	-5.183528	0.000000
6	-6.350249	-3.806982	0.000000
6	-4.043919	-3.546438	0.000000
1	-7.131641	-5.795248	0.000000
1	-7.307481	-3.302339	0.000000
1	-3.214390	-2.847907	0.000000
6	-2.544293	-5.489937	0.000000
6	-1.458815	-6.007049	0.000000
6	-0.171522	-6.622050	0.000000
6	2.340981	-7.824031	0.000000
6	-0.053764	-8.014824	0.000000
6	0.973714	-5.830017	0.000000
6	2.230637	-6.430725	0.000000
6	1.198700	-8.606544	0.000000
1	-0.948640	-8.621987	0.000000
1	0.885422	-4.752142	0.000000
1	1.283990	-9.684620	0.000000
1	3.321890	-8.279306	0.000000
6	3.394559	-5.606164	0.000000
6	4.357511	-4.885446	0.000000
6	5.464804	-3.996191	0.000000
6	7.523560	-2.182710	0.000000
6	6.786530	-4.448124	0.000000
6	5.246458	-2.618749	0.000000
7	6.258428	-1.755202	0.000000
6	7.822285	-3.531972	0.000000
1	6.984614	-5.511461	0.000000
1	4.244105	-2.208900	0.000000
1	8.854061	-3.852676	0.000000
1	8.291735	-1.420725	0.000000
53	5.854743	0.479130	0.000000
53	-5.548528	-0.758667	0.000000
15	-0.868921	0.912101	0.000000
9	-1.777297	2.266079	0.000000
9	-0.882586	0.919000	1.597270
9	-2.237710	0.031006	0.000000
9	-0.882586	0.919000	-1.597270
9	0.010240	-0.432737	0.000000
9	0.467570	1.817746	0.000000

[**2**-PF_6]$^+$

6	-4.823485	-1.096131	-0.890004
6	-4.823485	1.096131	0.890004
6	-4.835602	-1.281817	0.483862
6	-4.815747	0.209374	-1.356147
6	-4.835602	1.281817	-0.483862
6	-4.815747	-0.209374	1.356147
53	-0.000000	4.379213	0.000000
6	-4.863123	-2.256629	-1.847044
1	-5.845501	-2.729008	-1.817844
1	-4.688373	-1.902973	-2.861520
6	-4.863123	2.256629	1.847044
1	-5.845501	2.729008	1.817844
1	-4.688373	1.902973	2.861520
7	-3.890199	3.290392	1.510102
6	-2.630526	3.094460	1.094291
7	-2.061607	4.259904	0.857230
6	-2.977163	5.241570	1.128776
1	-2.748203	6.285342	1.006356
6	-4.126517	4.643534	1.537155
1	-5.077264	5.049614	1.833774
7	-3.890199	-3.290392	-1.510102
6	-2.630526	-3.094460	-1.094291
7	-2.061607	-4.259904	-0.857230
6	-2.977163	-5.241570	-1.128776

1	-2.748203	-6.285342	-1.006356
6	-4.126517	-4.643534	-1.537155
1	-5.077264	-5.049614	-1.833774
6	4.823485	1.096131	-0.890004
6	4.823485	-1.096131	0.890004
6	4.835602	1.281817	0.483862
6	4.815747	-0.209374	-1.356147
6	4.835602	-1.281817	-0.483862
6	4.815747	0.209374	1.356147
53	0.000000	-4.379213	0.000000
6	4.863123	2.256629	-1.847044
1	5.845501	2.729008	-1.817844
1	4.688373	1.902973	-2.861520
6	4.863123	-2.256629	1.847044
1	5.845501	-2.729008	1.817844
1	4.688373	-1.902973	2.861520
7	3.890199	-3.290392	1.510102
6	2.630526	-3.094460	1.094291
7	2.061607	-4.259904	0.857230
6	2.977163	-5.241570	1.128776
1	2.748203	-6.285342	1.006356
6	4.126517	-4.643534	1.537155
1	5.077264	-5.049614	1.833774
7	3.890199	3.290392	-1.510102
6	2.630526	3.094460	-1.094291
7	2.061607	4.259904	-0.857230
6	2.977163	5.241570	-1.128776
1	2.748203	6.285342	-1.006356
6	4.126517	4.643534	-1.537155
1	5.077264	5.049614	-1.833774
9	-4.876014	2.514179	-0.981754
9	-4.816442	0.447518	-2.663269
9	-4.816442	-0.447518	2.663269
9	-4.876014	-2.514179	0.981754
9	4.876014	2.514179	0.981754
9	4.816442	0.447518	2.663269
9	4.876014	-2.514179	-0.981754
9	4.816442	-0.447518	-2.663269
1	-2.163531	-2.127636	-0.961085
1	2.163531	-2.127636	0.961085
1	-2.163531	2.127636	0.961085
1	2.163531	2.127636	-0.961085
15	0.000000	0.000000	0.000000
9	-1.627215	-0.000000	-0.000000
9	0.008672	-1.134463	1.133974
9	-0.008672	-1.134463	-1.133974
9	0.008672	1.134463	-1.133974
9	-0.008672	1.134463	1.133974
9	1.627215	0.000000	-0.000000

[**3**-PF_6]$^+$

6	1.250824	-0.622693	5.219776
6	-1.250824	0.622693	5.219776
6	1.154614	0.763764	5.213827
6	0.086311	-1.380653	5.214729
6	-1.154614	-0.763764	5.213827
6	-0.086311	1.380653	5.214729
1	2.051543	1.371148	5.191796
1	0.147244	-2.462552	5.203162
1	-0.147244	2.462552	5.203162
53	-4.305987	-0.000686	-0.000023
1	-2.051543	-1.371148	5.191796
6	2.603165	-1.299247	5.233074
1	3.106898	-1.143952	6.187626
1	2.492091	-2.373660	5.090172
6	-2.603165	1.299247	5.233074
1	-3.106898	1.143952	6.187626
1	-2.492091	2.373660	5.090172
7	-3.484893	0.779729	4.196256
6	-3.390296	1.071573	2.883192
7	-4.244680	0.308028	2.218482
6	-4.897973	-0.494451	3.121702
1	-5.645464	-1.203241	2.811954
6	-4.430689	-0.206561	4.360511
1	-4.683519	-0.596004	5.330937
7	3.484893	-0.779729	4.196256
6	3.390296	-1.071573	2.883192

7	4.244680	-0.308028	2.218482
6	4.897973	0.494451	3.121702
1	5.645464	1.203241	2.811954
6	4.430689	0.206561	4.360511
1	4.683519	0.596004	5.330937
6	-1.250820	-0.622695	-5.220380
6	1.250820	0.622695	-5.220380
6	-1.154614	0.763766	-5.214435
6	-0.086305	-1.380662	-5.215328
6	1.154614	-0.763766	-5.214435
6	0.086305	1.380662	-5.215328
1	-2.051561	1.371132	-5.192433
1	-0.147248	-2.462562	-5.203766
1	0.147248	2.462562	-5.203766
53	4.305987	0.000686	-0.000023
1	2.051561	-1.371132	-5.192433
6	-2.603165	-1.299227	-5.233770
1	-3.106948	-1.143566	-6.188234
1	-2.492100	-2.373697	-5.091280
6	2.603165	1.299227	-5.233770
1	3.106948	1.143566	-6.188234
1	2.492100	2.373697	-5.091280
7	3.484840	0.780074	-4.196728
6	3.390176	1.072314	-2.883753
7	4.244829	0.309303	-2.218790
6	4.898333	-0.493287	-3.121759
1	5.646057	-1.201736	-2.811795
6	4.430957	-0.205963	-4.360669
1	4.683881	-0.595671	-5.330964
7	-3.484840	-0.780074	-4.196728
6	-3.390176	-1.072314	-2.883753
7	-4.244829	-0.309303	-2.218790
6	-4.898333	0.493287	-3.121759
1	-5.646057	1.201736	-2.811795
6	-4.430957	0.205963	-4.360669
1	-4.683881	0.595671	-5.330964
6	2.497927	2.125254	-2.339065
1	2.814585	3.105040	-2.703299
1	2.528712	2.117739	-1.253576
1	1.464869	1.945004	-2.636037
6	-2.497927	-2.125254	-2.339065
1	-1.464869	-1.945004	-2.636037
1	-2.814585	-3.105040	-2.703299
1	-2.528712	-2.117739	-1.253576
6	-2.498476	2.124699	2.338179
1	-2.529116	2.116719	1.252695
1	-1.465343	1.945183	2.635387
1	-2.815751	3.104465	2.701938
6	2.498476	-2.124699	2.338179
1	1.465343	-1.945183	2.635387
1	2.815751	-3.104465	2.701938
1	2.529116	-2.116719	1.252695
15	0.000000	0.000000	0.001074
9	-0.000987	1.607682	0.001096
9	-1.137487	0.015487	-1.142123
9	1.137487	-0.015487	-1.142123
9	1.137505	0.016879	1.144290
9	-1.137505	-0.016879	1.144290
9	0.000987	-1.607682	0.001096

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