Electronic Supplementary Materials for

Structural isolation of NIR Absorbing Ferrocenyl Bridged N-Confused Fused expanded Phlorin, N-Confused Porphodimethene and π-extended Corrorin isomer: Synthesis and characterization

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Materials and Methods:

1.1 Electronic absorption spectra were measured with a Perkin Elmer Lambda 950 UV-visible-NIR spectrophotometer. ^{1}H NMR spectra were recorded on a Bruker AVIII 500 MHz spectrometer, Bruker AVIII 400 MHz, Bruker DPX-300 MHz spectrometer and chemical shifts were reported as the delta scale in ppm relative to $CHCl_3$ (δ = 7.26 ppm) and CH_2Cl_2 (δ = 5.32 ppm) as internal reference for ^{1}H and ^{13}C NMR $CHCl_3$ (δ = 77.00 ppm) and CH_2Cl_2 (δ = 55.00 ppm). ESI HR-MS data were recorded using Waters QTOF Micro YA263 spectrometer. All solvents and chemicals were of reagent grade quality, obtained commercially and used without further purification except as noted. For spectral measurements, anhydrous dichloromethane was obtained by refluxing and distillation over CaH_2. Dry THF was obtained by refluxing and distillation over pressed Sodium metal. Thin layer chromatography (TLC) was carried out on alumina sheets coated with silica gel 60 F_{254} (Merck 5554) and gravity column chromatography were performed using Merck Silica Gel 230-400 mesh. Aluminum Oxide (Basic) grade II was purchased from Sigma Aldrich.

1.2 Theoretical Calculation

Macrocycle structures of **5** were modelled based on the observed ^{1}H NMR spectra and several isomers of **7** (**7a-7g**) were bulit based on the mechanistic possiblity for the formation of 7. Along with the modelled structures (**5** and **7a-7g**), X-ray crystal structure coordinates of **6,** were optimized using unrestricted hybrid density functional B3LYP[1a-c] and LanL2DZ[2a-c] (for metal atom) and 6-31G** basis set for rest of the atoms.[3] Hessian calculations were performed at same level of theory to ascertain the optimised structures are local minima. As deprotonation is the prevailing mechanism in anionic binding, the deprotonated state of **6** ([**6**]$^{-1}$) was also optimised at same level of theory and identified as a stationay point. Time dependent density functional (TD-DFT)[4] calculations were performed for **5, 6, deprotonated 6** and isomers of **7a-7g** in the presence of dichloromethane solvent with implicit polarizable continuum model (PCM) and the integral equation formalism variant (IEFPCM)[5] at same level of theory using Gaussian 16 A. 03.[6] The electronic structure and electonic excitation analysis of these macrocycles were analyzed through kohn sham molecular orbitals and natural transition orbitals which were obtained from Multiwfn program[7a] and Gauss Sum.[7b] The nature of aromaticity of 7 were assessed from the nuclear chemical independent shift [8a] NICS (0) value and Anisotropy of the current-induced density (ACID)[8b] that employs gauge independent atomic orbital (GIAO) method[8c-d] and the continuous set of gauge transformations (CSGT)[8e] methods respectively. AICD plot was plotted using POVRAY 3.7 for Windows. In addition, NICSzz (0) value was obtained from Multiwfn program.[7a]

References:

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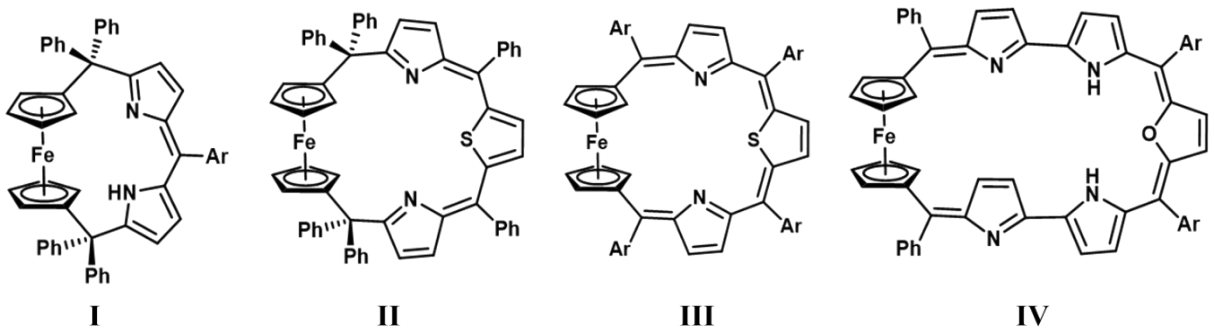
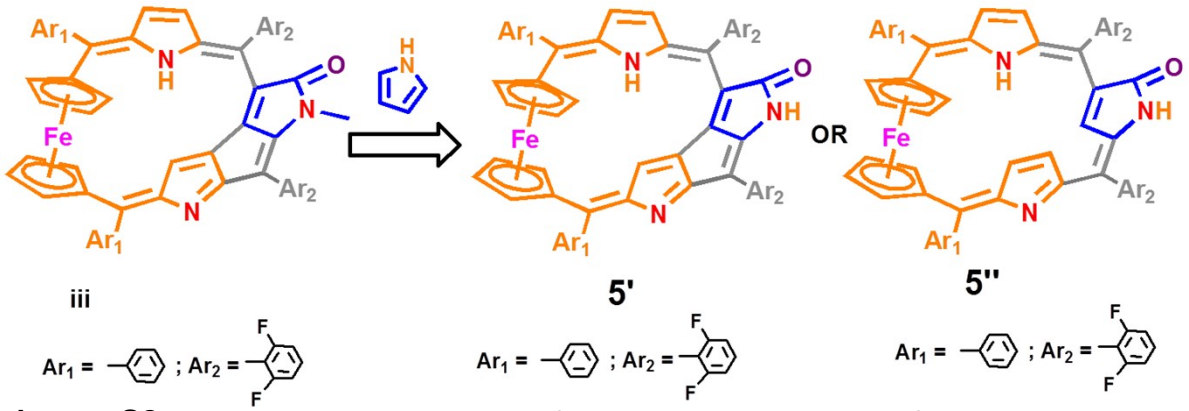
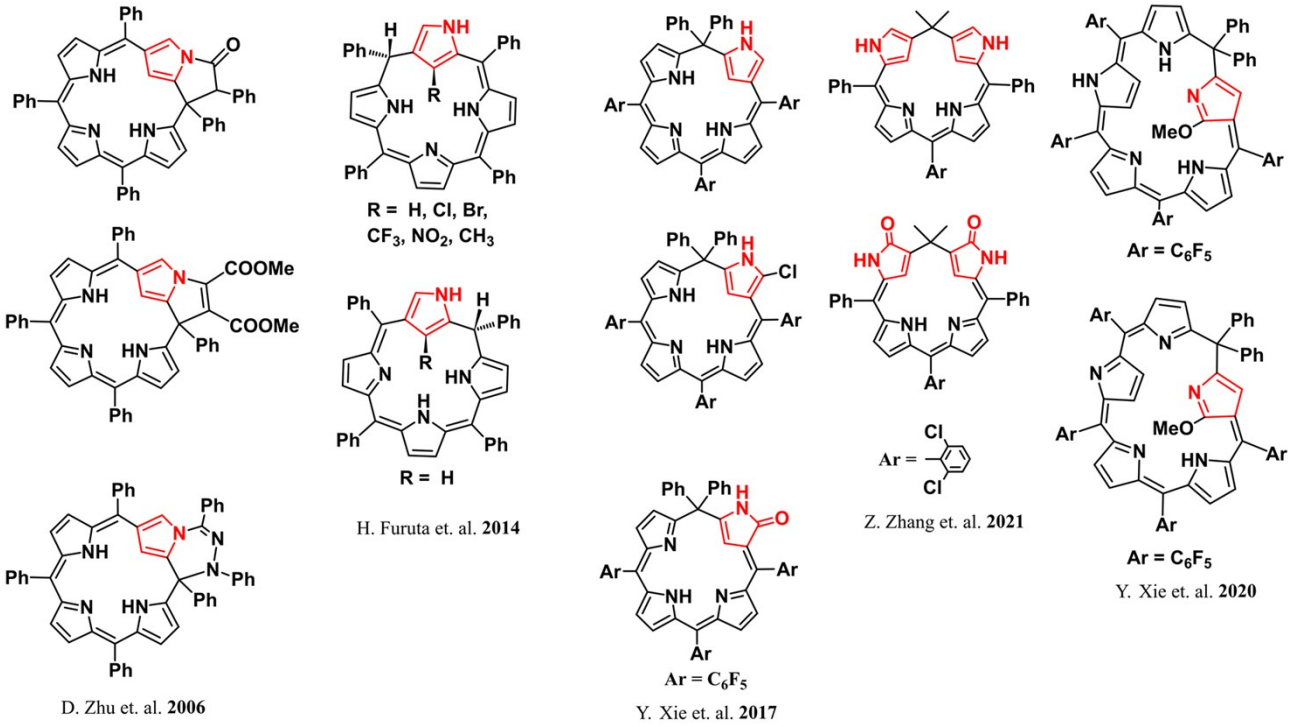


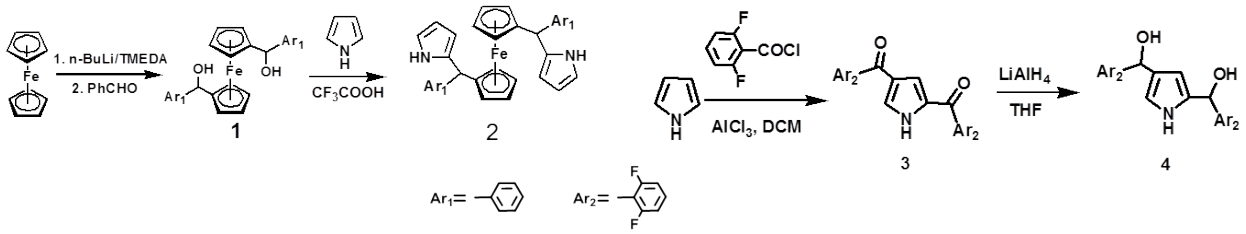
Scheme S1. Literature known Ferrocene bridged macrocycles



Scheme S2. Swapping N-Methyl N-Confused pyrrole with N-Confused pyrrole leading to the expected product of condensation between **2** and **4**



Scheme S3. Literature known N-Confused Phlorins and Expanded N-Confused Phlorins



Scheme S4. Syntheses of precursors for macrocycles **5**, **6** and **7**

Supplementary Data:

2.1 Mass Spectra

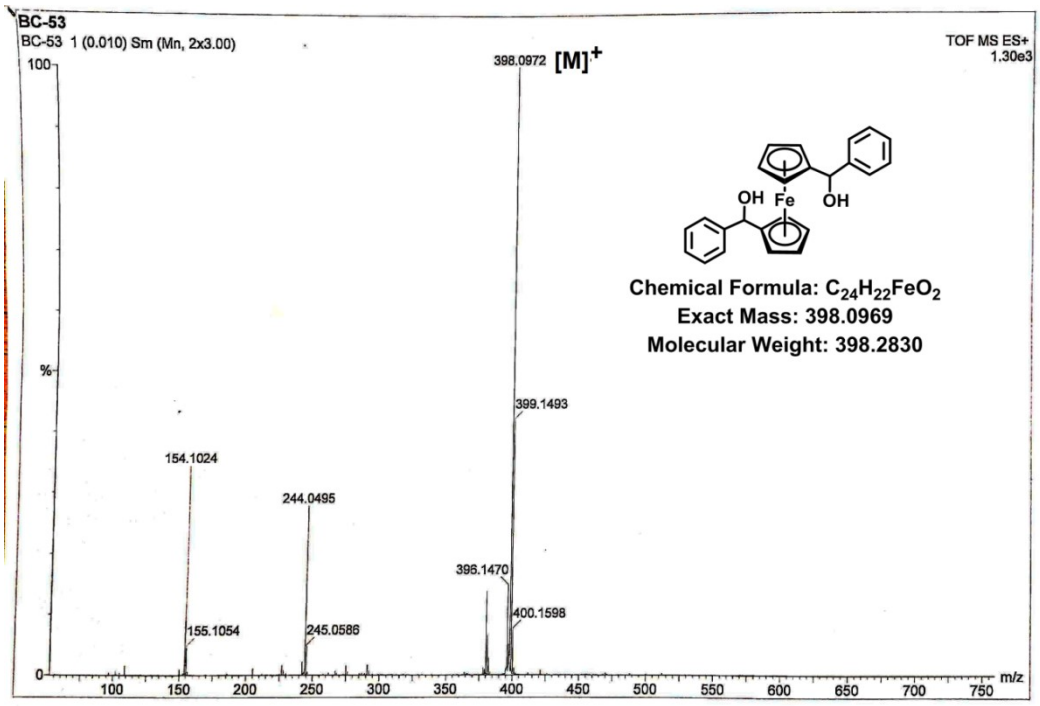


Fig. S1 HRMS Spectra of **1**

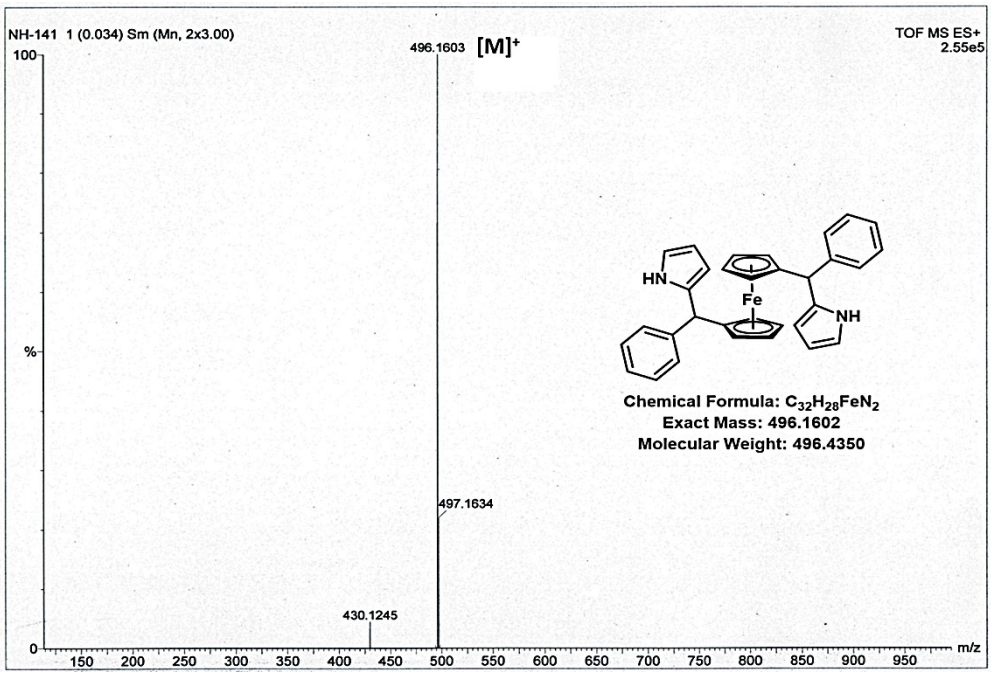


Fig. S2 HRMS Spectra of **2**

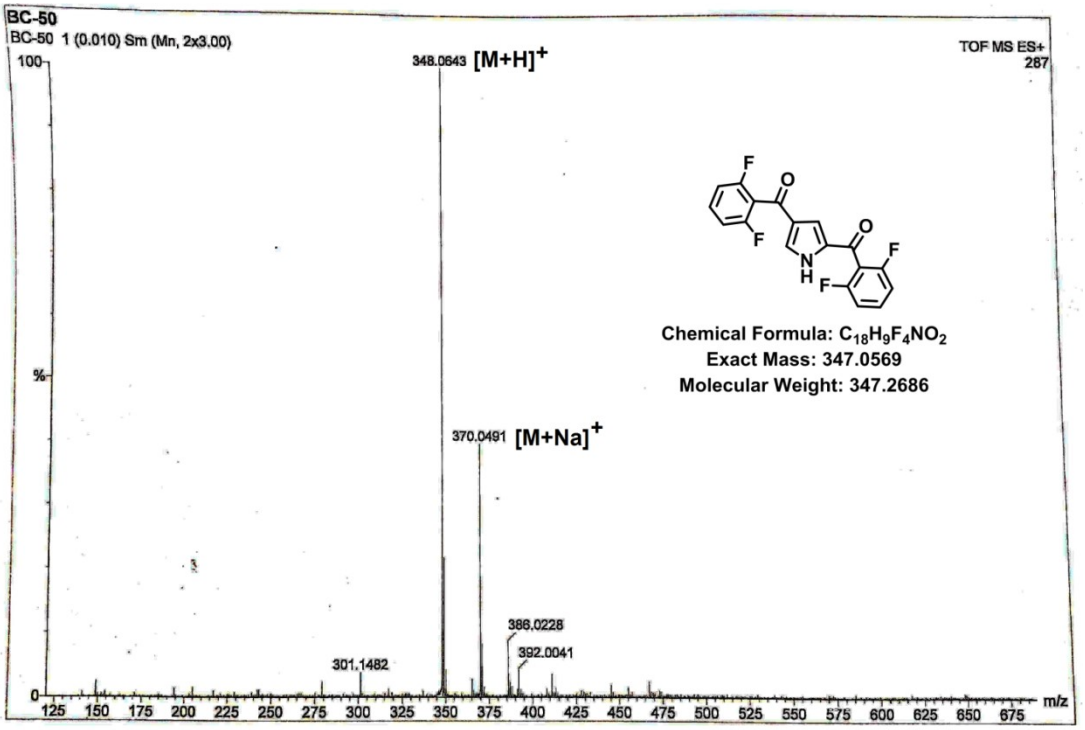


Fig. S3 HRMS Spectra of **3**

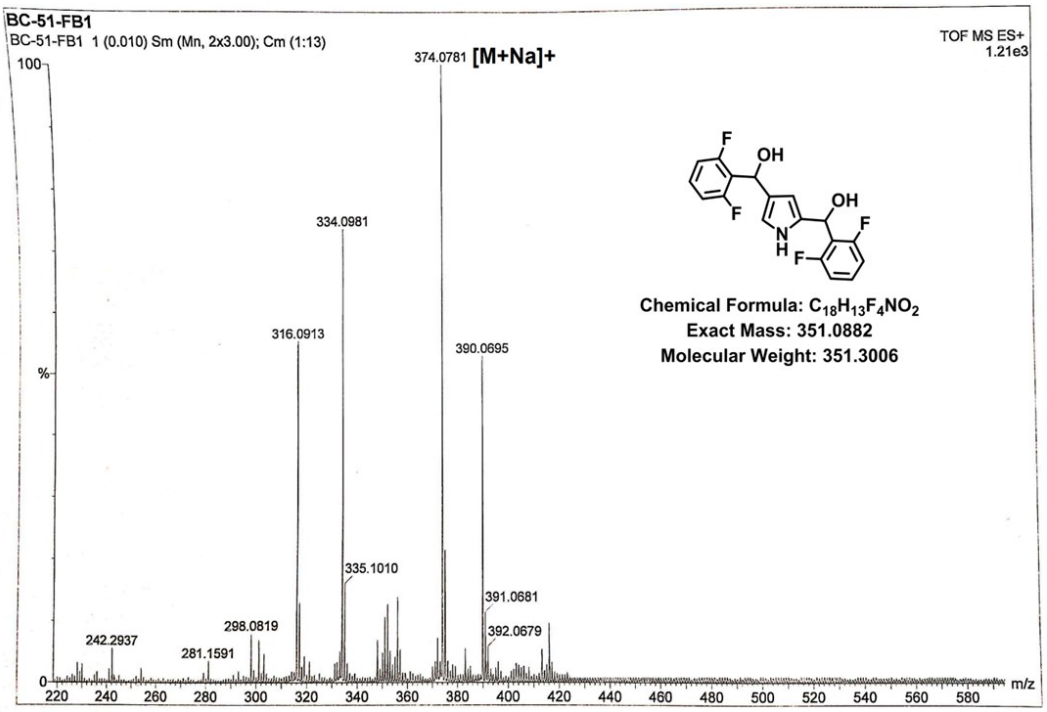


Fig. S4 HRMS Spectra of **4**

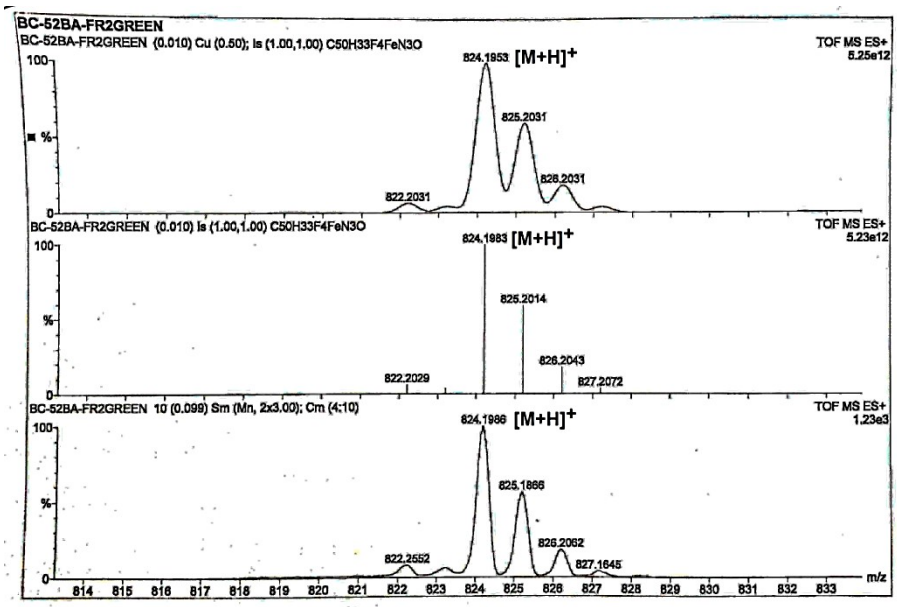


Fig. S5 HRMS Spectra of **5**

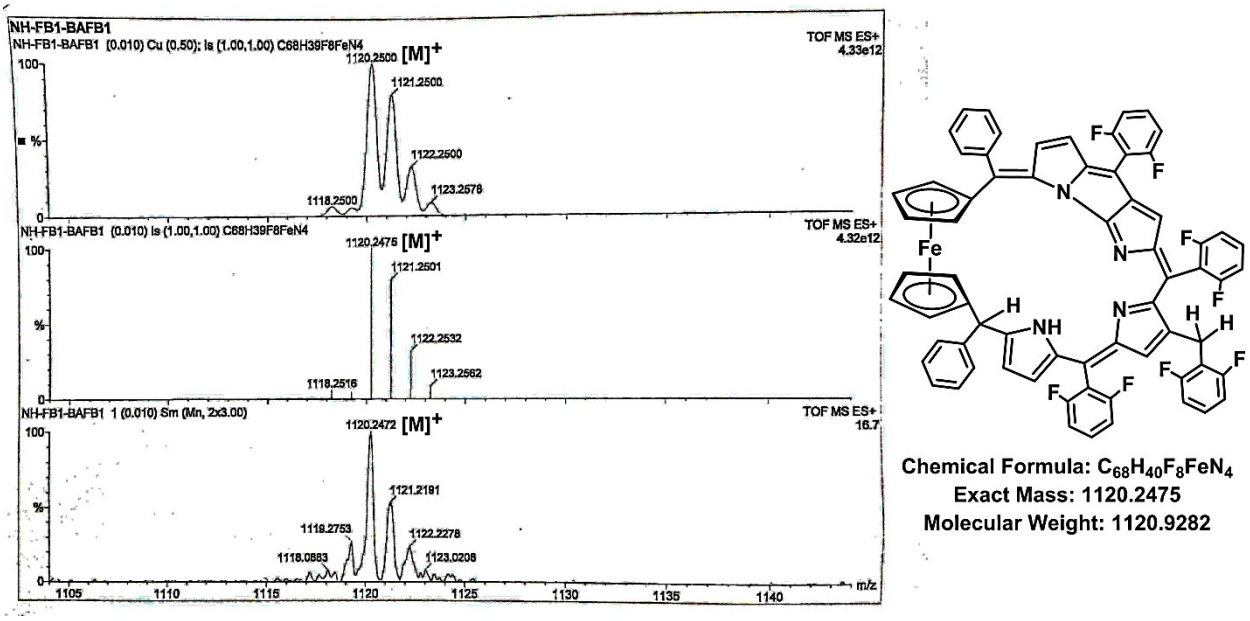
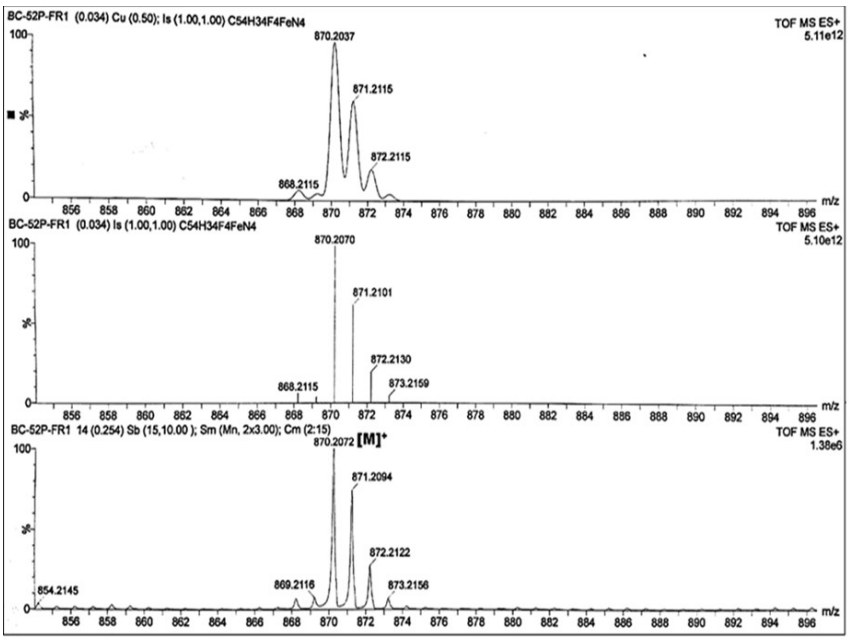
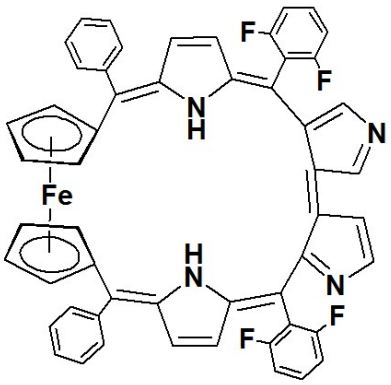


Fig. S6 HRMS Spectra of **6**





Chemical Formula: $C_{54}H_{34}F_4FeN_4$
Exact Mass: 870.2070
Molecular Weight: 870.7326

Fig. S7 HRMS Spectra of **7**

2.2 UV-vis Spectra

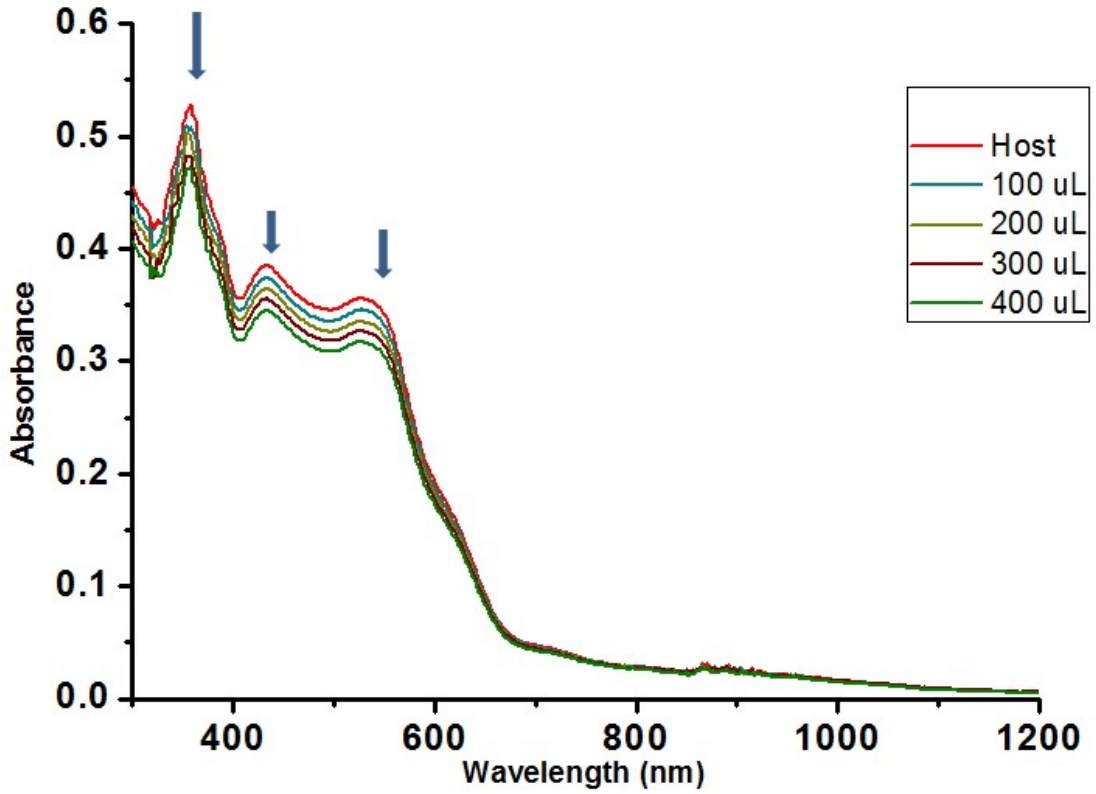


Fig. S8 Absorption spectra of **6** (2 x 10^{-5} M) upon addition of $TBAClO_4$ (0.7 M) in $CHCl_3$

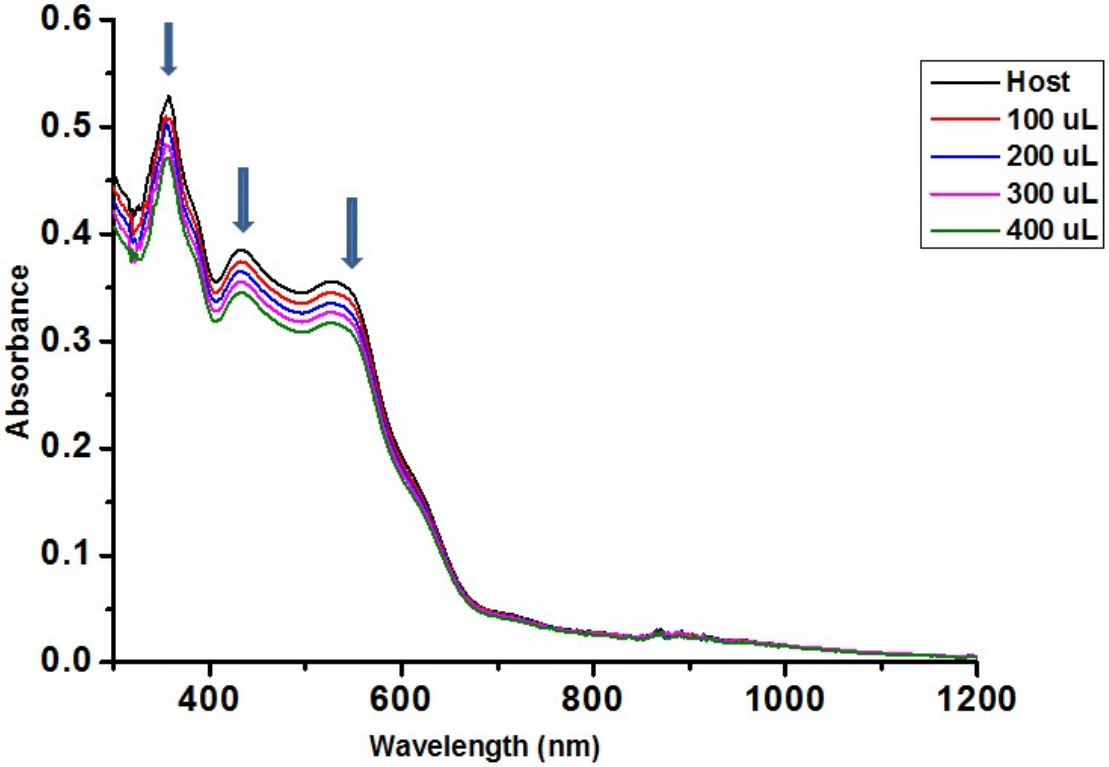


Fig. S9 Absorption spectra of **6** (2 x 10^{-5} M) upon addition of $TBAPF_6$ (0.7 M) in $CHCl_3$

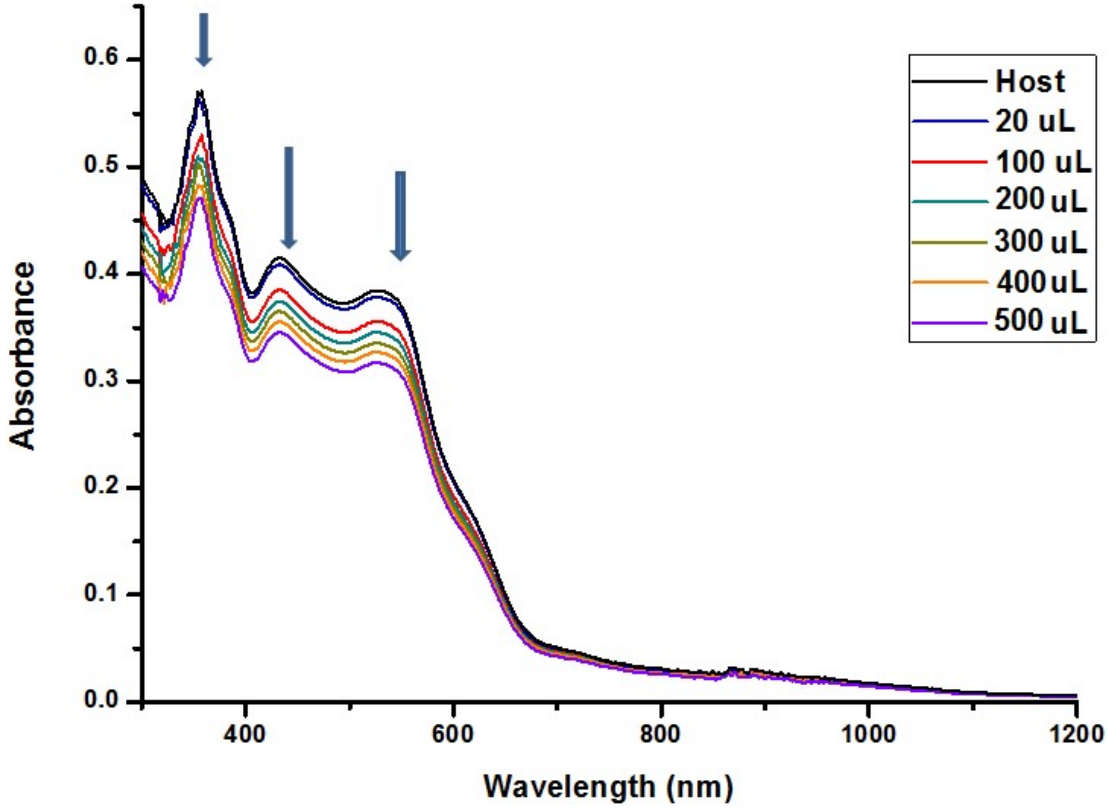


Fig. S10 Absorption spectra of **6** (2 x 10^{-5} M) upon addition of TBACl (0.7 M) in $CHCl_3$

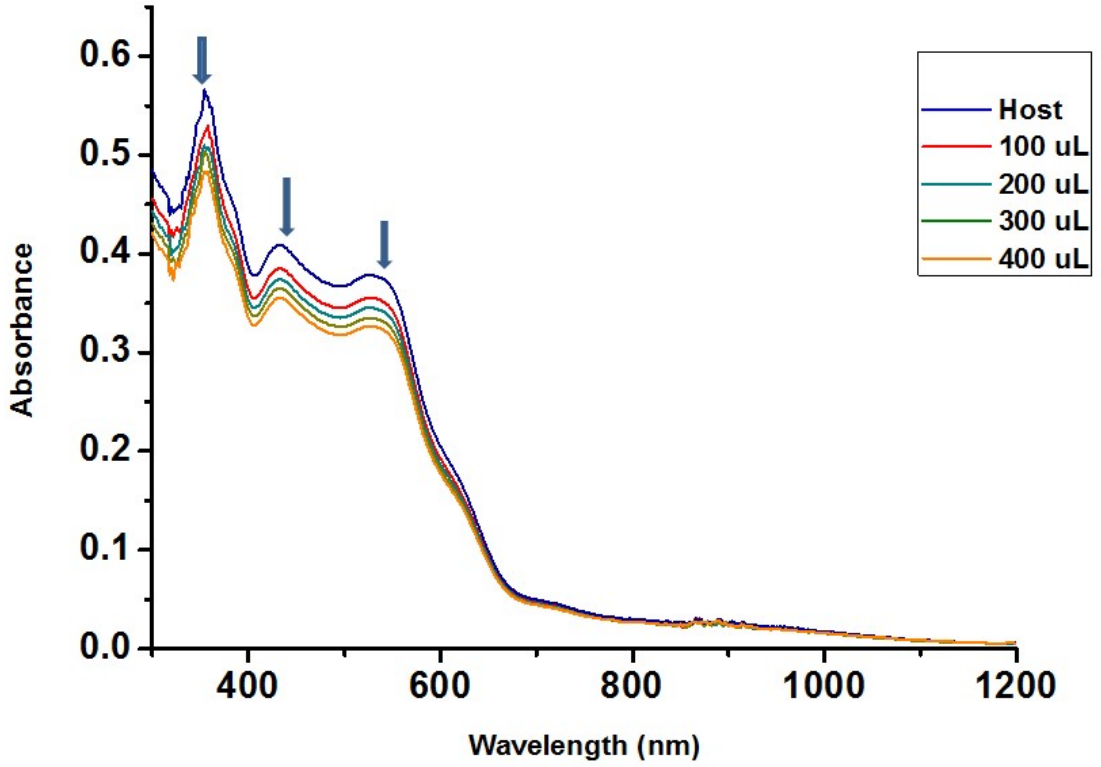


Fig. S11 Absorption spectra of **6** (2 x 10^{-5} M) upon addition of TBABr (0.7 M) in $CHCl_3$

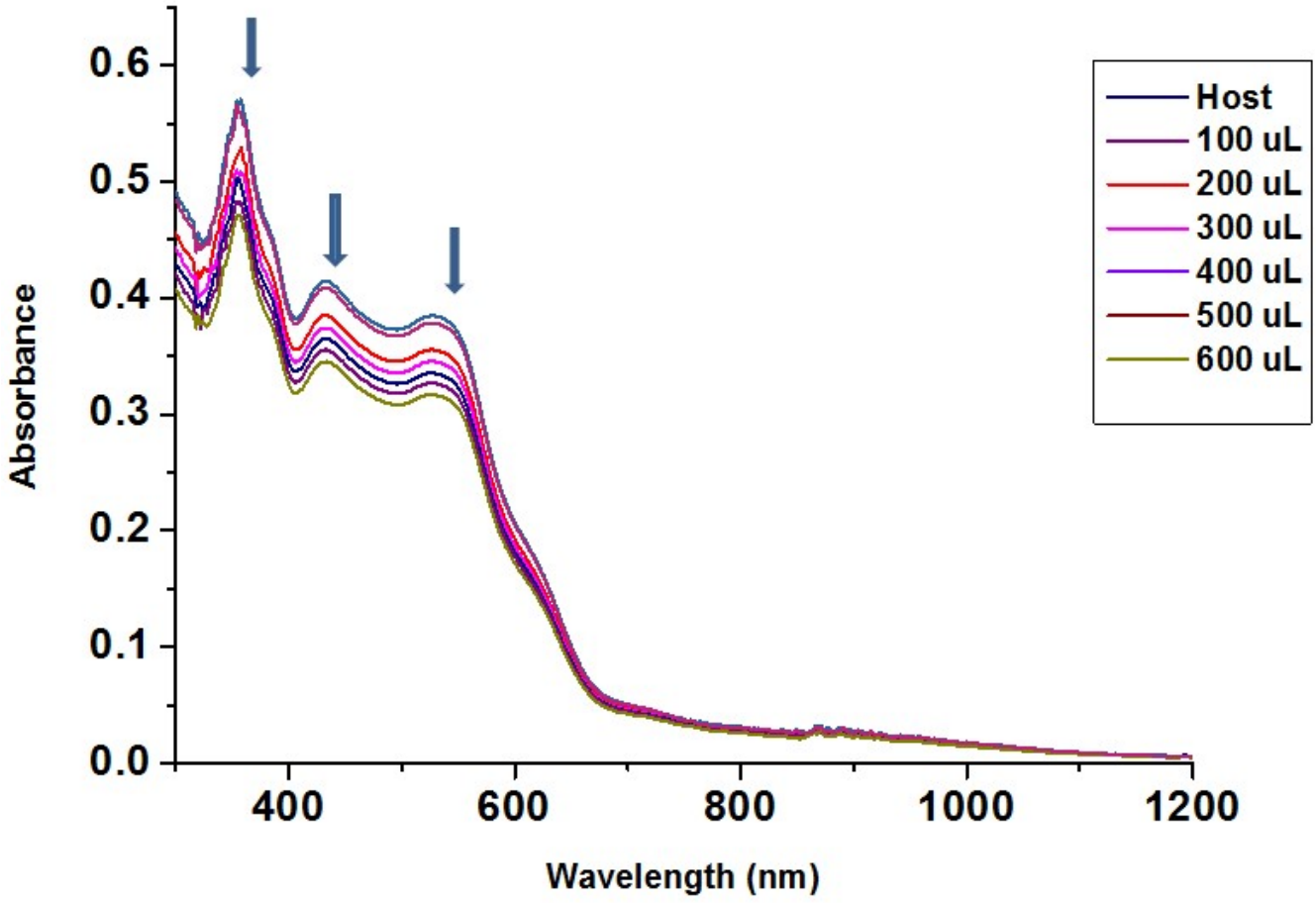


Fig. S12 Absorption spectra of **6** (2 x 10^{-5} M) upon addition of TBAI (0.7 M) in $CHCl_3$

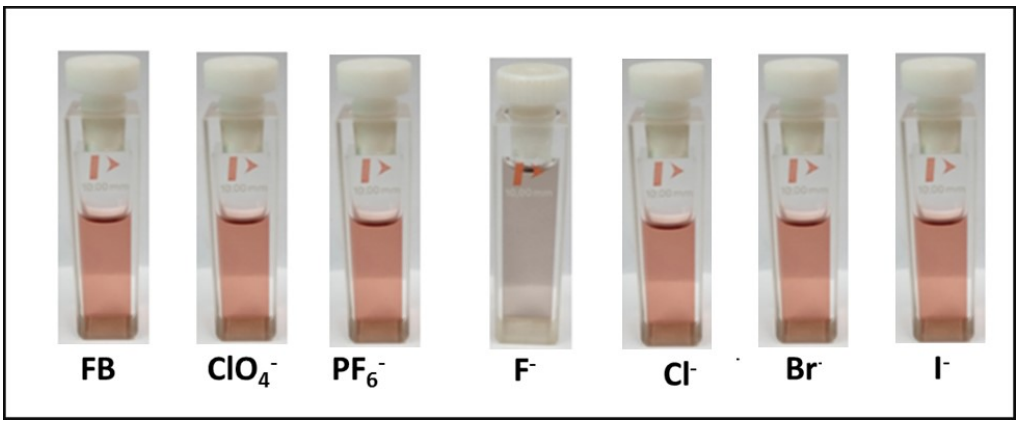


Fig. S13 Color Change induced upon addition of anions (excess equiv as the Bu_4N^+ salt) to receptor **6** in $CHCl_3$ at 298 K

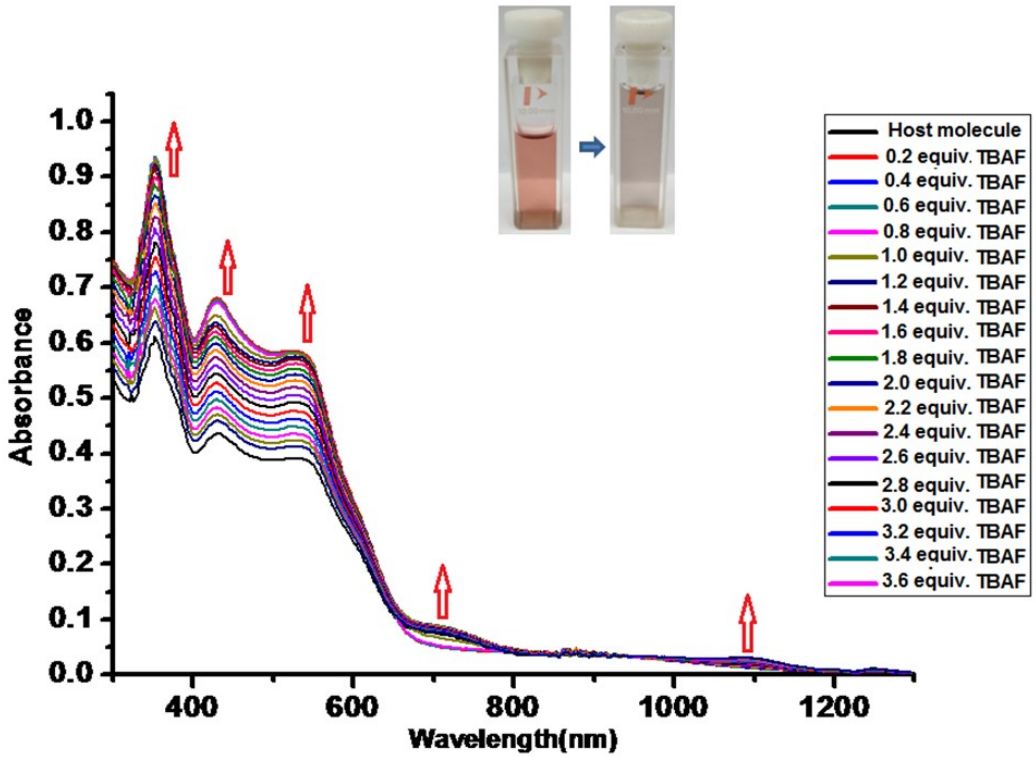


Fig. S14 Absorption spectra of **6** (2.6 x 10^{-5} M) upon addition of TBAF (0.007 M) in $CHCl_3$

2.3 IR spectra:

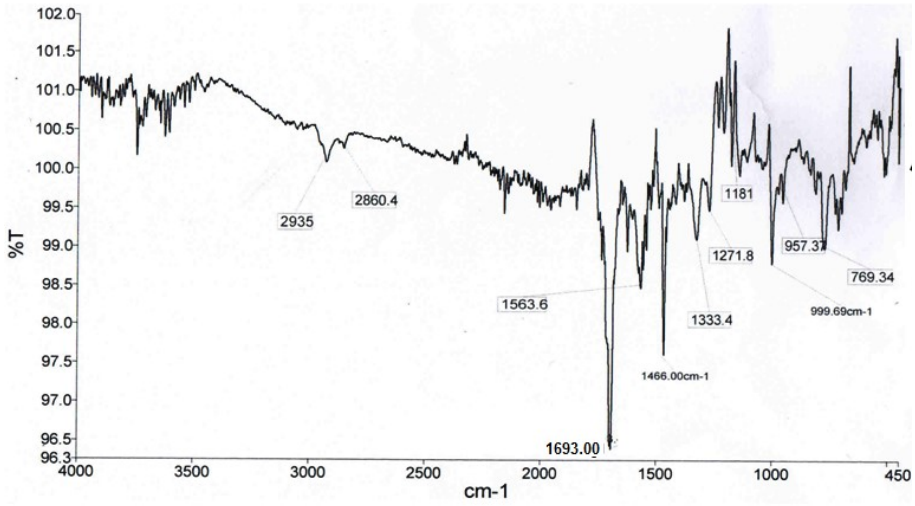


Fig. S15 IR Spectrum of **5**

2.4 NMR spectra:

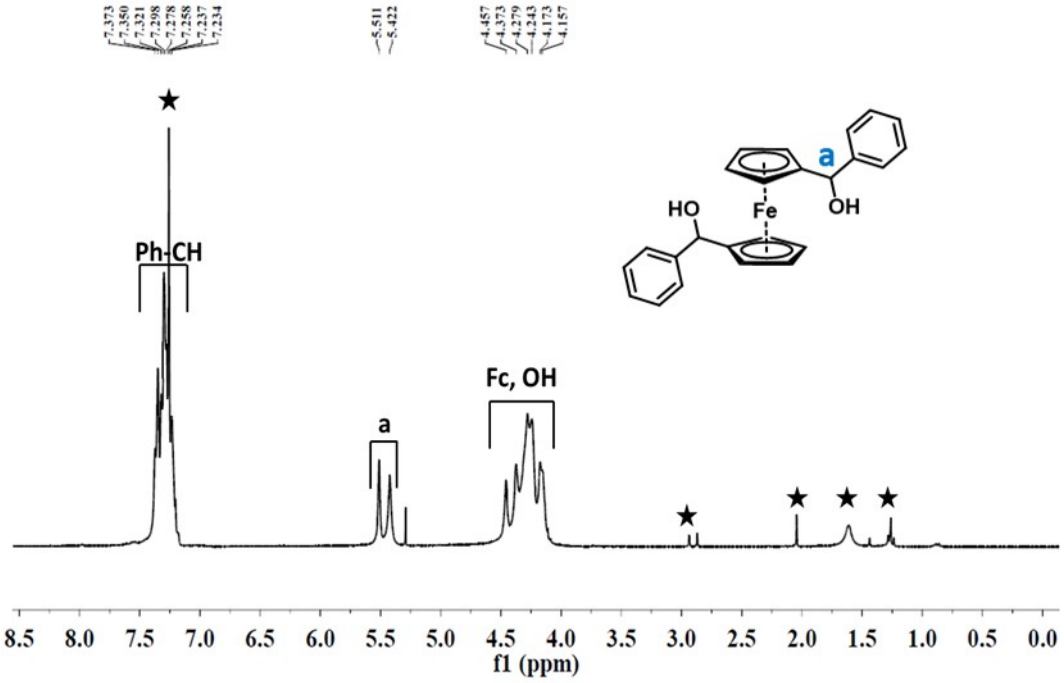


Fig. S16 ^{1}H NMR spectra of **1** in $CDCl_3$ at 298 K

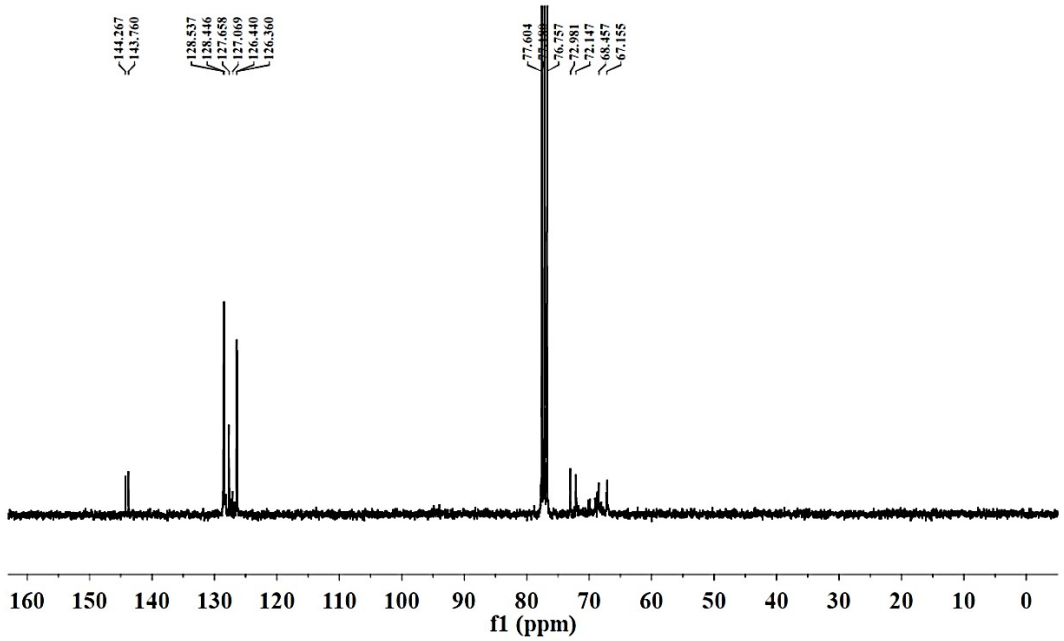


Fig. S17 ^{13}C NMR spectra of **1** in $CDCl_3$ at 298 K

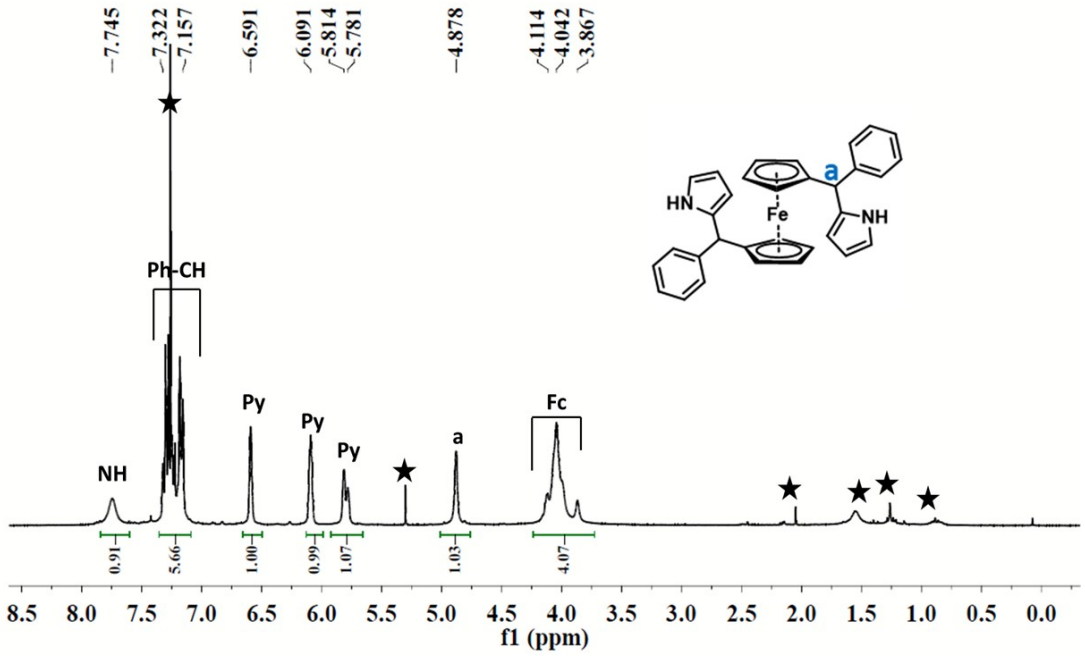


Fig. S18 ^{1}H NMR spectra of **2** in $CDCl_3$ at 298 K

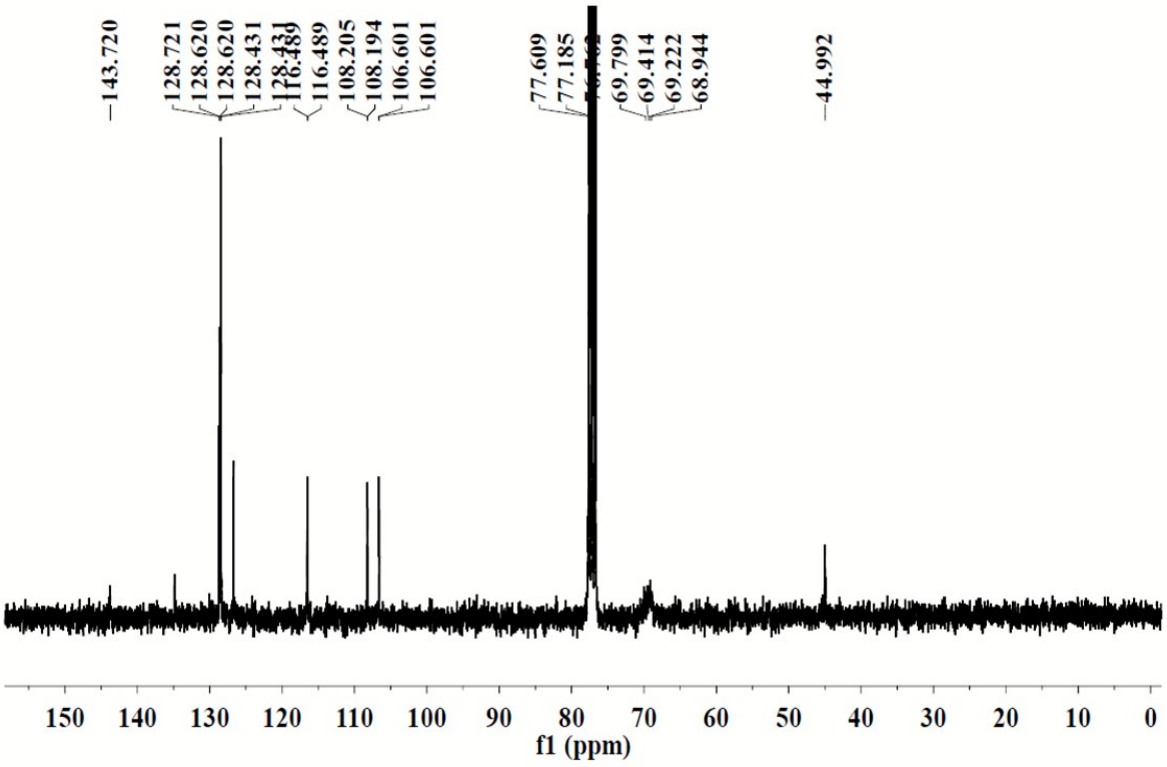


Fig. S19 ^{13}C NMR spectra of **2** in $CDCl_3$ at 298 K

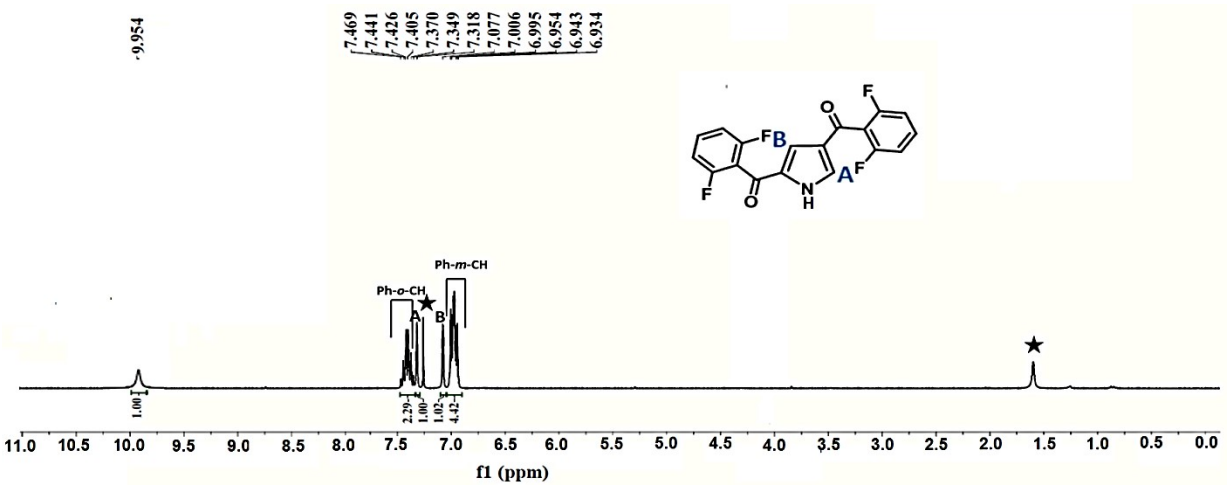


Fig. S20 ^{1}H NMR spectra of **3** in $CDCl_3$ at 298 K

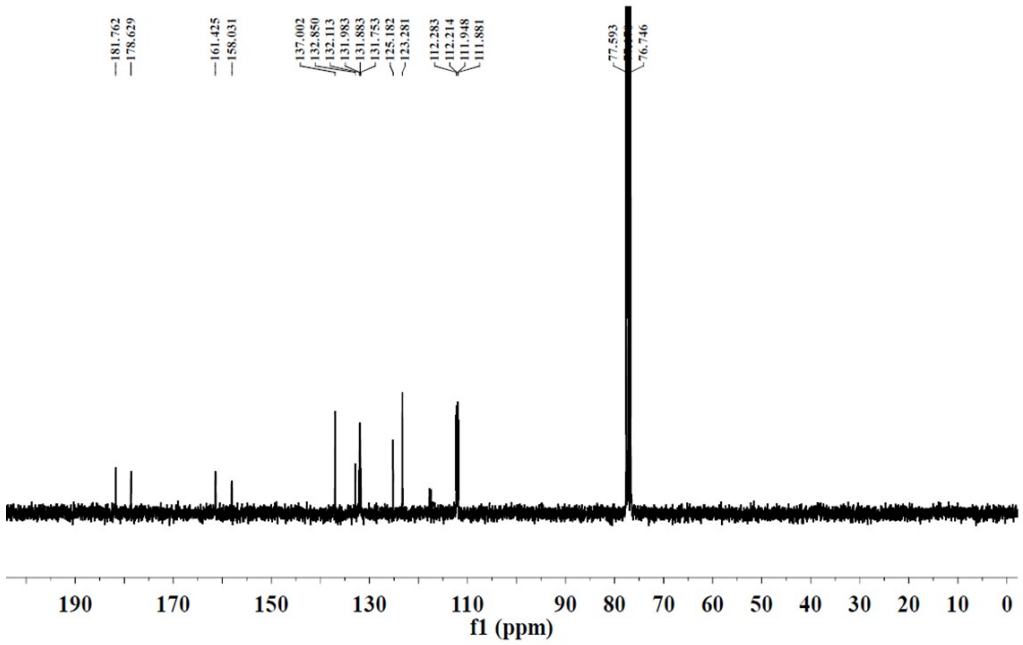


Fig. S21 ^{13}CNMR spectra of **3** in $CDCl_3$ at 298 K

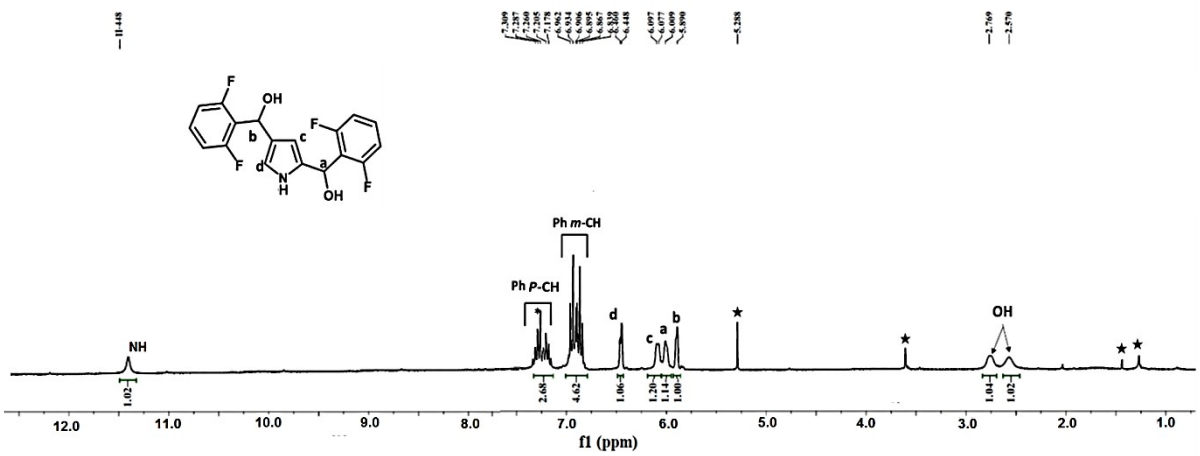


Fig. S22 ^{1}H NMR spectra of **4** in $CDCl_3$ at 298 K

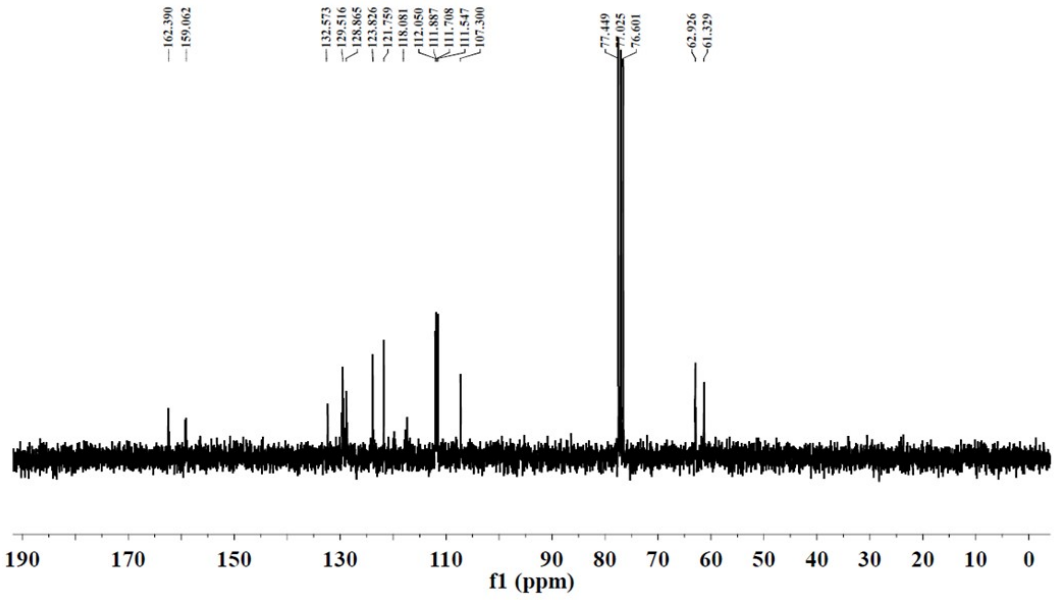


Fig. S23 ^{13}C NMR spectra of **4** in $CDCl_3$ at 298 K

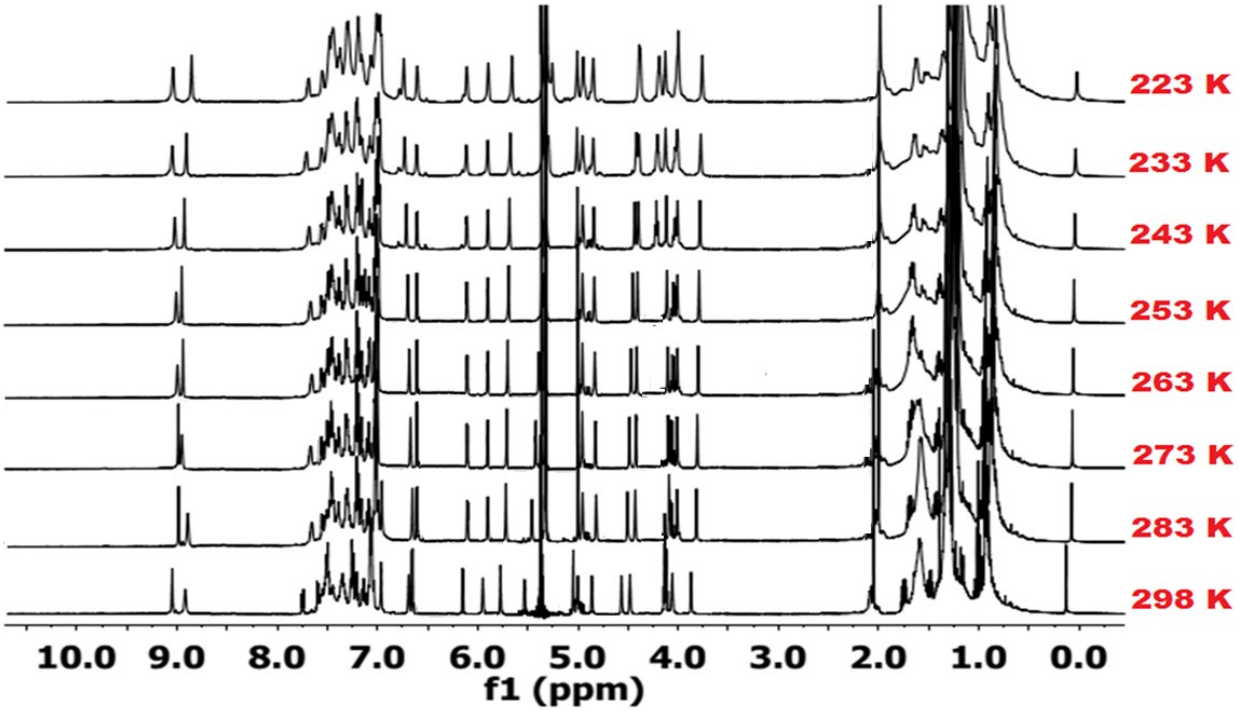
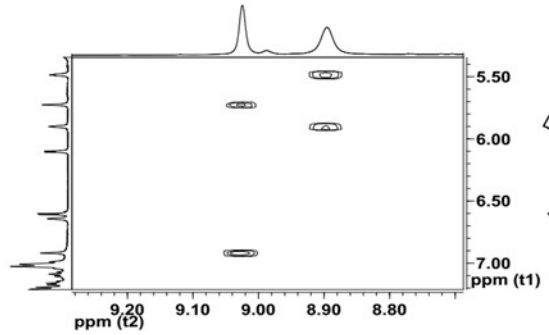
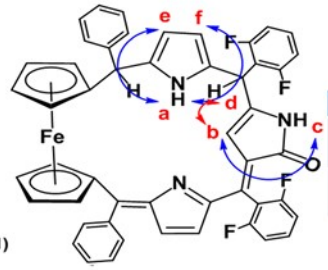


Fig. S24 Low VT ^{1}H NMR spectra of **5** in CD_2Cl_2





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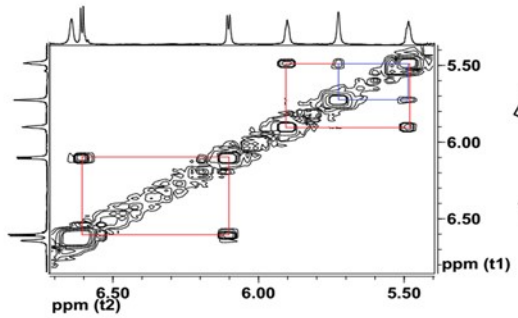
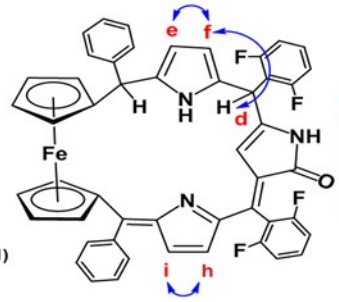
b	9.02	c d	6.92 5.72





Position	^{1}H-NMR	Position	^{1}H-NMR
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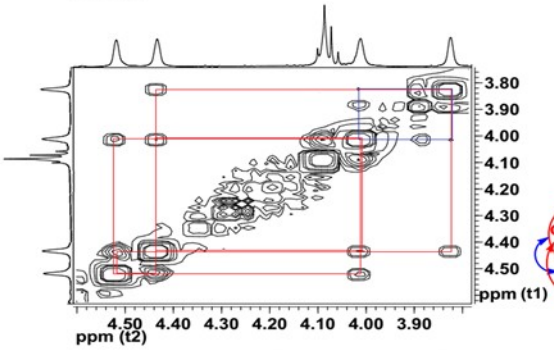
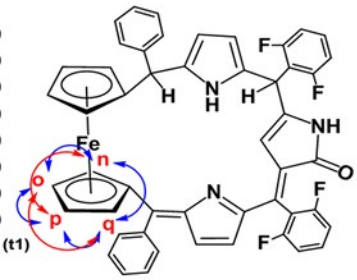
f	5.47	d	5.72
i	6.60	h	6.11





Position	^{1}H-NMR	Position	^{1}H-NMR
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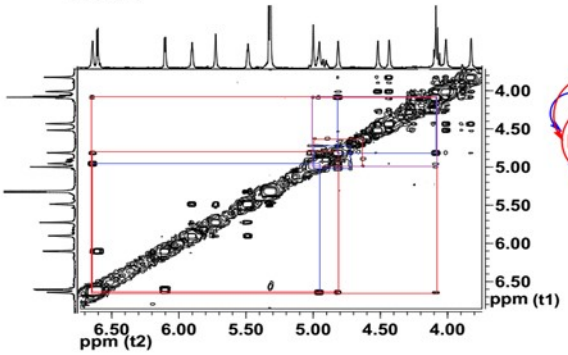
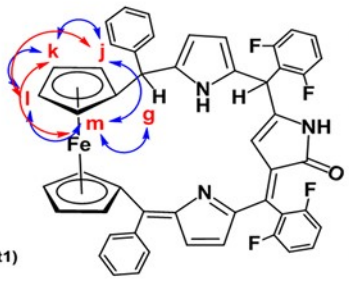
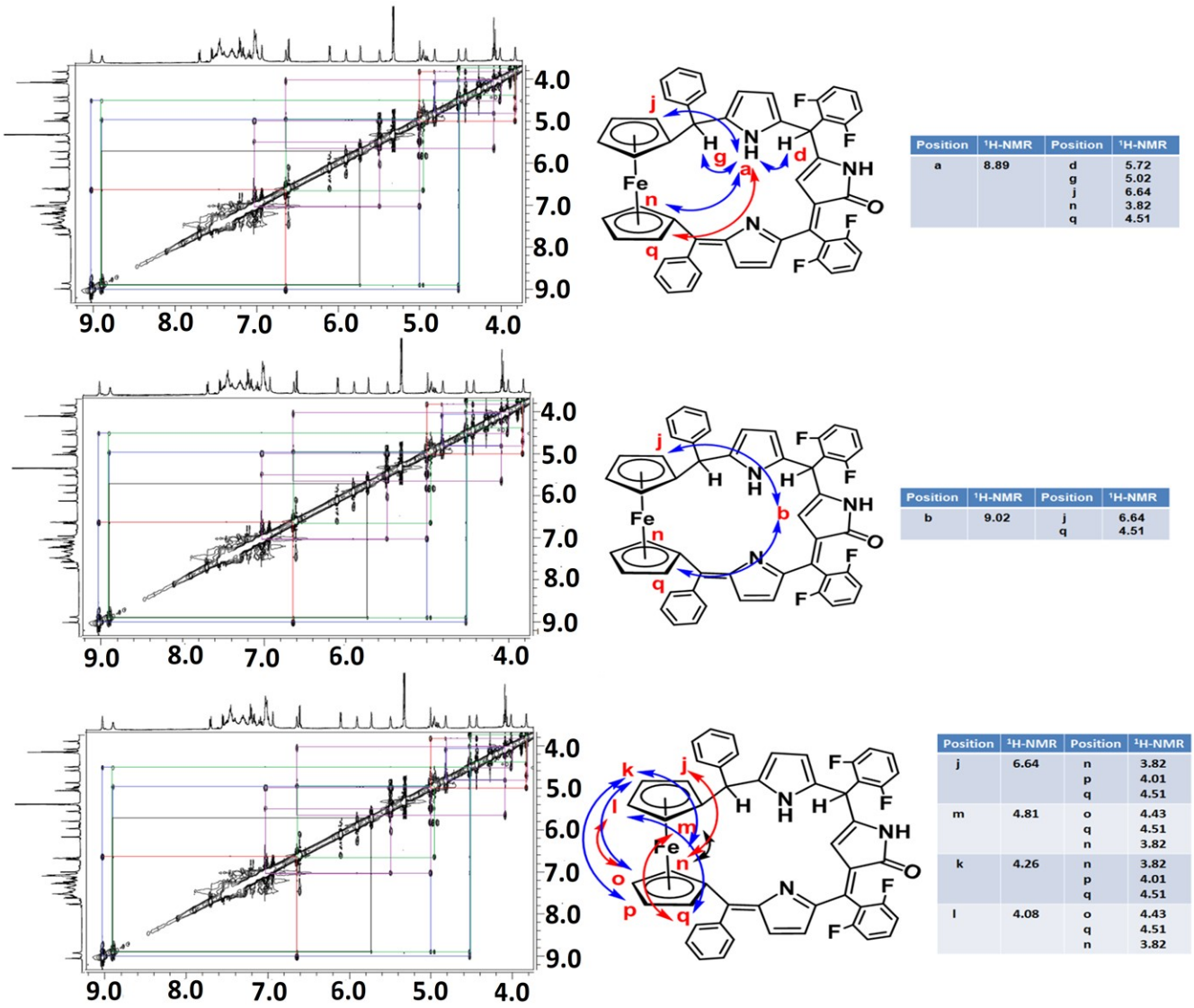
p	4.01	o q n	4.43 4.51 3.82
n	3.82	q	4.51





Position	^{1}H-NMR	Position	^{1}H-NMR
g	5.02	j m	6.64 4.81
j	6.64	m l g	4.81 4.08 5.02
m	4.81	l j	4.08 6.64
k	4.26	l	4.08

Fig. S25 ^{1}H -^{1}H 2D COSY NMR spectra of **5** in CD_2Cl_2 at 298 K



Position	^{1}H-NMR	Position	^{1}H-NMR
a	8.89	d	5.72
		g	5.02
		j	6.64
		n	3.82
		q	4.51

Position	^{1}H-NMR	Position	^{1}H-NMR
b	9.02	j	6.64
		q	4.51

Position	^{1}H-NMR	Position	^{1}H-NMR
j	6.64	n	3.82
		p	4.01
		q	4.51
m	4.81	o	4.43
		q	4.51
		n	3.82
k	4.26	n	3.82
		p	4.01
		q	4.51
l	4.08	o	4.43
		q	4.51
		n	3.82

Fig. S26 ^{1}H -^{1}H 2D ROESY NMR spectra of **5** in CD_2Cl_2 at 298 K

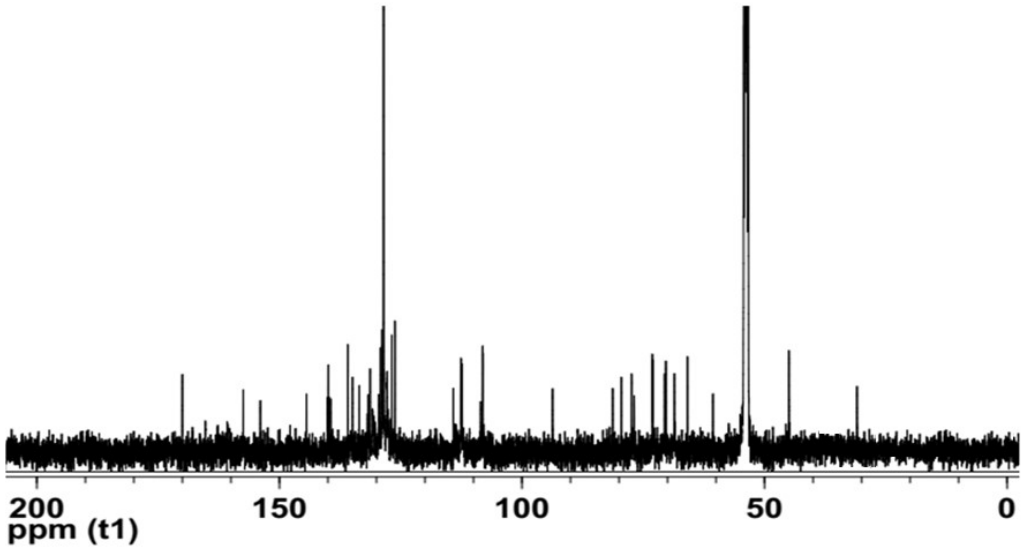
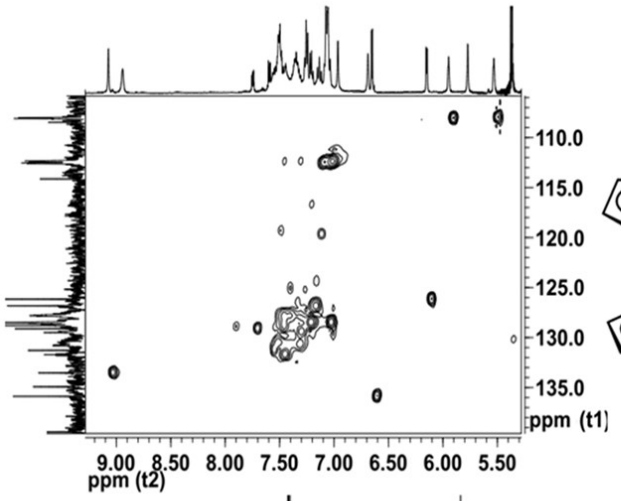
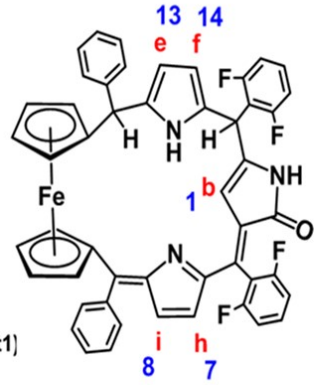
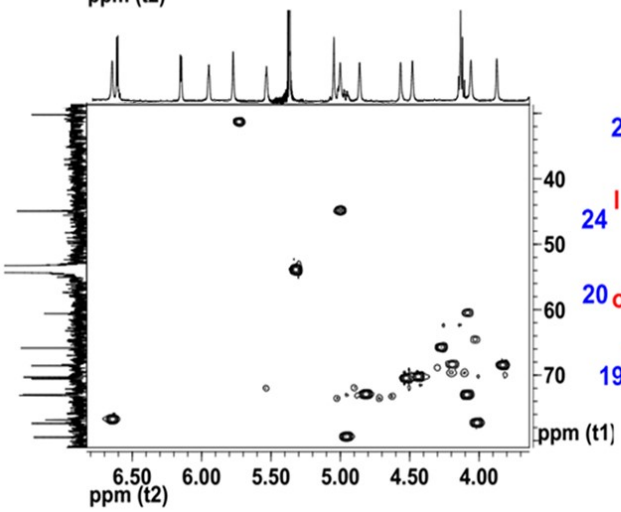


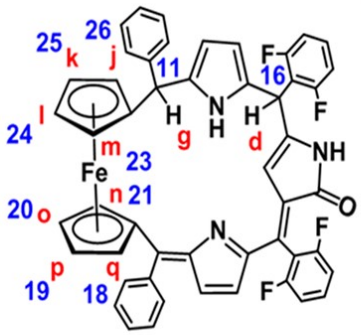
Fig. S27 ^{13}C NMR spectra of **5** in CD_2Cl_2 at 298 K





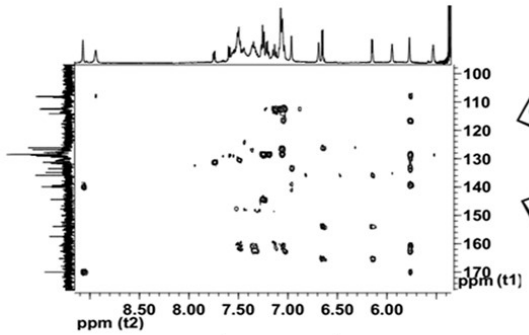
Position	^{1}H-NMR	Position	^{13}C-NMR
b	9.02	1	133.50
e	5.90	13	108.01
f	5.47	14	107.88
h	6.11	7	126.03
i	6.60	8	135.89

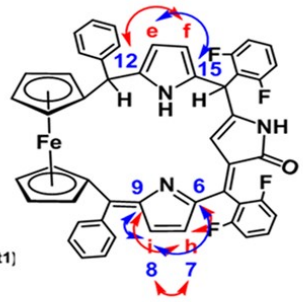




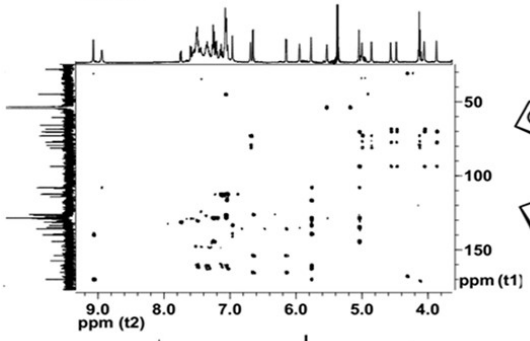
Position	^{1}H-NMR	Position	^{13}C-NMR
d	5.72	16	31.28
g	5.02	11	44.89
j	6.64	26	76.70
k	4.95	25	79.38
l	4.08	24	72.65
m	4.81	23	72.80
n	3.82	21	68.49
o	4.43	20	70.13
p	4.01	19	77.40
q	4.51	18	70.43

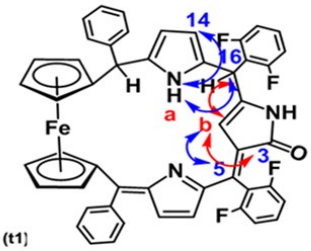
Fig. S28 HSQC NMR spectra of **5** in CD_2Cl_2 at 298 K



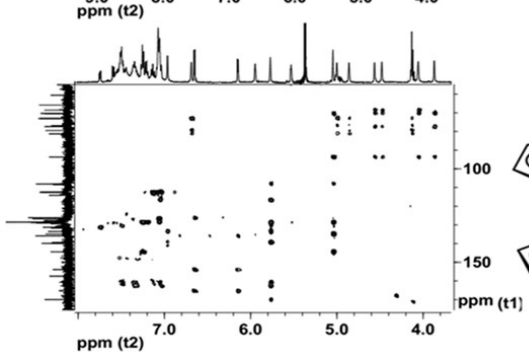


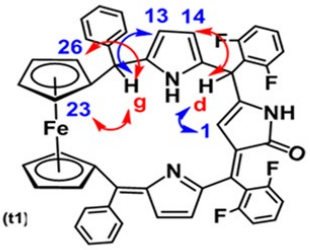
Position	^{1}H-NMR	Position	^{13}C-NMR
e	5.90	15	135.04
f	5.47	12	128.63
i	6.60	6	153.91
		7	126.03
		9	165.27
h	6.11	6	153.91
		8	135.89
		9	165.27



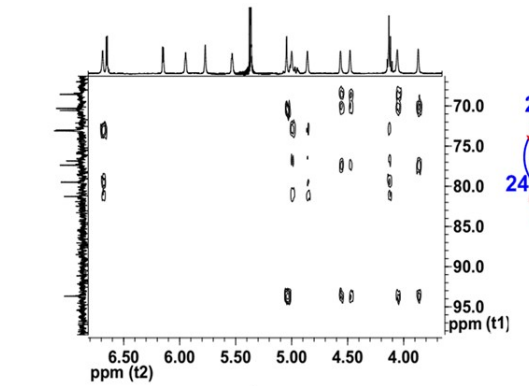


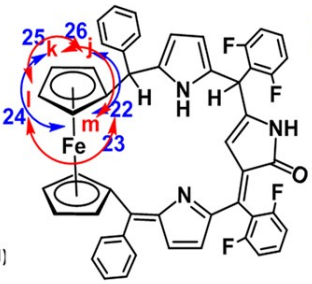
Position	^{1}H-NMR	Position	^{13}C-NMR
b	9.02	3	169.86
		16	31.28
		5	140.23
a	8.89	16	31.28
		14	107.88



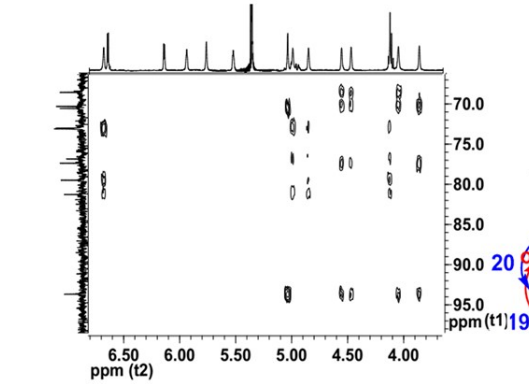


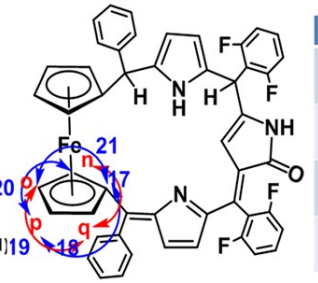
Position	^{1}H-NMR	Position	^{13}C-NMR
d	5.72	14	107.88
		1	133.50
g	5.02	13	108.01
		26	76.70
		23	72.80





Position	^{1}H-NMR	Position	^{13}C-NMR
j	6.64	24	72.65
		23	72.80
k	4.95	23	72.80
		22	93.81
l	4.08	26	76.70
		22	93.81
m	4.81	25	79.38
		26	76.70





Position	^{1}H-NMR	Position	^{13}C-NMR
n	3.82	18	70.43
		19	77.40
o	4.43	18	70.43
		17	81.90
p	4.01	17	81.90
		21	68.49
q	4.51	21	68.49
		20	70.13

Fig. S29 HMBC NMR spectra of **5** in CD_2Cl_2 at 298 K

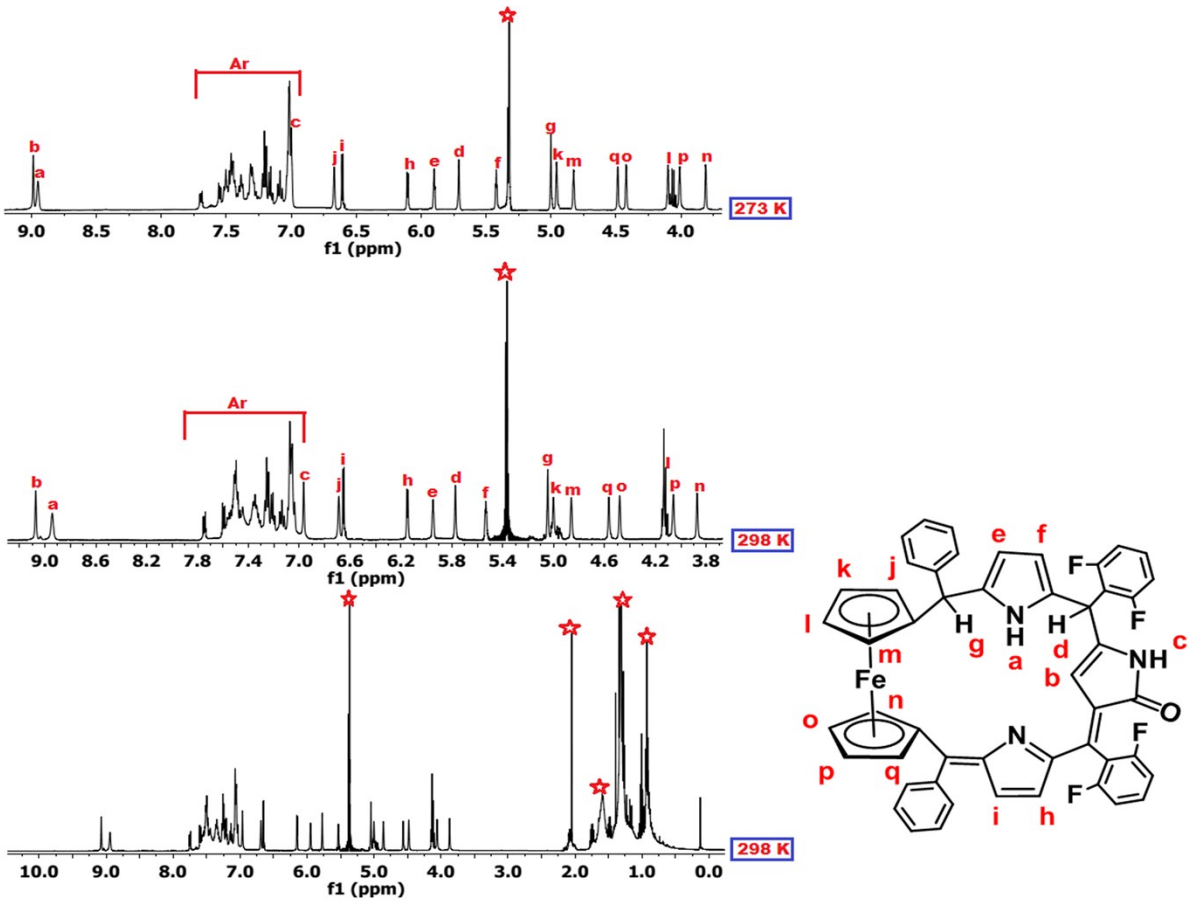


Fig. S30 Complete ^{1}H NMR spectral assignment of **5** in CD_2Cl_2 at 298 K

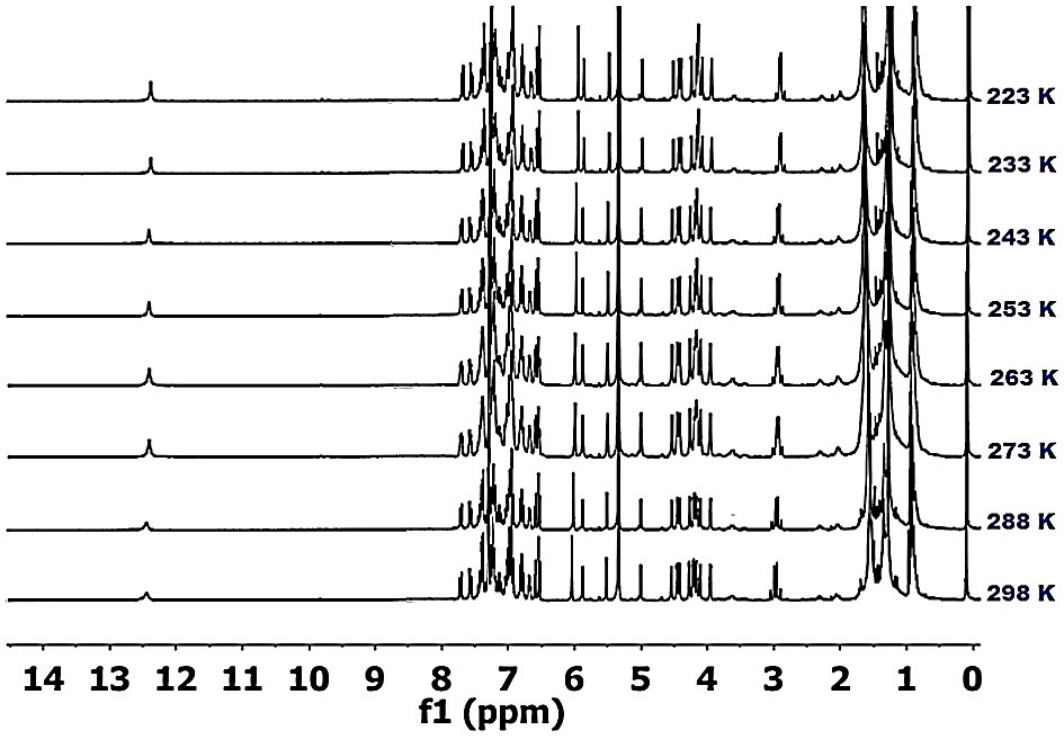
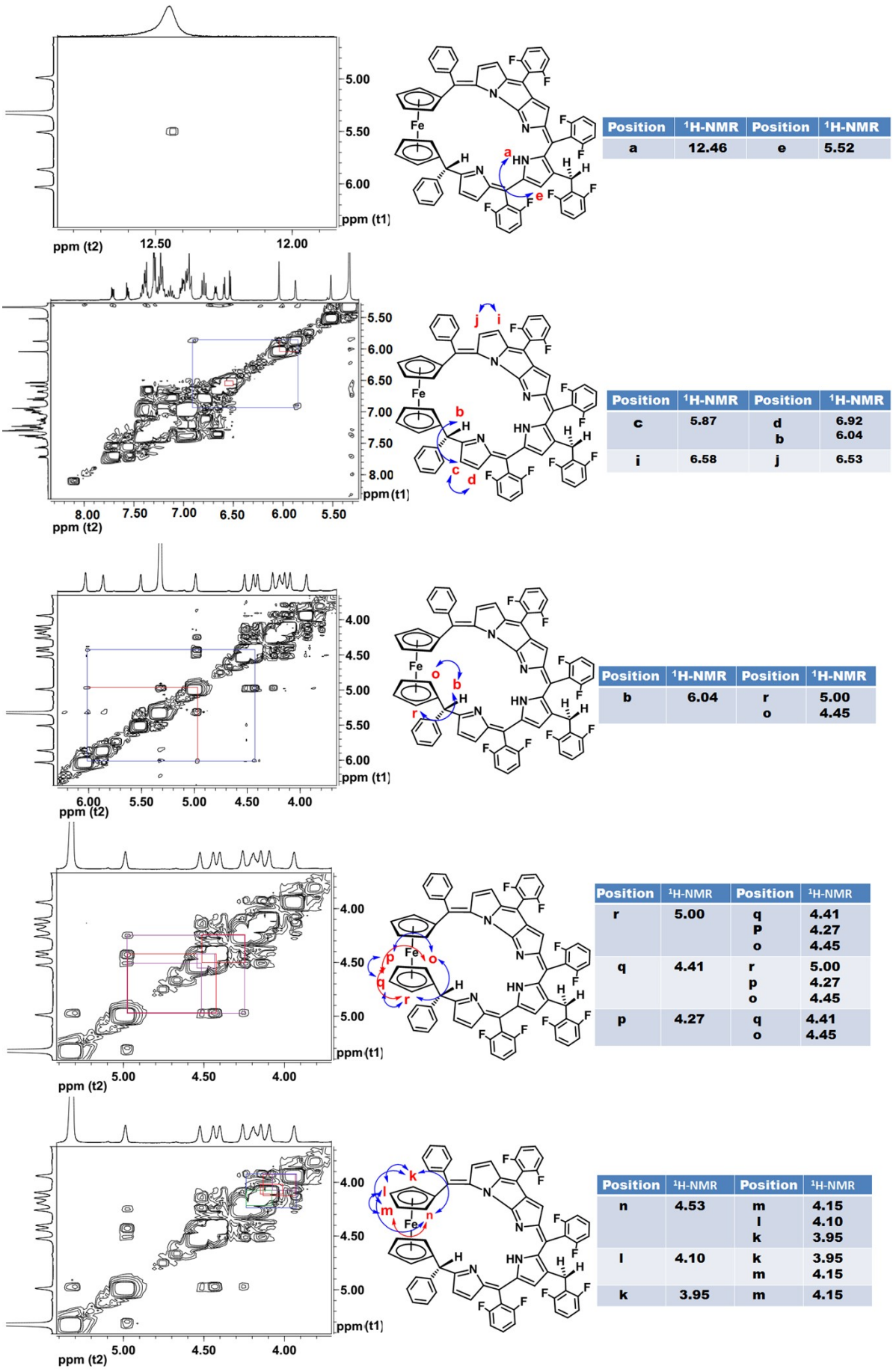


Fig. S31 Low VT ^{1}H NMR spectra of **6** in CD_2Cl_2



Position	^{1}H-NMR	Position	^{1}H-NMR
a	12.46	e	5.52

Position	^{1}H-NMR	Position	^{1}H-NMR
c	5.87	d b	6.92 6.04
i	6.58	j	6.53

Position	^{1}H-NMR	Position	^{1}H-NMR
b	6.04	r o	5.00 4.45

Position	^{1}H-NMR	Position	^{1}H-NMR
r	5.00	q P o	4.41 4.27 4.45
q	4.41	r p o	5.00 4.27 4.45
p	4.27	q o	4.41 4.45

Position	^{1}H-NMR	Position	^{1}H-NMR
n	4.53	m l k	4.15 4.10 3.95
l	4.10	k m	3.95 4.15
k	3.95	m	4.15

Fig. S32 ^{1}H -^{1}H 2D COSY NMR spectra of **6** in CD_2Cl_2 at 298 K

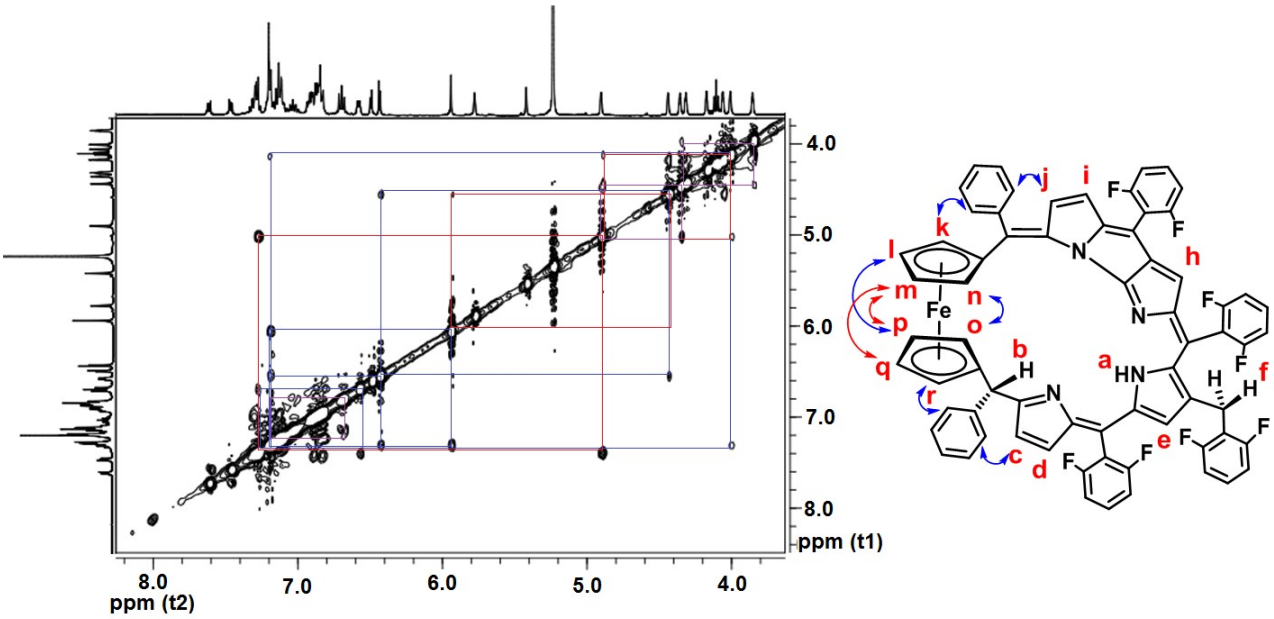


Fig. S33 ^{1}H -^{1}H 2D ROESY NMR spectra of **6** in CD_2Cl_2 at 298 K

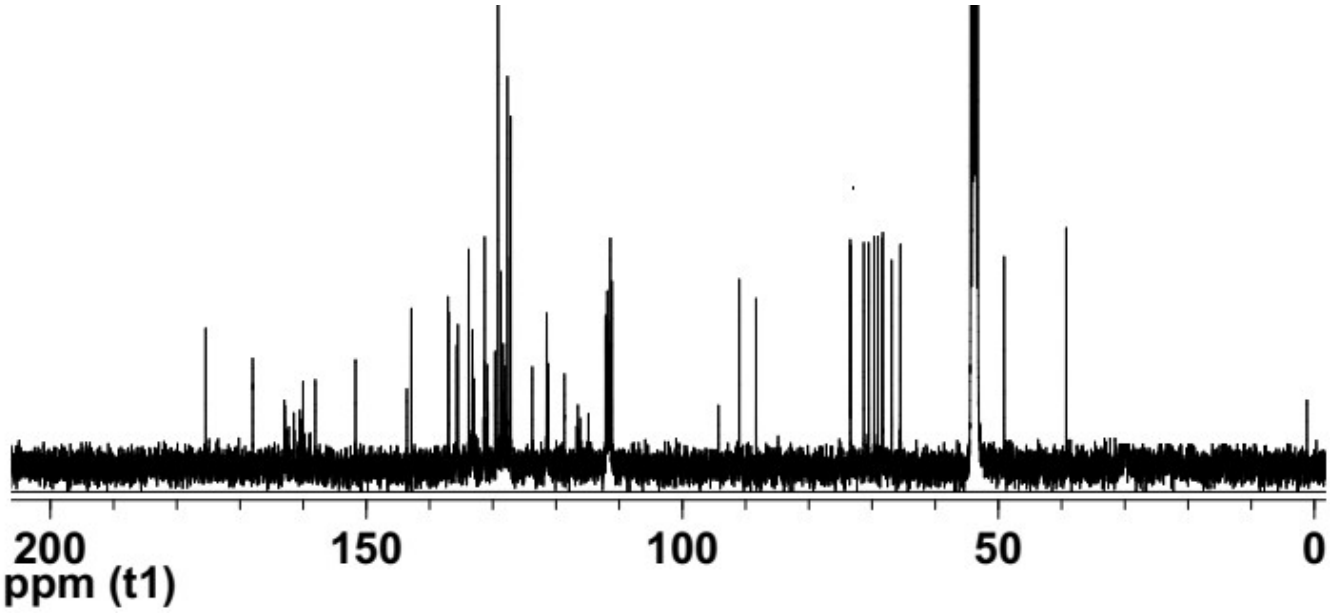
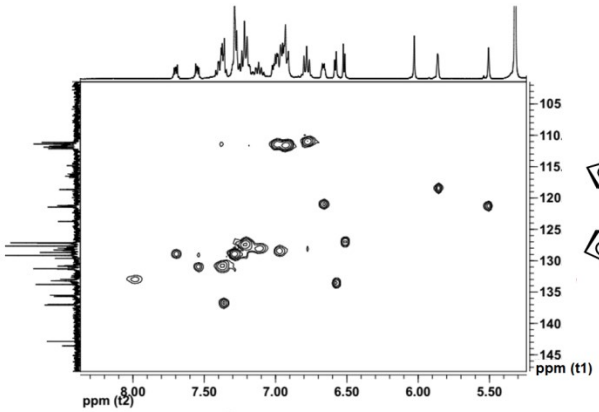
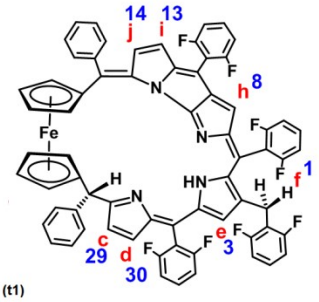
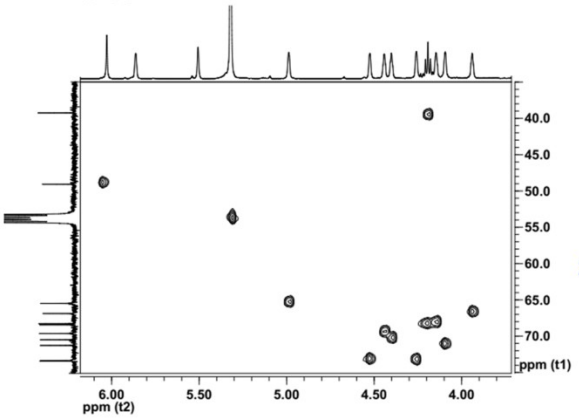


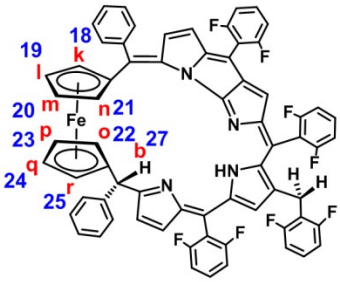
Fig. S34 ^{13}C NMR spectrum of **6** in CD_2Cl_2 at 298 K





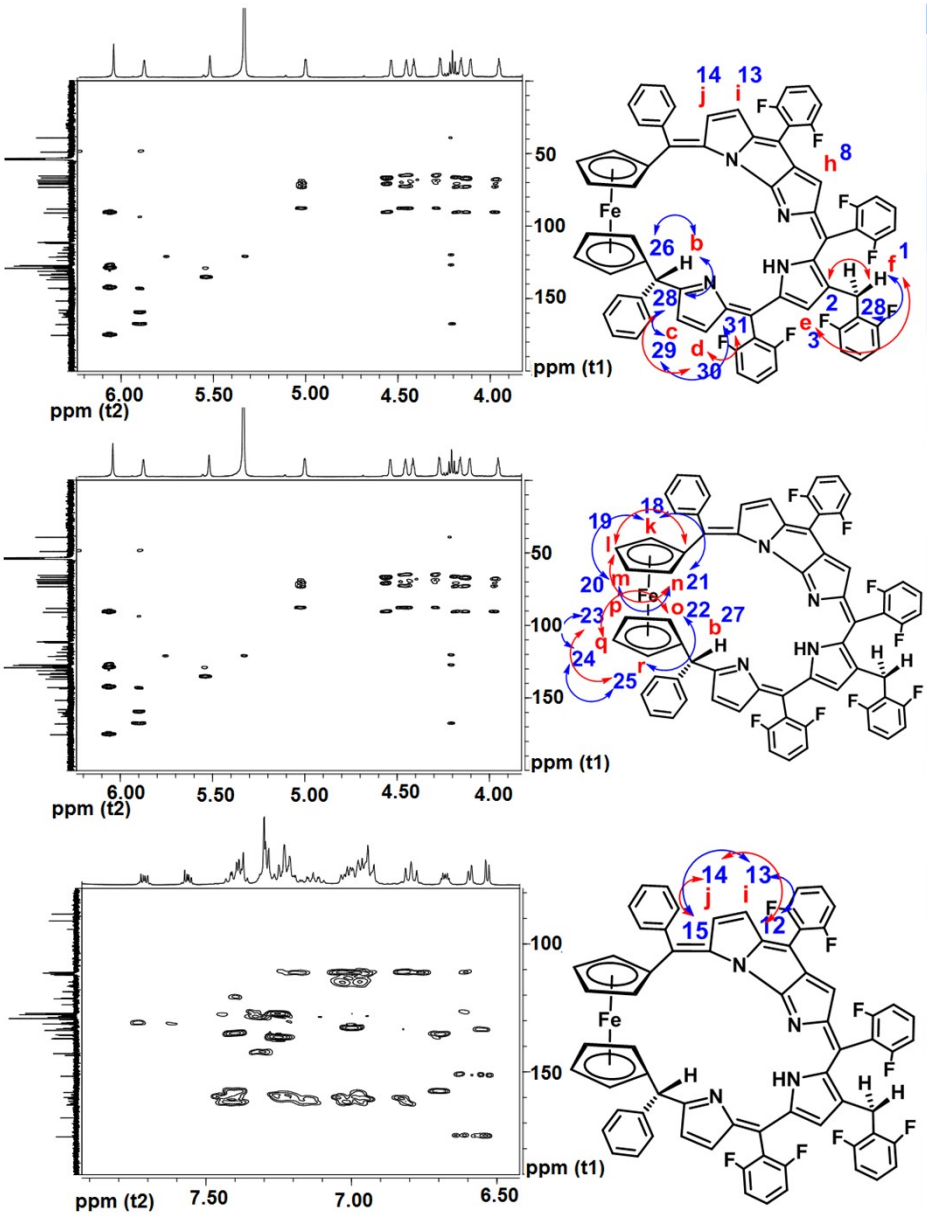
Position	^{1}H-NMR	Position	^{13}C-NMR
a	12.46	-	-
c	5.87	29	118.37
d	6.92	30	111.51
e	5.52	3	121.26
h	6.77	8	110.92
i	6.58	13	133.60
j	6.53	14	127.13





Position	^{1}H-NMR	Position	^{13}C-NMR
f	4.21	1	39.22
b	6.041	27	49.07
r	5.00	25	65.18
q	4.415	24	69.23
p	4.456	23	70.13
o	4.275	22	73.11
n	4.537	21	73.02
m	4.158	20	67.92
l	4.106	19	71.04
k	3.954	18	66.50

Fig. S35 HSQC NMR spectra of **6** in CD_2Cl_2 at 298 K



Position	^{1}H-NMR	Position	^{13}C-NMR
b	6.04	26 28	88.33 129.16
c	5.87	28 30 31	129.16 111.51 137.97
d	5.87	28 29 31	129.16 118.37 137.97
f	4.21	2 3 28	126.41 121.26 167.50

Position	^{1}H-NMR	Position	^{13}C-NMR
r	5.00	24 22 23	69.23 73.11 70.13
q	4.41	25 22 23	65.18 73.11 70.13
p	4.45	22 24 25	73.11 69.23 65.18
o	4.27	23 24 25	70.13 69.23 65.18
n	4.537	19 20 18	71.04 67.92 66.50
m	4.158	19 21 18	71.04 73.02 66.50
l	4.106	20 21 18	67.92 73.02 66.50
k	3.954	20 21 19	67.92 73.02 71.04

Position	^{1}H-NMR	Position	^{13}C-NMR
i	6.58	14 12 15	127.13 175.41 158.06
j	6.53	13 12 15	133.60 175.41 158.06

Fig. S36 HMBC NMR spectra of **6** in CD_2Cl_2 at 298 K

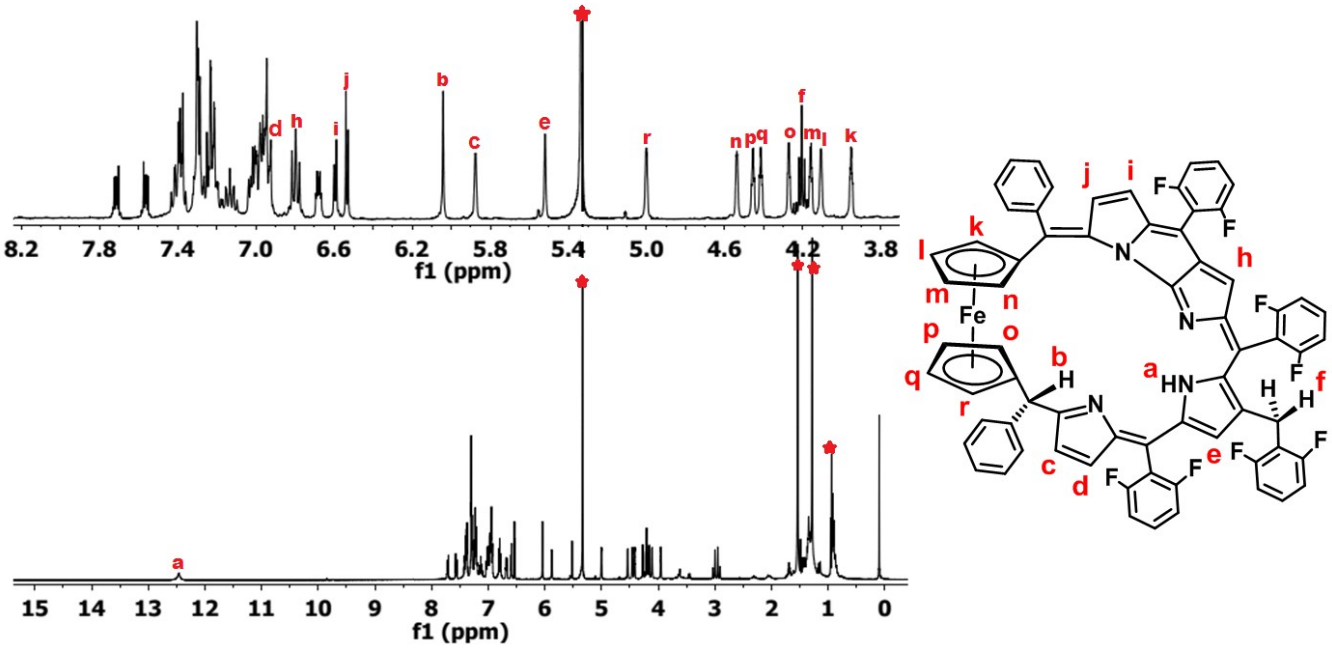


Fig. S37 Complete ^{1}H NMR spectral assignment of **6** in CD_2Cl_2 at 298 K

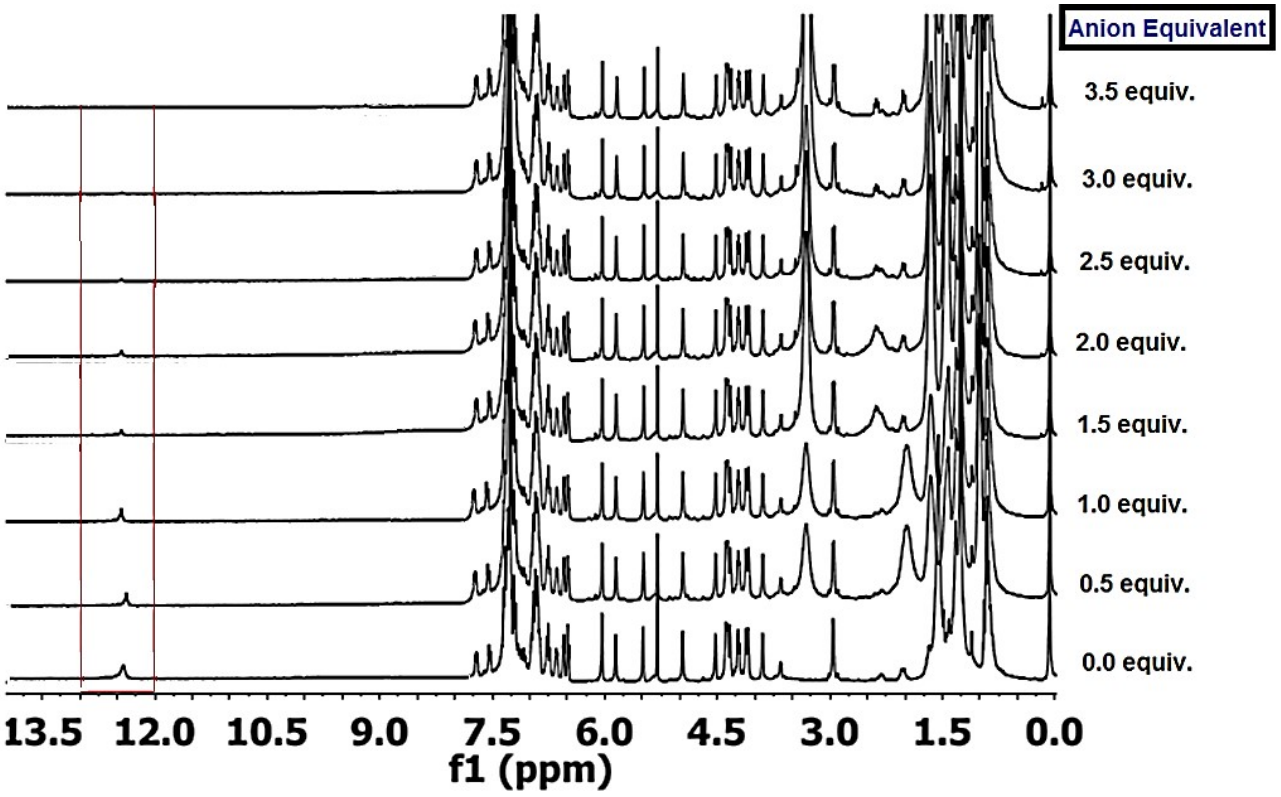


Fig. S38 ^{1}H NMR spectral pattern of **6** upon TBAF titration in $CDCl_3$

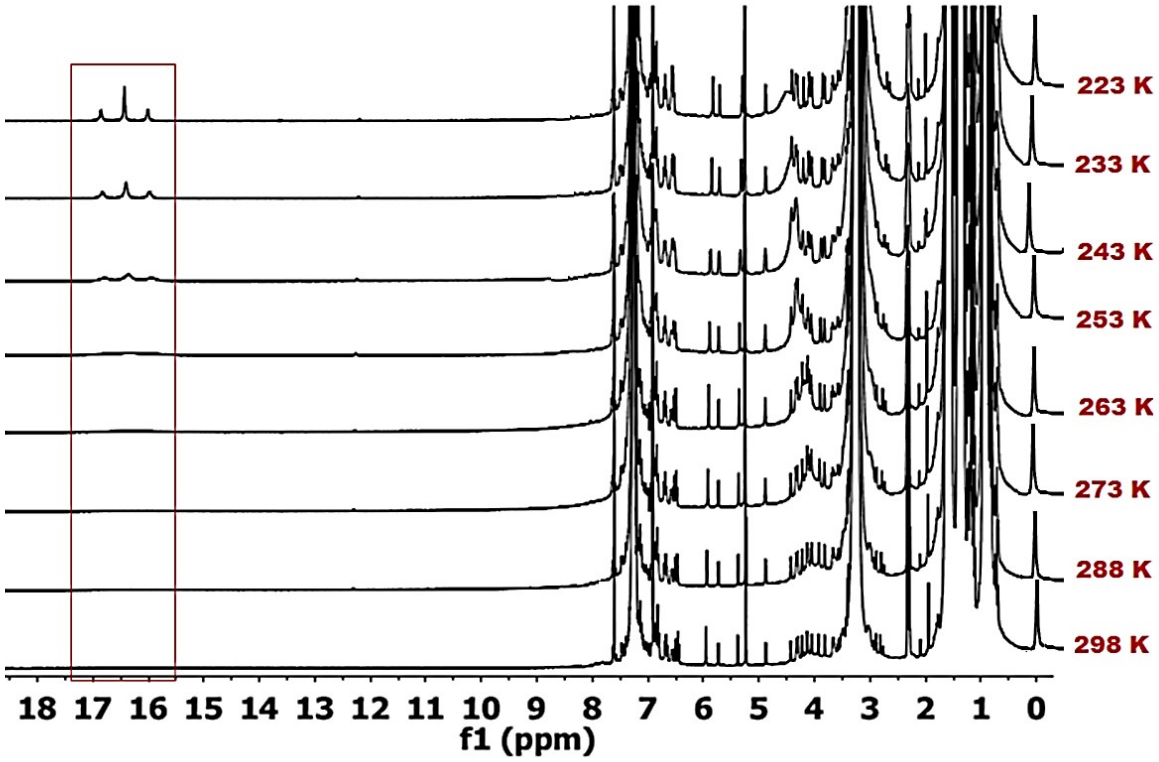


Fig. S39 Low VT ^{1}H NMR spectral pattern of **6** upon TBAF titration in $CDCl_3$

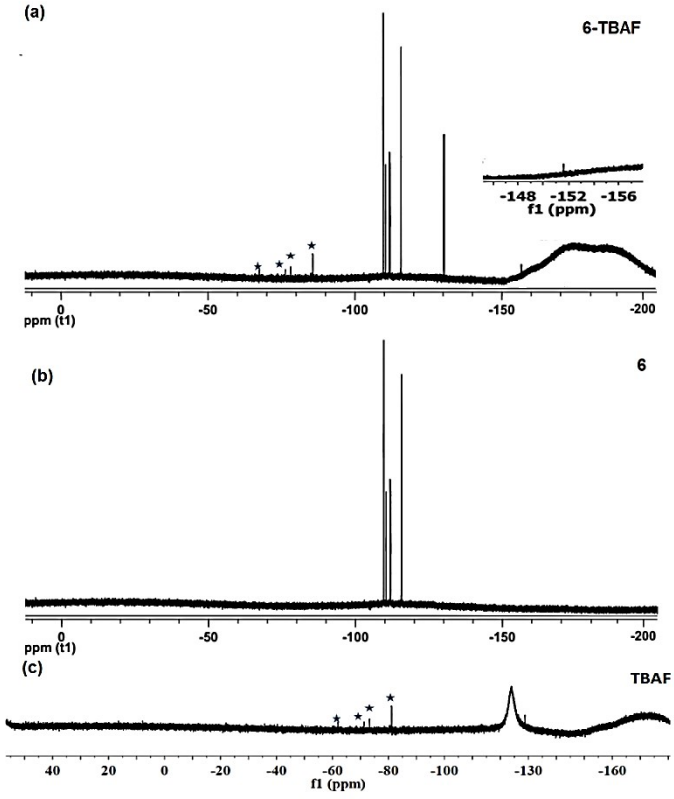


Fig. S40 ^{19}F NMR spectral pattern of (c) TBAF, (b) **6** and (a) **6**-TBAF in $CDCl_3$ at 298 K (* from -80 to -60 ppm correspond to unknown impurities of TBAF)

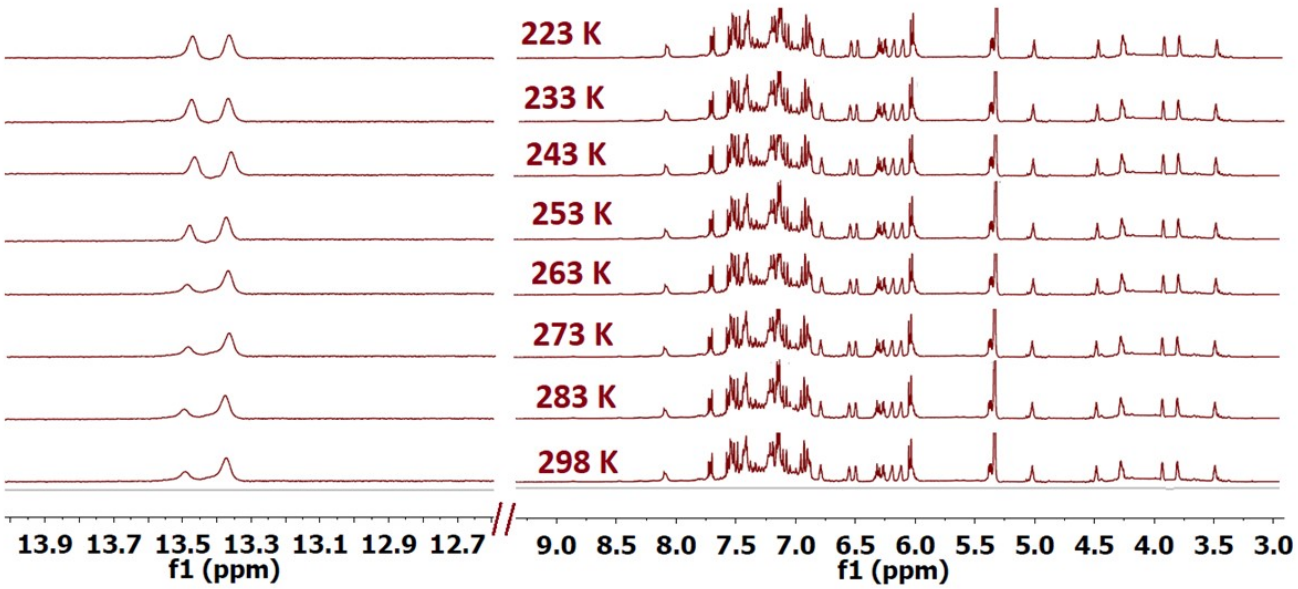
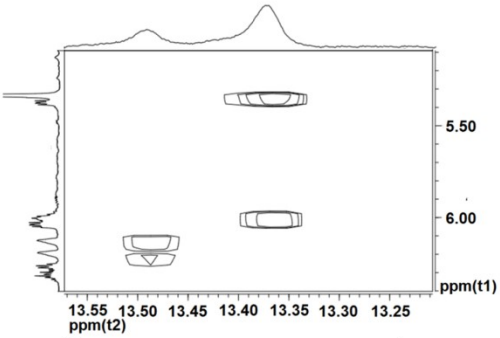
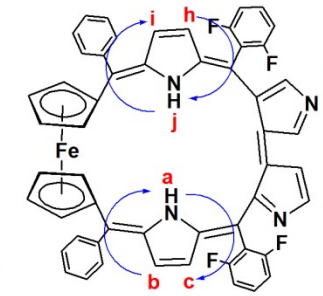
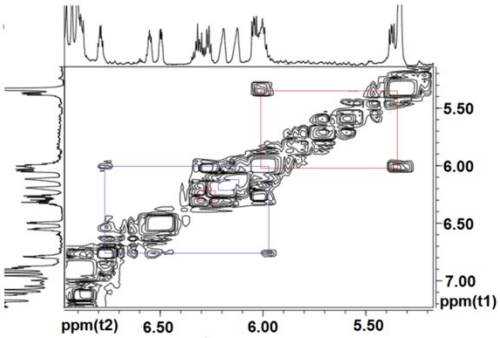


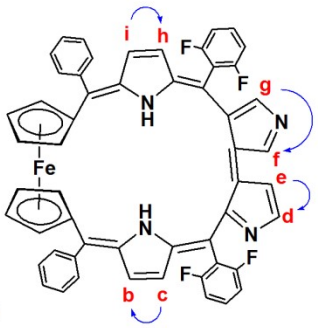
Fig. S41 Variable Low VT ^{1}H NMR spectra of **7** in CD_2Cl_2





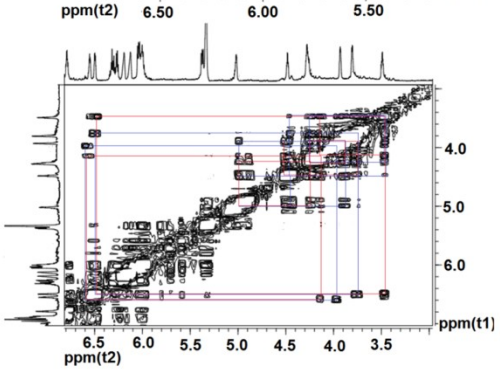
Position	^{1}H-NMR	Position	^{1}H-NMR
a	13.50	b	6.14
		c	6.19
j	13.37	h	6.05
		i	5.38

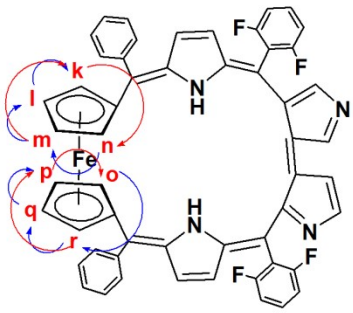




Position	^{1}H-NMR	Position	^{1}H-NMR
b	6.14	c	6.19
h	6.05	i	5.38

Position	^{1}H-NMR	Position	^{1}H-NMR
d	6.26	e	6.32
f	6.79	g	6.00





Position	^{1}H-NMR	Position	^{1}H-NMR
m	4.28	k	5.02
		l	3.49
		n	6.50
l	3.49	k	5.02
		n	6.50
k	5.02	n	6.50

Position	^{1}H-NMR	Position	^{1}H-NMR
p	3.94	o	6.55
		q	3.81
		r	4.48
q	3.81	o	6.55
		r	4.48
r	4.48	o	6.55

Fig. S42 ^{1}H-^{1}H 2D COSY spectra of **7** in CD_2Cl_2 at 298 K

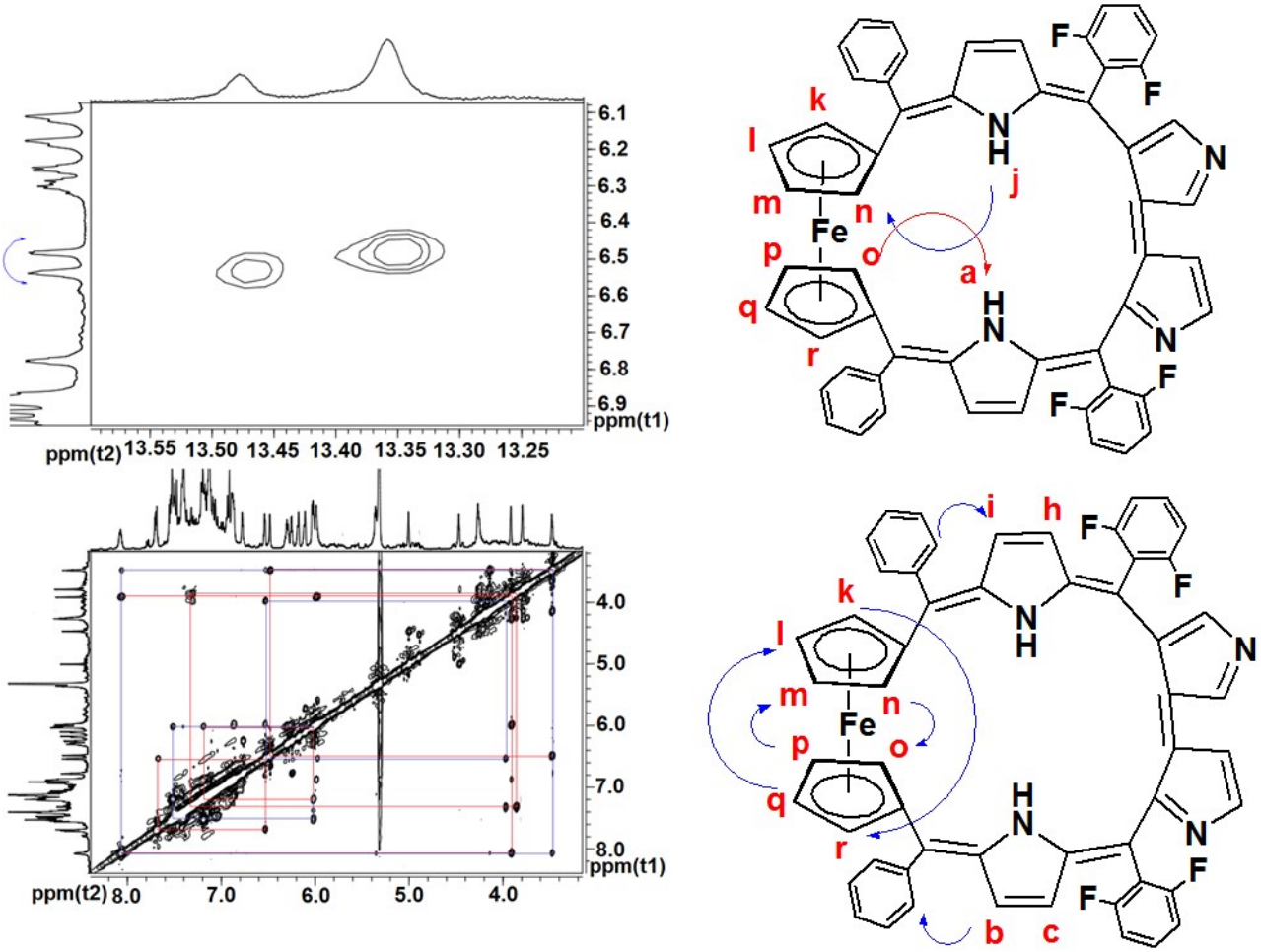


Fig. S43 ^{1}H-^{1}H 2D ROESY spectra of **7** in CD_2Cl_2 at 298 K

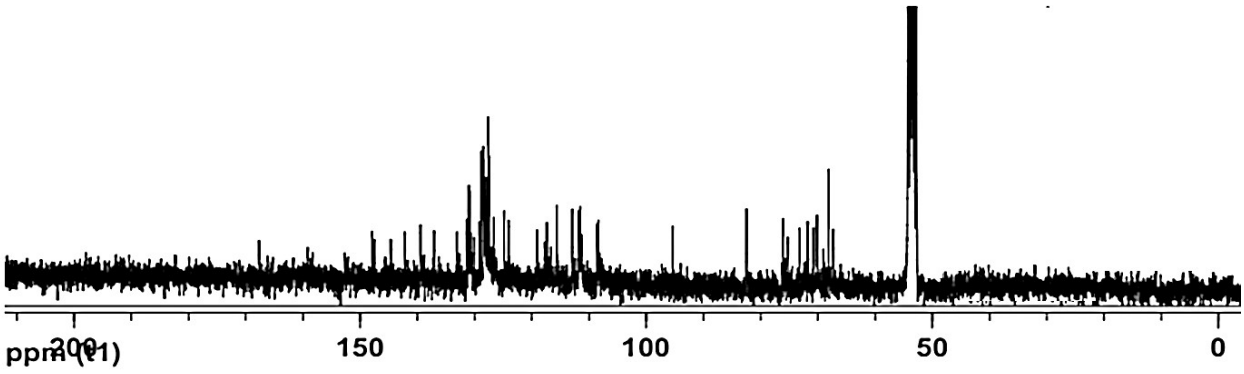
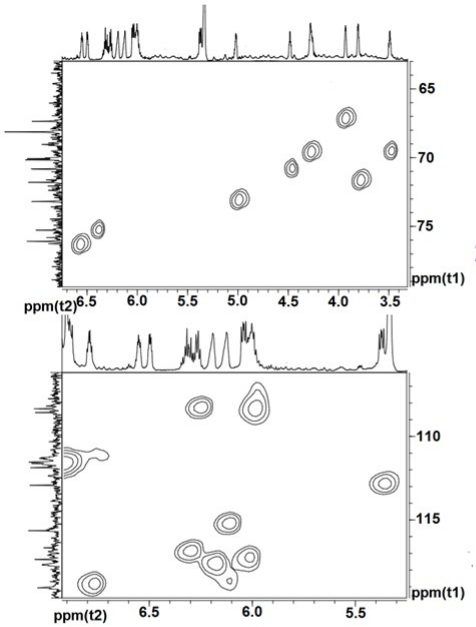
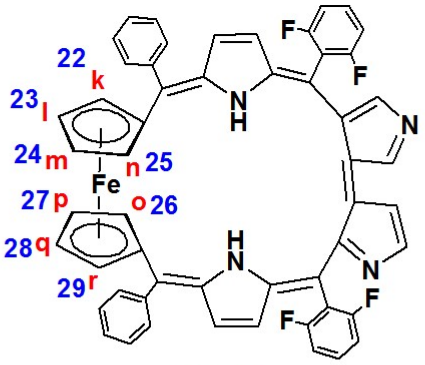
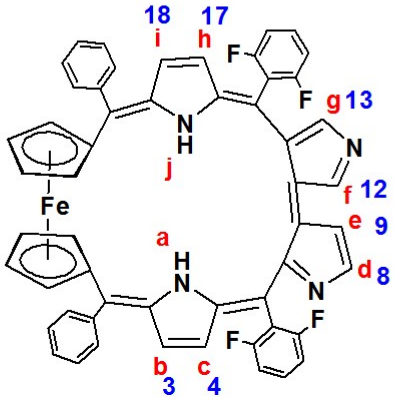


Fig. S44 ^{13}C NMR spectra of **7** in CD_2Cl_2 at 298 K



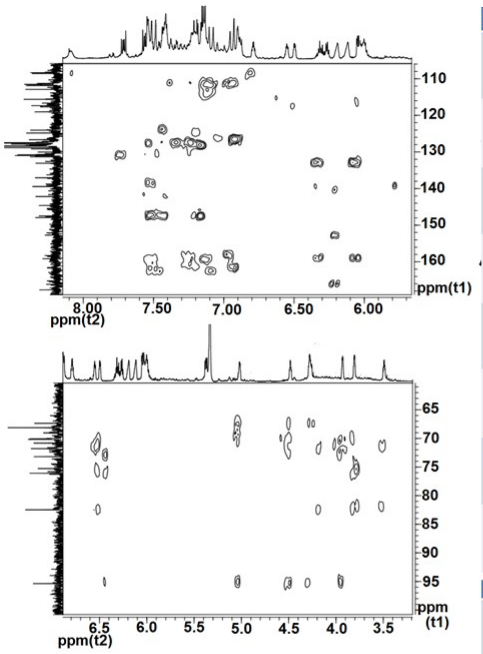


Position	^{1}H-NMR	Position	^{13}C-NMR
k	5.02	22	73.12
l	3.49	23	69.62
m	4.28	24	70.07
n	6.50	25	75.23
o	6.55	26	76.01
p	3.94	27	67.34
q	3.81	28	71.57
r	4.48	29	70.90



Position	^{1}H-NMR	Position	^{13}C-NMR
a	13.50	-	-
b	6.14	3	115.63
c	6.19	4	117.50
d	6.26	8	108.15
e	6.32	9	116.88
f	6.79	12	119.12
g	6.00	13	108.28
h	6.05	17	117.19
i	5.38	18	112.84
j	13.37	-	-

Fig. S45 HSQC NMR spectra of **7** in CD_2Cl_2 at 298 K



Position	^{1}H-NMR	Position	^{13}C-NMR
b	6.14	5	116.05
		2	126.26
		4	117.50
c	6.19	5	116.05
		2	126.26
		3	115.63
d	6.26	7	126.69
		10	127.97
		9	116.88
e	6.32	7	126.69
		10	127.97
		8	108.15
f	6.79	11	126.08
		13	108.28
		14	108.28
g	6.00	11	126.08
		12	119.12
		14	108.28
h	6.05	16	127.60
		19	121.27
		18	112.84
i	5.38	16	127.60
		19	121.27
		17	117.19

Position	^{1}H-NMR	Position	^{13}C-NMR
k l m n	5.02 3.49 4.28 6.50	21	95.09
o p q r	6.55 3.94 3.81 4.48	30	82.40

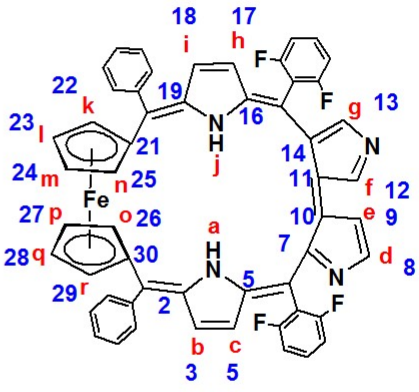


Fig. S46 HMBC NMR spectra of **7** in CD_2Cl_2 at 298 K

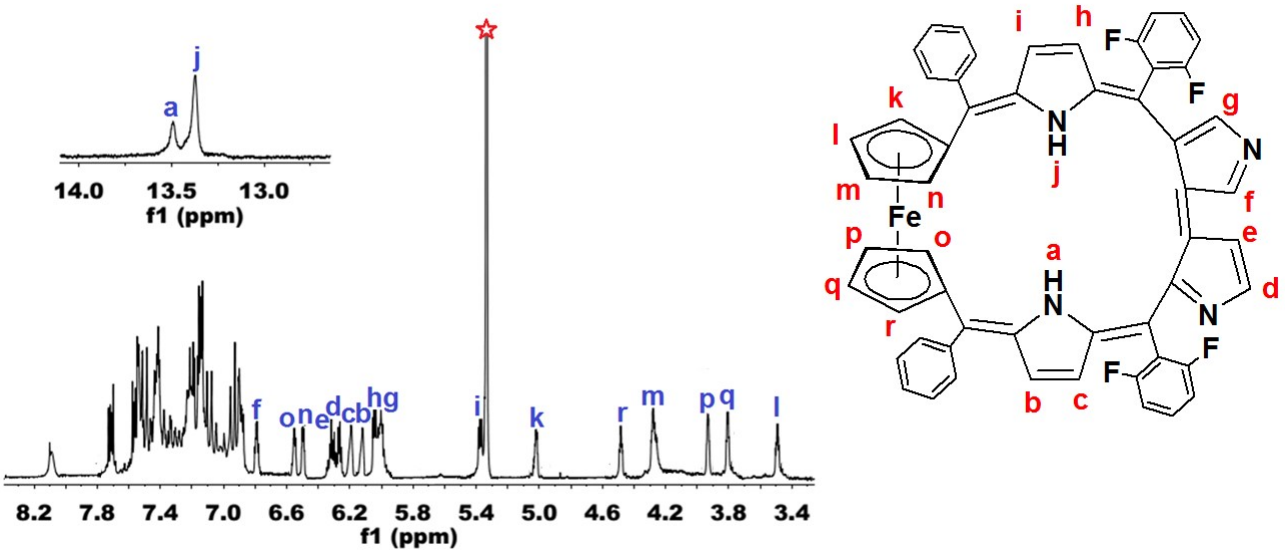


Fig. S47 Complete ^{1}H NMR spectral assignment of **7** in CD_2Cl_2 at 298 K

2.5. Electrochemistry

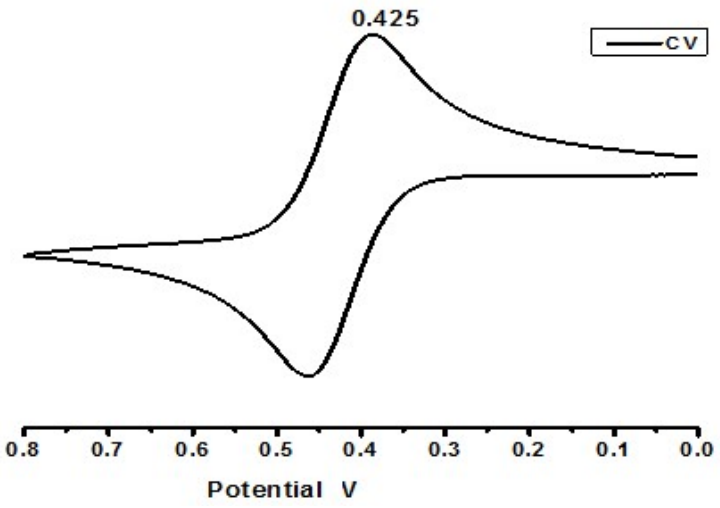


Fig. S48 Cyclic voltammogram of ferrocene in CH_2Cl_2 at 298 K

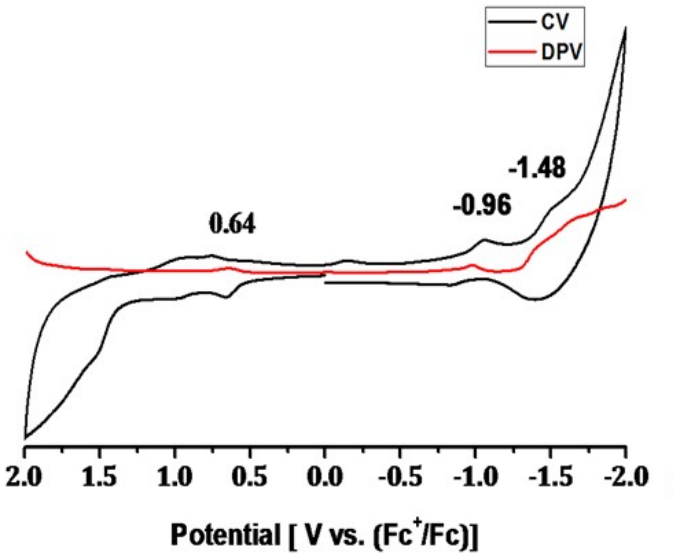


Fig. S49 Cyclic voltammogram of **5** in CH_2Cl_2 at 298 K

3. X-ray Crystal Data

Parameters	6
Chemical formula	$C_{68}H_{40}F_8FeN_4$
Formula weight	1120.89
Temperature	100 K
Crystal system	Triclinic
Space group	P-1
a (Å); α (°)	10.8521(18); 118.145(5)
b (Å); β(°)	17.560(3); 93.156(5)
c (Å); γ (°)	17.760(3); 99.868(5)
V (Å3); Z	2903.9(8); 2
ρ (calc.) g m-3	1.282
μ(Mo Kα) mm-1	0.701
2θmax (°)	54.542
R(int)	0.0821
Completeness to θ	0.984
Data / param.	10092/730
GOF	1.042
R1 [F>4σ(F)]	0.0756
wR2 (all data)	0.1880
max. peak/hole (e.Å-3)	0.46/-0.62
CCDC	2053405

4. Theoretical Calculation

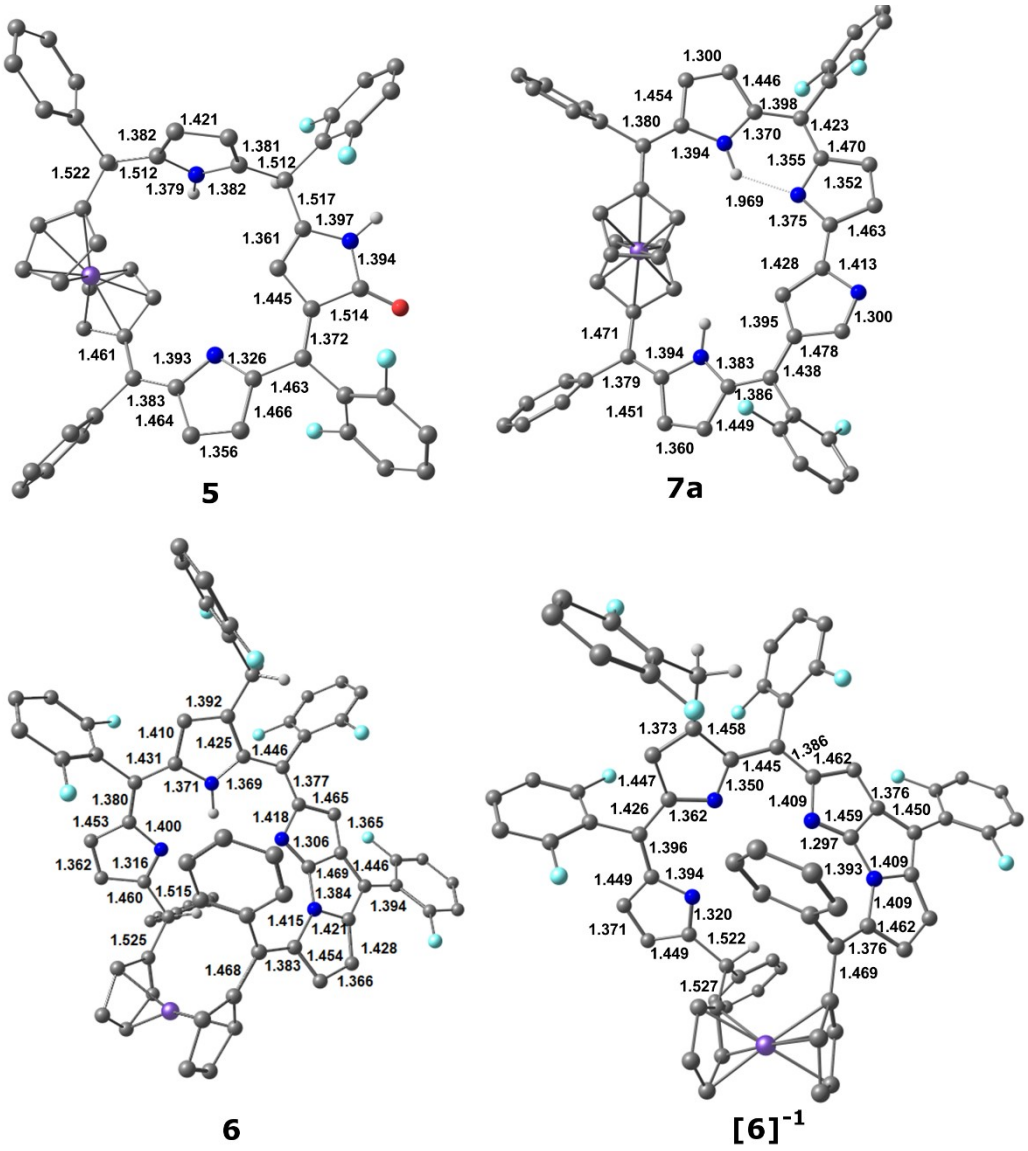


Fig. S50 DFT optimised geometries and key bond length parameters (Å) of **5**, **6**, **6**-deprotonated and **7a**, at uB3LYP/LanL2DZ (Fe) and 6-31+G** (for rest of the atoms) level of theory. Note that **6** is the optimised structure of X-ray crystal structure.

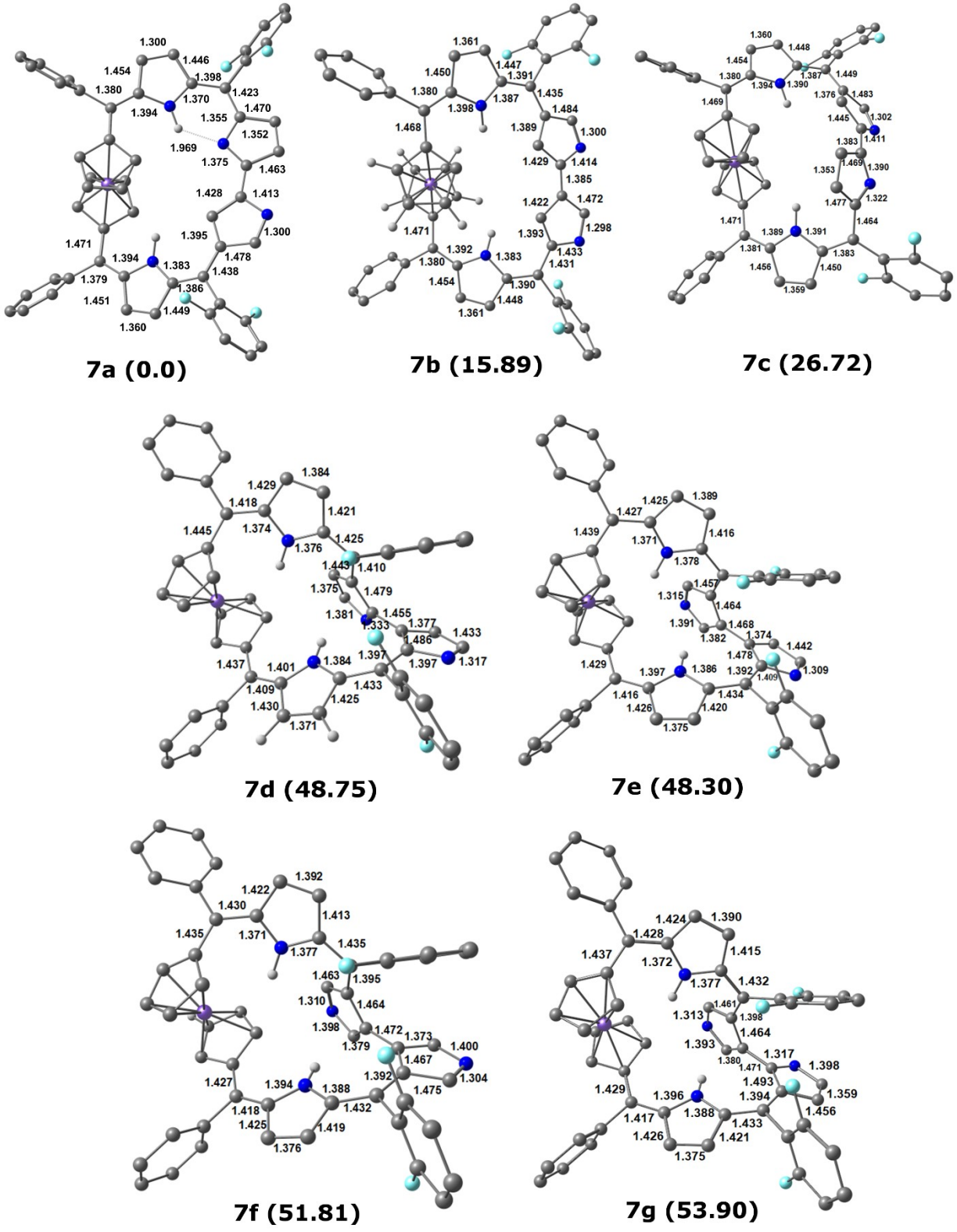


Fig. S51 DFT optimised geometries and key bond length parameters (Å) of isomers of **7a-7g**, at uB3LYP/LanL2DZ (Fe) and 6-31+G** (for rest of the atoms) level of theory.

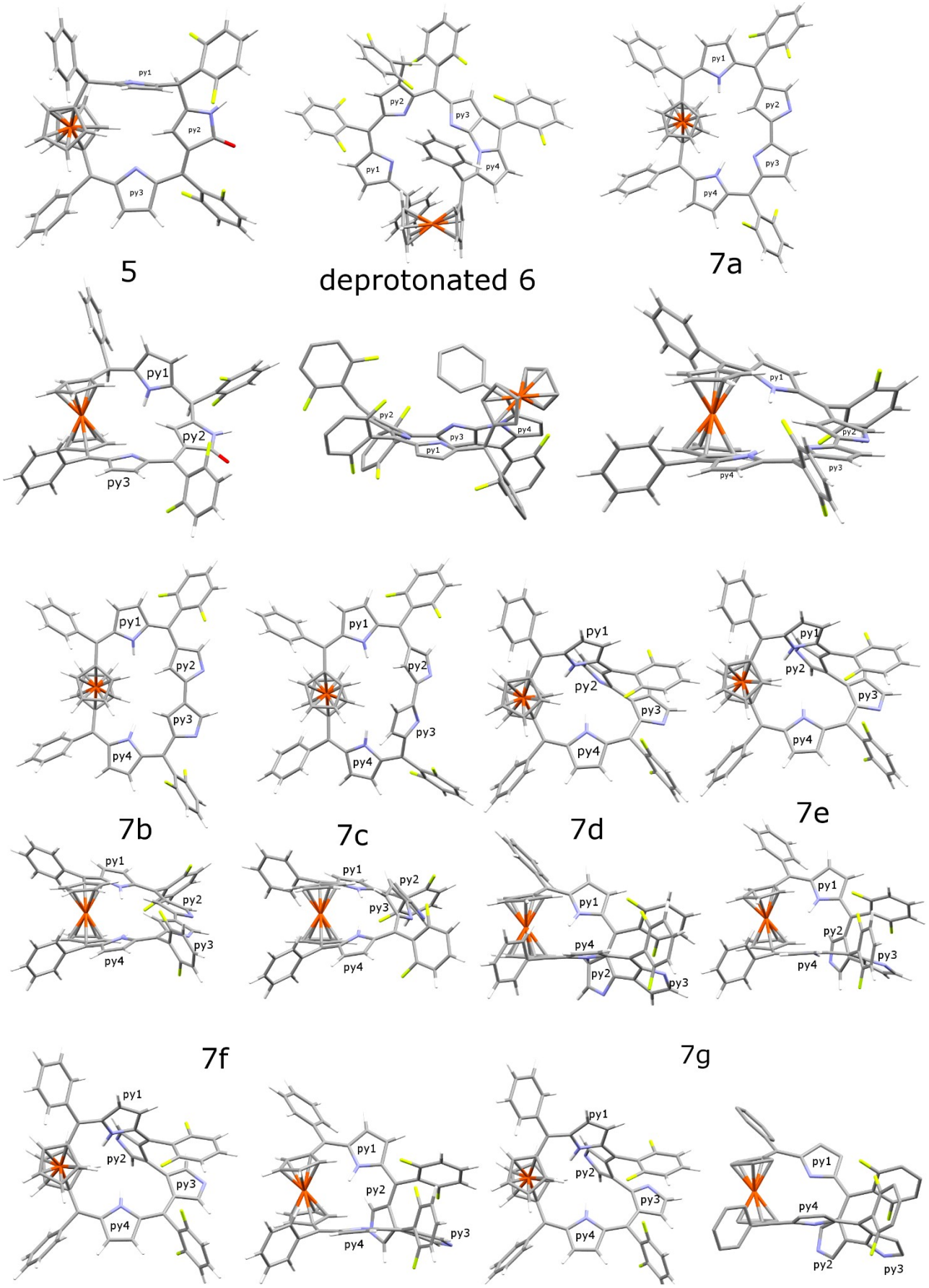


Fig. S52 Top and side view of DFT optimised geometries of **5**, **6-deprotonated** and **7a-7g**, at uB3LYP/LanL2DZ (Fe) and 6-31+G** (for rest of the atoms) level of theory.

Table S1: Dihedral angle planes of pyrrole rings for DFT optimised geometries of **5**, **6**, **deprotonated 6** and **7a-7g** at uB3LYP/LanL2DZ (Fe) and 6-31+G** (for rest of the atoms) level of theory.

S. No	5	6	Deprotonated $[6]^{-1}$	
1	py1—py2 -79.7	py1—py2 – 10.15	py1—py2 – 26.8	
2	py2—py3 – 25.8	py2—py3 – 33.08	py2—py3 – 45.5	
3	py3—cp1 – 7.2	py3—py4 – 4.59	py3—py4 – 9.73	
4	py1—cp2 -84.7	py4—cp1 – 37.47	py4—cp1 – 46.4	
5		py1—cp2 – 56.03	py1—cp2 – 89.1	
	7a	**7b**	**7c**	
1	py1—py2 – 12.1	py1—py2 – 10.8	py1—py2 – 39.9	
2	py2—py3 – 21.9	py2—py3 – 7.4	py2—py3 – 31.9	
3	py3—py4 – 33.5	py3—py4 – 30.9	py3—py4 – 64.3	
4	py4—cp1 – 12.8	py4—cp1 – 16.5	py4—cp1 – 0.0	
5	py1—cp2 – 29.7	py1—cp2 – 27.77	py1—cp2 – 18.2	
	7d	**7e**	**7f**	**7g**
1	py1—py2 – 54.6	py1—py2 – 52.9	py1—py2 – 52.9	py1—py2 – 54.26
2	py2—py3 – 55.5	py2—py3 – 66.5	py2—py3 – 71.2	py2—py3 – 65.63
3	py3—py4 – 37.8	py3—py4 – 27.6	py3—py4 – 23.8	py3—py4 – 27.46
	py4—cp1 – 10.1	py4—cp1 – 14.1	py4—cp1 – 14.9	py4—cp1 – 15.34
5	py1—cp2 – 54.0	py1—cp2 – 54.0	py1—cp2 – 53.3	py1—cp2 – 53.03

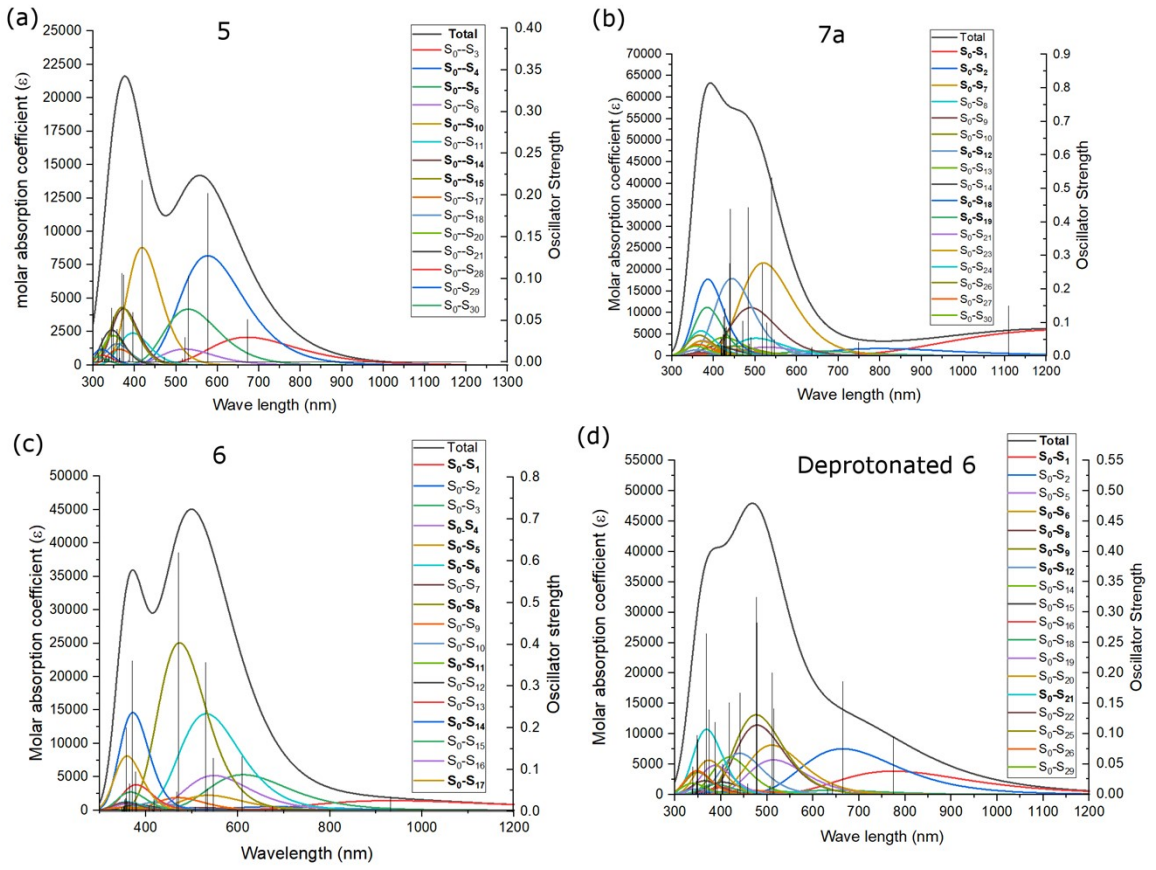


Fig. S53 Steady state absorption spectrum (total) and individual transitions that are predicted from TD-DFT calculation done with solvent (dichloromethane using a polarizable continuum model) and at uB3LYP/LanL2DZ (Fe) and 6-31G** (for rest of the atoms) level of theory. (a) **5**, (b) **7a** (c) **6** (d) deprotonated **6**.

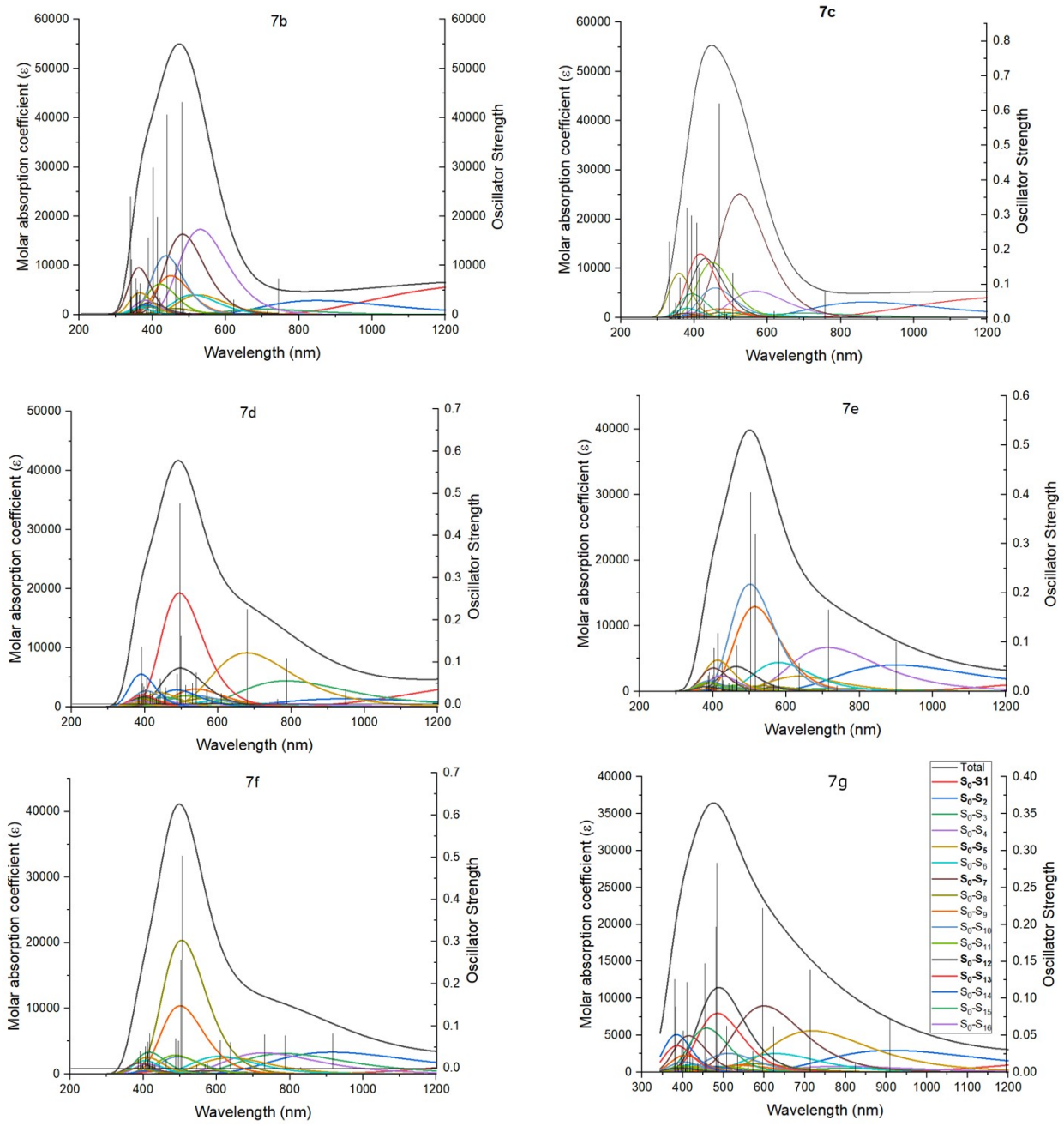


Fig. S54 Steady state absorption spectrum (total) and individual transitions of isomers of **7** (**7b-7g**) that are predicted from TD-DFT calculation done with solvent (dichloromethane using a polarizable continuum model) and at uB3LYP/LanL2DZ (Fe) and 6-31G** (for rest of the atoms) level of theory.

Table S2: Summary of UV-vis spectral data of **5**

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
2	14342.95	697.20	0.0003	Singlet-A	H-2->LUMO (54%), H-2->L+4 (18%)
3	14884.96	671.81	0.0515	Singlet-A	H-3->LUMO (25%), H-3->L+4 (14%), HOMO->LUMO (17%)
4	**17345.75**	**576.50**	**0.2023**	**Singlet-A**	**H-1->LUMO (23%), HOMO->LUMO (68%)**
5	**18885.47**	**529.50**	**0.1035**	**Singlet-A**	**H-2->L+3 (12%), H-1->LUMO (63%)**
6	19179.86	521.38	0.0296	Singlet-A	H-3->LUMO (19%), H-2->L+3 (26%)
7	19419.41	514.94	0.0039	Singlet-A	H-3->L+3 (32%), H-2->LUMO (16%), H-1->L+3 (11%)
8	21186.57	471.99	0.0065	Singlet-A	H-3->LUMO (28%)
9	22210.08	450.24	0.0038	Singlet-A	H-10->L+3 (11%), H-2->LUMO (15%), H-2->L+4 (19%)
10	**23908.69**	**418.25**	**0.2175**	**Singlet-A**	**H-4->LUMO (75%), HOMO->L+1 (11%)**
11	25274.18	395.66	0.0594	Singlet-A	H-7->LUMO (17%), H-6->LUMO (32%), H-5->LUMO (22%)
12	25791.19	387.72	0.0092	Singlet-A	H-7->LUMO (11%), H-6->LUMO (20%), H-5->LUMO (10%)
13	25979.11	384.92	0.0026	Singlet-A	H-9->LUMO (17%), H-8->LUMO (49%)
14	**26759.86**	**373.69**	**0.1044**	**Singlet-A**	**H-7->LUMO (15%), H-5->LUMO (17%), HOMO->L+1 (41%)**
15	**27040.54**	**369.81**	**0.1067**	**Singlet-A**	**H-6->LUMO (20%), H-5->LUMO (13%), HOMO->L+1 (27%)**
16	27444.62	364.37	0.0046	Singlet-A	H-16->LUMO (46%), H-9->LUMO (27%), H-8->LUMO (13%)
17	27575.28	362.64	0.0294	Singlet-A	H-16->LUMO (29%), H-9->LUMO (37%), H-8->LUMO (10%),
18	27978.56	357.41	0.0394	Singlet-A	H-12->LUMO (11%), H-10->LUMO (13%), H-7->LUMO (27%)
19	28281.83	353.58	0.0009	Singlet-A	H-10->L+3 (14%), H-5->L+3 (10%), H-2->L+1 (20%)
20	28672.20	348.76	0.0547	Singlet-A	H-1->L+1 (75%)
21	29000.47	344.82	0.0648	Singlet-A	H-14->LUMO (73%)
22	29646.52	337.30	0.0064	Singlet-A	H-14->LUMO (73%)
23	29815.89	335.39	0.005	Singlet-A	H-13->LUMO (13%), H-12->LUMO (47%), H-10->LUMO (12%)
24	30220.78	330.89	0.0071	Singlet-A	H-15->LUMO (10%), H-10->LUMO (19%), H-3->L+1 (27%)
25	30398.22	328.96	0.0012	Singlet-A	H-15->LUMO (69%)
26	30449.84	328.40	0.0036	Singlet-A	H-12->LUMO (10%), H-11->LUMO (27%), H-10->LUMO (11%)
27	30486.95	328.00	0.0032	Singlet-A	H-13->LUMO (63%), H-12->LUMO (13%)
28	30908.77	323.53	0.0176	Singlet-A	H-11->LUMO (22%), H-3->L+1 (19%), H-2->L+1 (22%)
29	31194.29	320.57	0.0289	Singlet-A	H-11->LUMO (11%), H-3->L+1 (25%)
30	32112.15	311.40	0.0151	Singlet-A	H-19->LUMO (69%)

Table S3: Summary of UV-vis spectral data of **6**

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	10717.49	933.05	0.0357	Singlet-A	HOMO->LUMO (98%)
2	14777.69	676.69	0.0133	Singlet-A	H-3->L+8 (10%), H-2->LUMO (20%), H-2->L+1 (11%), H-
3	15109.18	661.84	0.0039	Singlet-A	H-3->LUMO (19%), H-3->L+1 (11%), H-3->L+5 (10%), H-
4	**16350.47**	**611.60**	**0.1317**	**Singlet-A**	**H-1->LUMO (68%), HOMO->L+1 (12%)**
5	**18248.29**	**547.99**	**0.1285**	**Singlet-A**	**H-2->LUMO (61%), HOMO->L+1 (14%)**
6	18653.99	536.07	0.0555	Singlet-A	H-3->LUMO (60%), H-2->L+8 (16%)
7	**18816.10**	**531.45**	**0.3572**	**Singlet-A**	**H-1->LUMO (11%), HOMO->L+1 (41%), HOMO->L+2 (12%)**
8	19635.56	509.27	0.0106	Singlet-A	H-3->L+8 (21%)
9	20269.51	493.35	0.0022	Singlet-A	H-3->L+1 (14%), H-2->L+8 (20%)
10	**21120.43**	**473.47**	**0.6196**	**Singlet-A**	**HOMO->L+1 (11%), HOMO->L+2 (67%)**
11	21277.71	469.97	0.0469	Singlet-A	H-1->L+1 (93%)
12	23050.51	433.82	0.0017	Singlet-A	H-2->L+1 (61%)
13	23840.13	419.46	0.0289	Singlet-A	H-6->LUMO (55%), H-5->LUMO (11%), H-4->LUMO (27%)
14	23886.91	418.63	0.0011	Singlet-A	H-3->L+1 (57%)
15	24019.99	416.31	0.0055	Singlet-A	H-7->LUMO (34%), H-5->LUMO (50%)
16	24466.82	408.71	0.0136	Singlet-A	H-4->LUMO (31%), H-1->L+2 (49%)
17	24897.52	401.64	0.0034	Singlet-A	H-7->LUMO (45%), H-5->LUMO (17%), H-4->LUMO (13%)
18	26175.91	382.03	0.0206	Singlet-A	H-8->LUMO (55%)
19	26359.81	379.36	0.0948	Singlet-A	H-9->LUMO (40%)
20	**26868.74**	**372.17**	**0.3614**	**Singlet-A**	**H-6->LUMO (17%), H-4->LUMO (11%), H-2->L+2 (13%),**
21	27222.01	367.34	0.0674	Singlet-A	H-12->LUMO (12%), H-9->LUMO (32%), H-2->L+2 (10%)
22	27317.99	366.05	0.0069	Singlet-A	H-13->LUMO (12%), H-12->LUMO (13%), H-3->L+2 (18%),
23	27643.84	361.74	0.0239	Singlet-A	H-13->LUMO (21%), H-9->LUMO (11%), H-8->LUMO (18%),
24	**27809.99**	**359.58**	**0.2007**	**Singlet-A**	**H-14->LUMO (16%), H-13->LUMO (12%), H-11->LUMO (11%)**
25	27906.78	358.33	0.0311	Singlet-A	H-14->LUMO (12%), H-13->LUMO (13%), H-12->LUMO (13%)
26	28092.29	355.96	0.0285	Singlet-A	H-13->LUMO (16%), H-11->LUMO (71%)
27	28168.91	355.00	0.012	Singlet-A	H-15->LUMO (20%), H-14->LUMO (35%)
28	28251.98	353.95	0.0099	Singlet-A	H-15->LUMO (34%), H-12->LUMO (28%), H-10->LUMO (23%)
29	28471.37	351.23	0.0015	Singlet-A	H-16->LUMO (90%)
30	28549.60	350.26	0.0107	Singlet-A	H-15->LUMO (33%), H-14->LUMO (18%), H-10->LUMO (24%)

Table S4: Summary of UV-vis spectral data of deprotonated **6 [6]$^{-1}$**

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	12920.19	773.98	0.095	Singlet-A	HOMO->LUMO (91%)
2	**15047.07**	**664.58**	**0.1861**	**Singlet-A**	**H-1->LUMO (80%)**
3	15567.30	642.37	0.0171	Singlet-A	H-3->L+6 (12%), H-2->LUMO (15%)
4	15826.21	631.86	0.0078	Singlet-A	H-3->LUMO (10%), H-2->L+6 (15%)
5	19442.80	514.32	0.141	**Singlet-A**	H-3->L+6 (23%), H-2->LUMO (10%), HOMO->L+1 (14%)
6	**19579.91**	**510.72**	**0.2006**	**Singlet-A**	**H-1->L+1 (25%), HOMO->L+1 (56%)**
7	19748.48	506.36	0.0135	Singlet-A	H-3->LUMO (15%), H-2->L+6 (27%)
8	**20888.14**	**478.74**	**0.2826**	**Singlet-A**	**H-4->LUMO (21%), H-3->LUMO (16%), H-2->LUMO (13%**
9	**20980.90**	**476.62**	**0.3244**	**Singlet-A**	**H-4->LUMO (34%), H-1->L+1 (34%), HOMO->L+1 (10%)**
10	21840.68	457.86	0.0179	Singlet-A	H-4->LUMO (25%), H-2->LUMO (31%)
11	22217.34	450.09	0.0035	Singlet-A	H-3->LUMO (38%), H-2->LUMO (14%)
12	**22669.82**	**441.11**	**0.1675**	**Singlet-A**	**HOMO->L+2 (62%)**
13	22882.75	437.01	0.0094	Singlet-A	H-6->LUMO (17%), H-5->LUMO (64%)
14	23906.27	418.30	0.1515	Singlet-A	H-1->L+2 (79%)
15	24766.06	403.77	0.0498	Singlet-A	H-8->LUMO (74%)
16	24826.55	402.79	0.0283	Singlet-A	H-7->LUMO (26%), H-6->LUMO (36%), H-5->LUMO (28%
17	25480.66	392.45	0.0102	Singlet-A	H-9->LUMO (11%), H-2->L+1 (59%)
18	25748.44	388.37	0.0413	Singlet-A	H-4->L+1 (18%), H-3->L+1 (38%)
19	25812.16	387.41	0.1185	Singlet-A	H-7->LUMO (23%), H-4->L+1 (26%), H-3->L+1 (26%)
20	26738.08	373.99	0.1395	Singlet-A	H-9->LUMO (46%), H-3->L+1 (15%), H-2->L+1 (13%)
21	**27112.32**	**368.83**	**0.2647**	**Singlet-A**	**H-7->LUMO (15%), H-4->L+1 (41%)**
22	27424.46	364.63	0.0557	Singlet-A	H-10->LUMO (20%), H-9->LUMO (15%)
23	27929.36	358.04	0.0023	Singlet-A	HOMO->L+6 (13%)
24	28279.41	353.61	0.0014	Singlet-A	H-11->LUMO (35%), H-10->LUMO (50%)
25	28586.70	349.81	0.0902	Singlet-A	H-14->LUMO (10%), H-12->LUMO (18%)
26	28702.04	348.40	0.0969	Singlet-A	HOMO->L+3 (76%)
27	28830.28	346.85	0.0221	Singlet-A	H-11->LUMO (11%), H-4->L+2 (44%)
28	29027.08	344.50	0.0042	Singlet-A	H-6->L+1 (17%), H-5->L+1 (53%)
29	29481.98	339.19	0.0456	Singlet-A	HOMO->L+4 (62%), HOMO->L+5 (16%)
30	29614.25	337.67	0.0086	Singlet-A	HOMO->L+5 (65%)

Table S5: Summary of UV-vis spectral data of **7a**

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	**7817.125**	**1279.2**	**0.1511**	**Singlet-A**	**HOMO->LUMO (100%)**
2	12533.04	797.89	0.0414	Singlet-A	H-3->LUMO (12%), H-2->LUMO (11%), H-1->LUMO (45%)
3	12601.60	793.54	0.0036	Singlet-A	H-3->LUMO (14%), H-2->LUMO (49%), H-2->L+4 (10%)
4	15442.29	647.57	0.026	Singlet-A	H-3->LUMO (30%), H-1->LUMO (31%), HOMO->L+1 (17%)
5	18149.08	550.99	0.0024	Singlet-A	H-9->LUMO (17%), H-9->L+4 (10%), H-2->L+3 (25%)
6	18950.80	527.68	0.0497	Singlet-A	H-3->L+3 (31%), H-2->LUMO (10%), H-1->L+3 (15%)
7	**19241.96**	**519.69**	**0.5325**	**Singlet-A**	**HOMO->L+1 (53%), HOMO->L+2 (15%)**
8	19907.37	502.32	0.1005	Singlet-A	H-3->LUMO (20%), HOMO->L+2 (35%)
9	20417.92	489.76	0.2757	Singlet-A	HOMO->L+1 (12%), HOMO->L+2 (30%)
10	22077.00	452.95	0.0555	Singlet-A	H-4->LUMO (26%), H-2->L+4 (11%), H-1->L+1 (11%)
11	22331.87	447.79	0.037	Singlet-A	H-4->LUMO (34%), H-2->L+4 (10%)
12	**22528.67**	**443.87**	**0.4429**	**Singlet-A**	**H-5->LUMO (72%)**
13	23484.44	425.81	0.1055	Singlet-A	H-7->LUMO (31%), H-1->L+1 (55%)
14	24513.60	407.93	0.0562	Singlet-A	H-9->LUMO (23%), H-2->L+3 (14%), H-1->L+2 (28%)
15	25634.71	390.09	0.001	Singlet-A	H-6->LUMO (74%)
16	25687.95	389.28	0.0034	Singlet-A	H-8->LUMO (88%), H-7->LUMO (10%)
17	25766.99	388.09	0.014	Singlet-A	HOMO->L+3 (87%)
18	**25900.07**	**386.09**	**0.439**	**Singlet-A**	**H-16->LUMO (10%), H-11->LUMO (16%), H-7->LUMO (19%)**
19	**26008.15**	**384.49**	**0.2771**	**Singlet-A**	**H-16->LUMO (11%), H-12->LUMO (12%), H-10->LUMO (13%)**
20	26243.66	381.04	0.0032	Singlet-A	H-17->LUMO (21%), H-15->LUMO (13%), H-10->LUMO (18%)
21	26738.89	373.98	0.0864	Singlet-A	H-13->LUMO (30%), H-12->LUMO (13%),
22	26855.03	372.36	0.0024	Singlet-A	H-12->LUMO (16%), H-2->L+1 (58%)
23	26939.72	371.19	0.0838	Singlet-A	H-11->LUMO (25%), HOMO->L+4 (34%)
24	27056.67	369.59	0.1426	Singlet-A	H-11->LUMO (13%), H-3->L+1 (14%), H
25	27172.01	368.02	0.0171	Singlet-A	H-17->LUMO (12%), H-16->LUMO (17%),
26	27362.35	365.46	0.1169	Singlet-A	H-3->L+1 (23%), H-1->L+2 (31%)
27	27476.88	363.94	0.0645	Singlet-A	H-14->LUMO (51%), H-10->LUMO (25%)
28	27768.86	360.11	0.0094	Singlet-A	H-15->LUMO (37%), H-10->LUMO (12%)
29	27864.84	358.87	0.0326	Singlet-A	H-20->LUMO (13%), H-15->LUMO (10%),
30	27985.82	357.32	0.0546	Singlet-A	H-20->LUMO (17%), H-3->L+1 (25%),

Table S6: Summary of UV-vis spectral data of **7b**

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	**7238.826**	**1381.44**	**0.1542**	**Singlet-A**	**HOMO->LUMO (100%)**
2	11785.37	848.50	0.071	Singlet-A	H-2->LUMO (13%), H-1->LUMO (61%)
3	12323.34	811.46	0.0046	Singlet-A	H-3->LUMO (65%), H-3->L+2 (10%), H-3->L+4 (14%)
4	14264.72	701.03	0.0282	Singlet-A	H-2->LUMO (46%), H-1->LUMO (25%)
5	17916.80	558.13	0.001	Singlet-A	H-9->LUMO (13%), H-3->L+3 (28%)
6	18594.30	537.79	0.0078	Singlet-A	H-3->LUMO (15%), H-2->L+3 (34%), H-1->L+3 (12%),
7	**18837.88**	**530.84**	**0.4287**	**Singlet-A**	**H-2->LUMO (13%), HOMO->L+1 (59%)**
8	18969.35	527.16	0.0995	Singlet-A	H-2->L+3 (10%), HOMO->L+2 (63%)
9	19581.52	510.68	0.0997	Singlet-A	H-3->L+3 (17%), H-2->LUMO (20%), HOMO->L+1 (12%)
10	**20712.31**	**482.80**	**0.4039**	**Singlet-A**	**H-4->LUMO (61%), HOMO->L+2 (11%)**
11	21765.67	459.43	0.0314	Singlet-A	H-9->L+3 (11%), H-3->LUMO (15%), H-3->L+2 (14%),
12	**22206.05**	**450.32**	**0.1961**	**Singlet-A**	**H-5->LUMO (58%), H-1->L+1 (20%)**
13	**22866.62**	**437.31**	**0.2961**	**Singlet-A**	**H-5->LUMO (16%), H-1->L+1 (62%)**
14	23342.49	428.40	0.0078	Singlet-A	H-8->LUMO (21%), H-6->LUMO (56%)
15	**23772.38**	**420.65**	**0.1534**	**Singlet-A**	**H-9->LUMO (14%), H-3->L+3 (13%), H-1->L+2 (41%)**
16	24175.66	413.63	0.0083	Singlet-A	H-14->LUMO (12%), H-8->LUMO (26%), H-6->LUMO (36%)
17	24970.92	400.46	0.0051	Singlet-A	H-7->LUMO (93%)
18	25405.65	393.61	0.0609	Singlet-A	H-14->LUMO (10%), H-12->LUMO (15%), H-8->LUMO (26%)
19	25517.76	391.88	0.0375	Singlet-A	H-9->LUMO (34%), H-1->L+2 (22%)
20	25727.47	388.68	0.0052	Singlet-A	H-16->LUMO (23%), H-11->LUMO (14%), HOMO->L+3 (14%)
21	26017.02	384.36	0.0483	Singlet-A	H-14->LUMO (10%), H-12->LUMO (14%), H-11->LUMO (13%), H
22	26063.80	383.67	0.0413	Singlet-A	H-14->LUMO (11%), H-12->LUMO (34%), HOMO->L+3 (30%)
23	26290.44	380.36	0.0712	Singlet-A	H-11->LUMO (35%), H-10->LUMO (37%)
24	26734.85	374.04	0.0038	Singlet-A	H-3->L+1 (88%)
25	26851.00	372.42	0.0029	Singlet-A	H-13->LUMO (39%), H-2->L+1 (29%), HOMO->L+4 (13%)
26	26902.62	371.71	0.0041	Singlet-A	H-13->LUMO (42%), H-2->L+1 (33%), HOMO->L+4 (16%)
27	27125.23	368.66	0.0083	Singlet-A	H-16->LUMO (35%), H-14->LUMO (17%), H-11->LUMO (14%)
28	27342.19	365.73	0.1097	Singlet-A	H-20->LUMO (10%), H-17->LUMO (10%), HOMO->L+4 (22%)
29	27428.49	364.58	0.0341	Singlet-A	H-20->LUMO (11%), H-17->LUMO (12%), H-15->LUMO (13%)
30	**27566.41**	**362.76**	**0.2361**	**Singlet-A**	**H-15->LUMO (13%), H-2->L+1 (16%), HOMO->L+4 (33%)**

Table S7: Summary of UV-vis spectral data of **7c**

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	**7476.759**	**1337.4**	**0.1067**	**Singlet-A**	**HOMO->LUMO (100%)**
2	11497.43	869.75	0.0778	Singlet-A	H-1->LUMO (75%)
3	12744.36	784.66	0.0051	Singlet-A	H-2->LUMO (54%), H-2->L+3 (12%)
4	14219.55	703.25	0.022	Singlet-A	H-3->LUMO (39%), H-1->LUMO (20%)
5	17647.41	566.65	0.133	Singlet-A	HOMO->L+1 (57%), HOMO->L+2 (30%)
6	18216.83	548.94	0.0029	Singlet-A	H-3->LUMO (10%), H-2->L+4 (29%)
7	18290.23	546.73	0.0149	Singlet-A	H-3->L+4 (25%), H-2->LUMO (16%), H-1->L+4 (11%)
8	18493.48	540.73	0.0259	Singlet-A	H-3->LUMO (23%)
9	**19081.46**	**524.06**	**0.6204**	**Singlet-A**	**HOMO->L+1 (32%), HOMO->L+2 (57%)**
10	20804.26	480.67	0.0256	Singlet-A	H-2->L+3 (12%), H-1->L+1 (14%), H-1->L+2 (10%)
11	21140.59	473.02	0.0448	Singlet-A	H-4->LUMO (12%), H-1->L+1 (27%), H-1->L+2 (27%)
12	21864.88	457.35	0.1487	Singlet-A	H-8->LUMO (24%), H-4->LUMO (46%), H-1->L+1 (13%)
13	**22226.22**	**449.91**	**0.2772**	**Singlet-A**	**H-5->LUMO (22%), H-2->L+4 (10%), H-1->L+1 (18%),**
14	**23181.98**	**431.36**	**0.2974**	**Singlet-A**	**H-8->LUMO (26%), H-5->LUMO (18%), H-4->LUMO (14%)**
15	**23977.25**	**417.06**	**0.3204**	**Singlet-A**	**H-8->LUMO (11%), H-5->LUMO (17%), H-3->L+2 (10%)**
16	24599.10	406.51	0.0083	Singlet-A	H-17->LUMO (15%), H-14->LUMO (11%), H-9->LUMO (16%)
17	24853.16	402.36	0.0152	Singlet-A	H-6->LUMO (91%)
18	25360.49	394.31	0.1193	Singlet-A	H-17->LUMO (18%), H-16->LUMO (10%), H-9->LUMO (30%)
19	25432.27	393.20	0.0092	Singlet-A	H-7->LUMO (88%)
20	25708.92	388.97	0.0076	Singlet-A	H-2->L+1 (49%), H-2->L+2 (29%)
21	25837.97	387.02	0.0244	Singlet-A	H-17->LUMO (10%), H-15->LUMO (15%), H-10->LUMO (31%),
22	26264.63	380.74	0.0212	Singlet-A	H-3->L+1 (34%), H-3->L+2 (22%), H-2->L+2 (16%)
23	26324.32	379.87	0.0472	Singlet-A	H-17->LUMO (11%), H-15->LUMO (16%), H-14->LUMO (25%),
24	26406.59	378.69	0.0044	Singlet-A	H-3->L+2 (18%), H-2->L+1 (11%), H-2->L+2 (13%), H-1->
25	26770.34	373.54	0.0206	Singlet-A	H-12->LUMO (12%), H-11->LUMO (68%)
26	27148.62	368.34	0.0062	Singlet-A	H-10->LUMO (14%), H-3->L+1 (10%), H-3->L+2 (15%), H-1
27	27347.84	365.65	0.0022	Singlet-A	H-13->LUMO (16%), HOMO->L+4 (51%)
28	27403.49	364.91	0.0043	Singlet-A	H-13->LUMO (48%), H-12->LUMO (17%), HOMO->L+4 (14%)
29	27503.50	363.59	0.0056	Singlet-A	H-15->LUMO (30%), H-14->LUMO (26%), H-10->LUMO (12%),
30	**27834.19**	**359.27**	**0.2224**	**Singlet-A**	**H-21->LUMO (32%), H-18->LUMO (10%), H-12->LUMO (14%)**

Table S8: Summary of UV-vis spectral data of **7d**

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	**5802.352**	**1723.43**	**0.1322**	**Singlet-A**	**HOMO->LUMO (100%)**
2	10554.57	947.45	0.0334	Singlet-A	H-1->LUMO (75%)
3	12720.16	786.15	0.1084	Singlet-A	H-2->LUMO (54%), H-2->L+3 (12%)
4	13145.22	760.73	0.0127	Singlet-A	H-3->LUMO (39%), H-1->LUMO (20%)
5	**14729.29**	**678.91**	**0.2259**	**Singlet-A**	**HOMO->L+1 (57%), HOMO->L+2 (30%)**
6	16459.35	607.55	0.0253	Singlet-A	H-3->LUMO (10%), H-2->L+4 (29%)
7	17187.67	581.81	0.0137	Singlet-A	H-3->L+4 (25%), H-2->LUMO (16%), H-1->L+4 (11%)
8	17610.30	567.84	0.0352	Singlet-A	H-3->LUMO (23%)
9	18519.29	539.97	0.0744	Singlet-A	HOMO->L+1 (32%), HOMO->L+2 (57%)
10	18907.24	528.89	0.0497	Singlet-A	H-2->L+3 (12%), H-1->L+1 (14%), H-1->L+2 (10%)
11	19606.53	510.03	0.0458	Singlet-A	H-4->LUMO (12%), H-1->L+1 (27%), H-1->L+2 (27%)
12	20113.04	497.18	0.1619	Singlet-A	H-8->LUMO (24%), H-4->LUMO (46%), H-1->L+1 (13%)
13	**20198.54**	**495.08**	**0.4759**	**Singlet-A**	**H-5->LUMO (22%), H-2->L+4 (10%), H-1->L+1 (18%),**
14	20543.74	486.76	0.0709	Singlet-A	H-8->LUMO (26%), H-5->LUMO (18%), H-4->LUMO (14%)
15	21981.83	454.92	0.0398	Singlet-A	H-8->LUMO (11%), H-5->LUMO (17%), H-3->L+2 (10%)
16	22146.37	451.54	0.0223	Singlet-A	H-17->LUMO (15%), H-14->LUMO (11%), H-9->LUMO (16%)
17	22683.53	440.84	0.06	Singlet-A	H-6->LUMO (91%)
18	22945.66	435.81	0.0146	Singlet-A	H-17->LUMO (18%), H-16->LUMO (10%), H-9->LUMO (30%)
19	23247.31	430.15	0.0132	Singlet-A	H-7->LUMO (88%)
20	23515.09	425.25	0.0023	Singlet-A	H-2->L+1 (49%), H-2->L+2 (29%)
21	23807.06	420.04	0.022	Singlet-A	H-17->LUMO (10%), H-15->LUMO (15%), H-10->LUMO (31%),
22	24165.98	413.80	0.0304	Singlet-A	H-3->L+1 (34%), H-3->L+2 (22%), H-2->L+2 (16%)
23	24749.12	404.05	0.0665	Singlet-A	H-17->LUMO (11%), H-15->LUMO (16%), H-14->LUMO (25%),
24	25012.05	399.80	0.0362	Singlet-A	H-3->L+2 (18%), H-2->L+1 (11%), H-2->L+2 (13%), H-1->
25	25206.43	396.72	0.0417	Singlet-A	H-12->LUMO (12%), H-11->LUMO (68%)
26	25440.33	393.07	0.0494	Singlet-A	H-10->LUMO (14%), H-3->L+1 (10%), H-3->L+2 (15%), H-1
27	25629.07	390.18	0.136	Singlet-A	H-13->LUMO (16%), HOMO->L+4 (51%)
28	26056.54	383.78	0.0136	Singlet-A	H-13->LUMO (48%), H-12->LUMO (17%), HOMO->L+4 (14%)
29	26125.10	382.77	0.0252	Singlet-A	H-15->LUMO (30%), H-14->LUMO (26%), H-10->LUMO (12%),
30	26289.64	380.37	0.0171	Singlet-A	H-21->LUMO (32%), H-18->LUMO (10%), H-12->LUMO (14%)

Table S9: Summary of UV-vis spectral data of **7e**

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	4615.910	2166.42	0.09060	Singlet-A	HOMO->LUMO (117%)
2	11126.41	898.76	0.09960	Singlet-A	H-2->LUMO (22%), HOMO->L+1 (71%)
3	12239.46	817.03	0.00040	Singlet-A	H-3->LUMO (65%), H-1->LUMO (16%)
4	13556.56	737.65	0.01110	Singlet-A	H-2->LUMO (11%), H-1->LUMO (74%)
5	**14017.10**	**713.41**	**0.16550**	**Singlet-A**	**H-2->LUMO (34%), HOMO->L+1 (20%), HOMO->L+2 (10%)**
6	15776.20	633.87	0.05700	Singlet-A	H-5->LUMO (10%), HOMO->L+2 (66%)
7	**17256.23**	**579.50**	**0.10870**	**Singlet-A**	**H-5->LUMO (11%), H-4->LUMO (48%), H-2->LUMO (10%)**
8	17342.53	576.62	0.00150	Singlet-A	H-3->L+4 (12%), H-2->L+1 (20%), H-2->L+3 (17%)
9	17712.74	564.57	0.01350	Singlet-A	H-4->LUMO (15%), H-3->L+1 (16%), H-3->L+3 (28%)
10	18589.46	537.94	0.02060	Singlet-A	H-10->LUMO (29%), H-6->LUMO (18%)
11	**19429.08**	**514.69**	**0.31940**	**Singlet-A**	**H-5->LUMO (49%)**
12	**19945.28**	**501.37**	**0.40410**	**Singlet-A**	**H-6->LUMO (67%)**
13	20473.57	488.43	0.00430	Singlet-A	H-10->L+3 (13%), H-2->L+4 (22%)
14	21532.58	464.41	0.02290	Singlet-A	H-10->LUMO (11%), H-2->L+1 (14%), H-1->L+1 (17%),
15	21580.17	463.39	0.09370	Singlet-A	H-2->L+1 (18%), H-1->L+1 (59%)
16	22121.36	452.05	0.01350	Singlet-A	H-7->LUMO (70%)
17	22599.65	442.48	0.01620	Singlet-A	H-10->LUMO (10%), H-3->L+4 (14%), HOMO->L+3 (15%)
18	23160.21	431.78	0.00210	**Singlet-A**	H-8->LUMO (78%), H-7->LUMO (10%)
19	23448.95	426.46	0.02220	**Singlet-A**	H-11->LUMO (58%), HOMO->L+3 (10%)
20	23536.87	424.87	0.00220	Singlet-A	H-9->LUMO (73%)
21	23619.94	423.37	0.05830	Singlet-A	H-11->LUMO (15%), H-9->LUMO (15%), H-3->L+1 (18%)
22	**24233.73**	**412.65**	**0.11780**	**Singlet-A**	**H-10->LUMO (11%), H-2->L+1 (26%)**
23	24549.90	407.33	0.01230	Singlet-A	H-12->LUMO (75%)
24	24915.27	401.36	0.08790	Singlet-A	H-14->LUMO (12%), H-13->LUMO (54%)
25	25153.20	397.56	0.03230	Singlet-A	H-4->L+1 (63%)
26	25380.65	394.00	0.01040	Singlet-A	H-15->LUMO (11%), H-3->L+1 (24%)
27	25528.25	391.72	0.00460	Singlet-A	H-14->LUMO (69%), H-13->LUMO (17%)
28	25723.44	388.75	0.03890	Singlet-A	H-15->LUMO (37%), H-1->L+2 (40%)
29	25928.30	385.68	0.03220	Singlet-A	H-15->LUMO (21%), H-1->L+2 (38%)
30	26192.85	381.78	0.01780	Singlet-A	H-5->L+1 (64%)

Table S10: Summary of UV-vis spectral data of **7f**

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	4615.910	2166.42	0.09060	Singlet-A	HOMO->LUMO (117%)
2	11126.41	898.76	0.09960	Singlet-A	H-2->LUMO (22%), HOMO->L+1 (71%)
3	12239.46	817.03	0.00040	Singlet-A	H-3->LUMO (65%), H-1->LUMO (16%)
4	13556.56	737.65	0.01110	Singlet-A	H-2->LUMO (11%), H-1->LUMO (74%)
5	**14017.10**	**713.41**	**0.16550**	**Singlet-A**	**H-2->LUMO (34%), HOMO->L+1 (20%), HOMO->L+2 (10%)**
6	15776.20	633.87	0.05700	Singlet-A	H-5->LUMO (10%), HOMO->L+2 (66%)
7	**17256.23**	**579.50**	**0.10870**	**Singlet-A**	**H-5->LUMO (11%), H-4->LUMO (48%), H-2->LUMO (10%)**
8	17342.53	576.62	0.00150	Singlet-A	H-3->L+4 (12%), H-2->L+1 (20%), H-2->L+3 (17%)
9	17712.74	564.57	0.01350	Singlet-A	H-4->LUMO (15%), H-3->L+1 (16%), H-3->L+3 (28%)
10	18589.46	537.94	0.02060	Singlet-A	H-10->LUMO (29%), H-6->LUMO (18%)
11	**19429.08**	**514.69**	**0.31940**	**Singlet-A**	**H-5->LUMO (49%)**
12	**19945.28**	**501.37**	**0.40410**	**Singlet-A**	**H-6->LUMO (67%)**
13	20473.57	488.43	0.00430	Singlet-A	H-10->L+3 (13%), H-2->L+4 (22%)
14	21532.58	464.41	0.02290	Singlet-A	H-10->LUMO (11%), H-2->L+1 (14%), H-1->L+1 (17%),
15	21580.17	463.39	0.09370	Singlet-A	H-2->L+1 (18%), H-1->L+1 (59%)
16	22121.36	452.05	0.01350	Singlet-A	H-7->LUMO (70%)
17	22599.65	442.48	0.01620	Singlet-A	H-10->LUMO (10%), H-3->L+4 (14%), HOMO->L+3 (15%)
18	23160.21	431.78	0.00210	**Singlet-A**	H-8->LUMO (78%), H-7->LUMO (10%)
19	23448.95	426.46	0.02220	**Singlet-A**	H-11->LUMO (58%), HOMO->L+3 (10%)
20	23536.87	424.87	0.00220	Singlet-A	H-9->LUMO (73%)
21	23619.94	423.37	0.05830	Singlet-A	H-11->LUMO (15%), H-9->LUMO (15%), H-3->L+1 (18%)
22	**24233.73**	**412.65**	**0.11780**	**Singlet-A**	**H-10->LUMO (11%), H-2->L+1 (26%)**
23	24549.90	407.33	0.01230	Singlet-A	H-12->LUMO (75%)
24	24915.27	401.36	0.08790	Singlet-A	H-14->LUMO (12%), H-13->LUMO (54%)
25	25153.20	397.56	0.03230	Singlet-A	H-4->L+1 (63%)
26	25380.65	394.00	0.01040	Singlet-A	H-15->LUMO (11%), H-3->L+1 (24%)
27	25528.25	391.72	0.00460	Singlet-A	H-14->LUMO (69%), H-13->LUMO (17%)
28	25723.44	388.75	0.03890	Singlet-A	H-15->LUMO (37%), H-1->L+2 (40%)
29	25928.30	385.68	0.03220	Singlet-A	H-15->LUMO (21%), H-1->L+2 (38%)
30	26192.85	381.78	0.01780	Singlet-A	H-5->L+1 (64%)

Table S11: Summary of UV-vis spectral data of **7g**

No.	Energy (cm^{-1})	Wavelength (nm)	Oscillator Strength	Symmetry	Major contributions
1	4615.910	2166.42	0.09060	Singlet-A	HOMO->LUMO (117%)
2	11126.41	898.76	0.09960	Singlet-A	H-2->LUMO (22%), HOMO->L+1 (71%)
3	12239.46	817.03	0.00040	Singlet-A	H-3->LUMO (65%), H-1->LUMO (16%)
4	13556.56	737.65	0.01110	Singlet-A	H-2->LUMO (11%), H-1->LUMO (74%)
5	**14017.10**	**713.41**	**0.16550**	**Singlet-A**	**H-2->LUMO (34%), HOMO->L+1 (20%), HOMO->L+2 (10%)**
6	15776.20	633.87	0.05700	Singlet-A	H-5->LUMO (10%), HOMO->L+2 (66%)
7	**17256.23**	**579.50**	**0.10870**	**Singlet-A**	**H-5->LUMO (11%), H-4->LUMO (48%), H-2->LUMO (10%)**
8	17342.53	576.62	0.00150	Singlet-A	H-3->L+4 (12%), H-2->L+1 (20%), H-2->L+3 (17%)
9	17712.74	564.57	0.01350	Singlet-A	H-4->LUMO (15%), H-3->L+1 (16%), H-3->L+3 (28%)
10	18589.46	537.94	0.02060	Singlet-A	H-10->LUMO (29%), H-6->LUMO (18%)
11	**19429.08**	**514.69**	**0.31940**	**Singlet-A**	**H-5->LUMO (49%)**
12	**19945.28**	**501.37**	**0.40410**	**Singlet-A**	**H-6->LUMO (67%)**
13	20473.57	488.43	0.00430	Singlet-A	H-10->L+3 (13%), H-2->L+4 (22%)
14	21532.58	464.41	0.02290	Singlet-A	H-10->LUMO (11%), H-2->L+1 (14%), H-1->L+1 (17%),
15	21580.17	463.39	0.09370	Singlet-A	H-2->L+1 (18%), H-1->L+1 (59%)
16	22121.36	452.05	0.01350	Singlet-A	H-7->LUMO (70%)
17	22599.65	442.48	0.01620	Singlet-A	H-10->LUMO (10%), H-3->L+4 (14%), HOMO->L+3 (15%)
18	23160.21	431.78	0.00210	**Singlet-A**	H-8->LUMO (78%), H-7->LUMO (10%)
19	23448.95	426.46	0.02220	**Singlet-A**	H-11->LUMO (58%), HOMO->L+3 (10%)
20	23536.87	424.87	0.00220	Singlet-A	H-9->LUMO (73%)
21	23619.94	423.37	0.05830	Singlet-A	H-11->LUMO (15%), H-9->LUMO (15%), H-3->L+1 (18%)
22	**24233.73**	**412.65**	**0.11780**	**Singlet-A**	**H-10->LUMO (11%), H-2->L+1 (26%)**
23	24549.90	407.33	0.01230	Singlet-A	H-12->LUMO (75%)
24	24915.27	401.36	0.08790	Singlet-A	H-14->LUMO (12%), H-13->LUMO (54%)
25	25153.20	397.56	0.03230	Singlet-A	H-4->L+1 (63%)
26	25380.65	394.00	0.01040	Singlet-A	H-15->LUMO (11%), H-3->L+1 (24%)
27	25528.25	391.72	0.00460	Singlet-A	H-14->LUMO (69%), H-13->LUMO (17%)
28	25723.44	388.75	0.03890	Singlet-A	H-15->LUMO (37%), H-1->L+2 (40%)
29	25928.30	385.68	0.03220	Singlet-A	H-15->LUMO (21%), H-1->L+2 (38%)
30	26192.85	381.78	0.01780	Singlet-A	H-5->L+1 (64%)

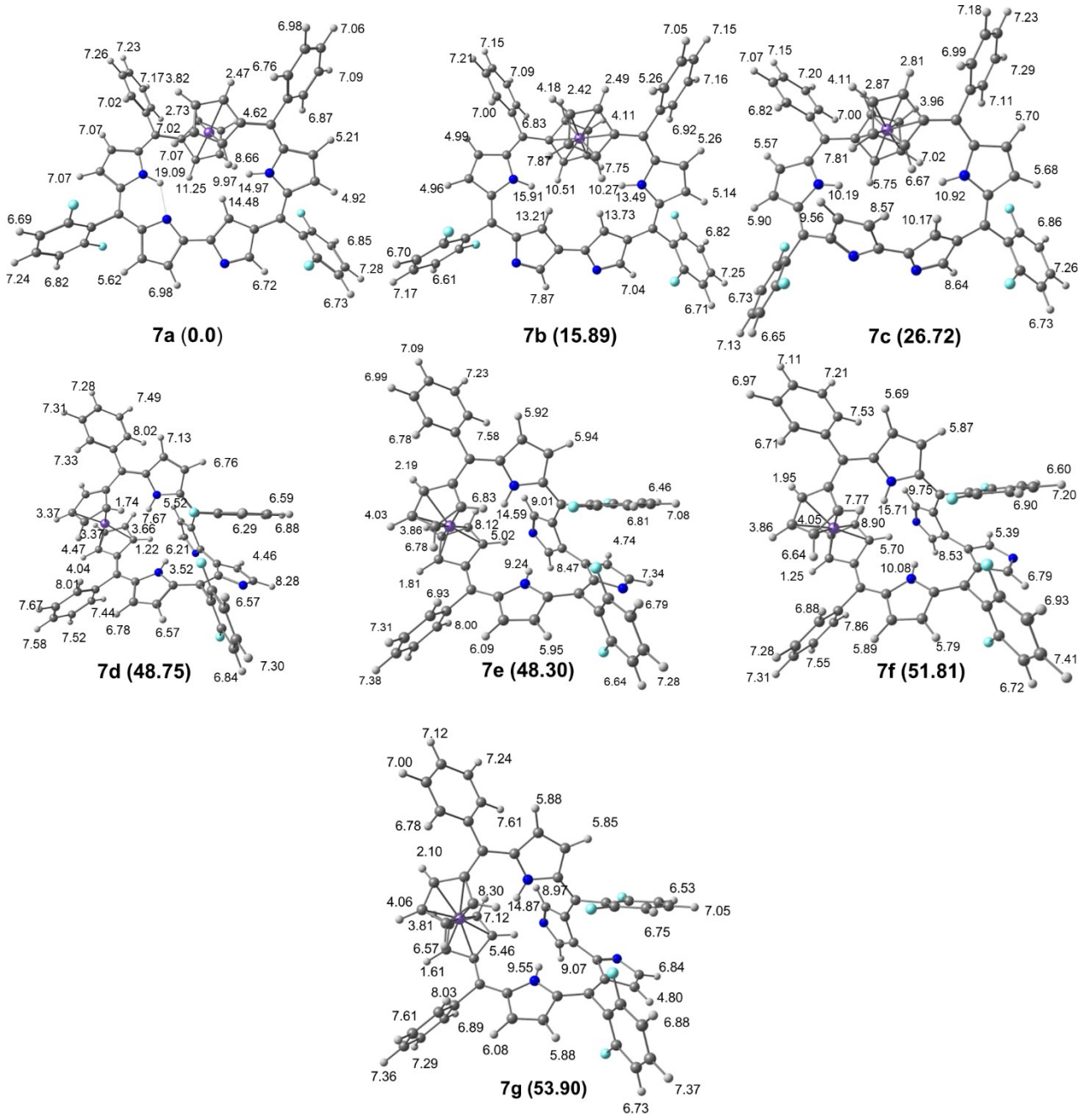


Fig. S55 ^{1}H chemical shifts predicted for the Isomers of **7** at uB3LYP/LanL2DZ(Fe) and 6-31G** (for rest of the atoms) level of theory.

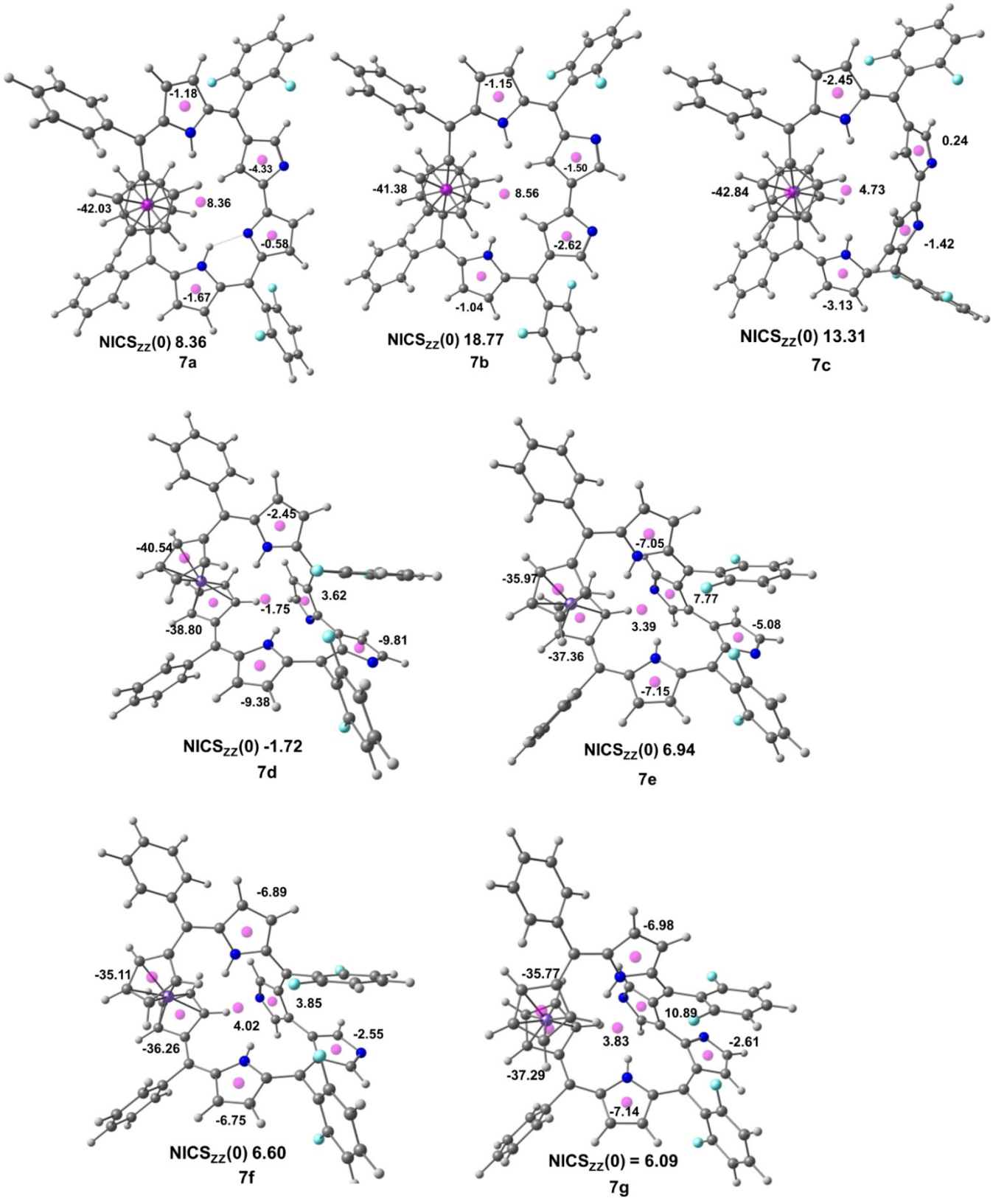


Fig. S56 NICS (0) and NICSzz(0) value for Isomers of **7** at uB3LYP/LanL2DZ(Fe) and 6-31G** (for rest of the atoms) level of theory.

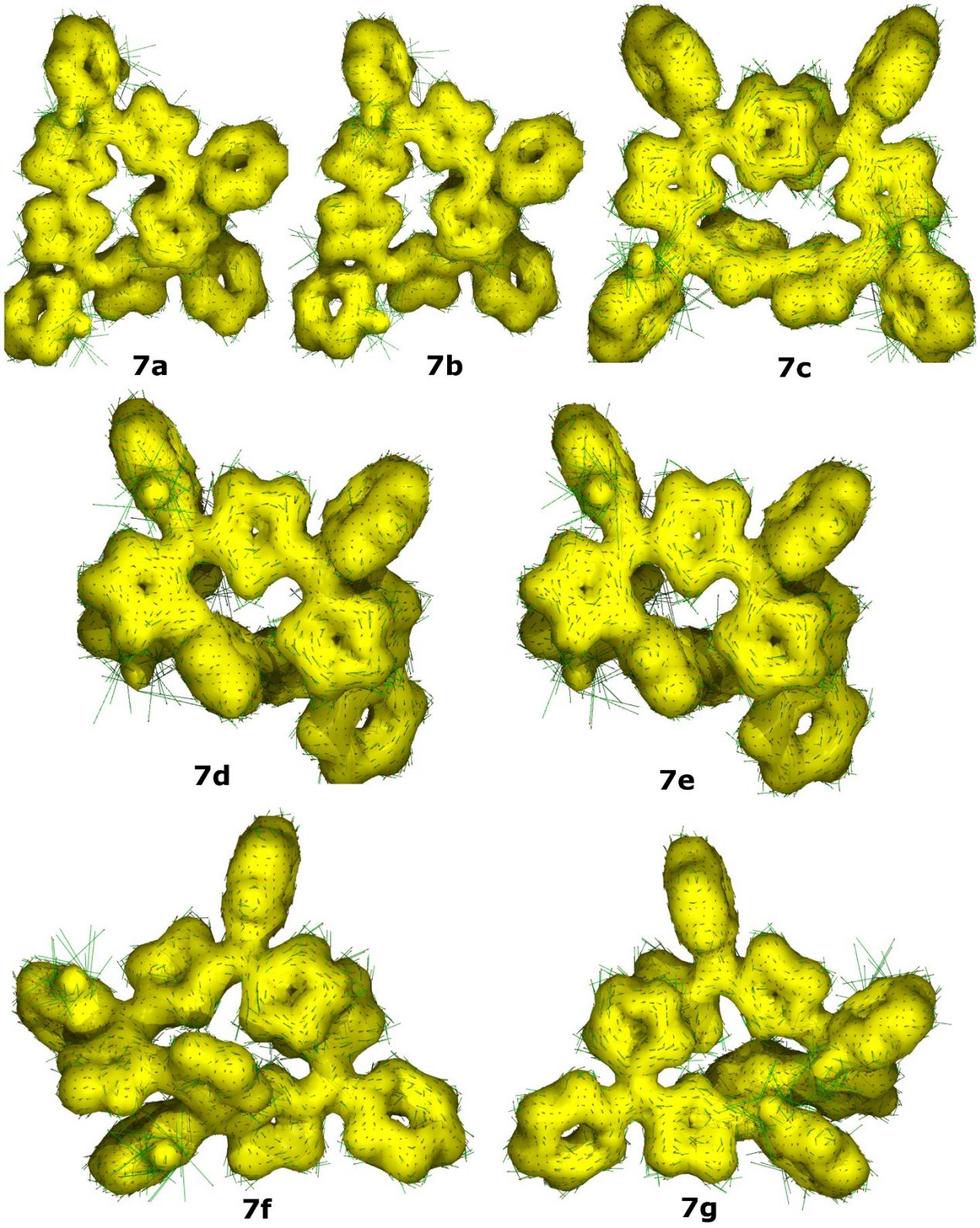


Fig. S57 AICD plot for Isomers of **7** at uB3LYP/LanL2DZ(Fe) and 6-31G** (for rest of the atoms) level of theory.

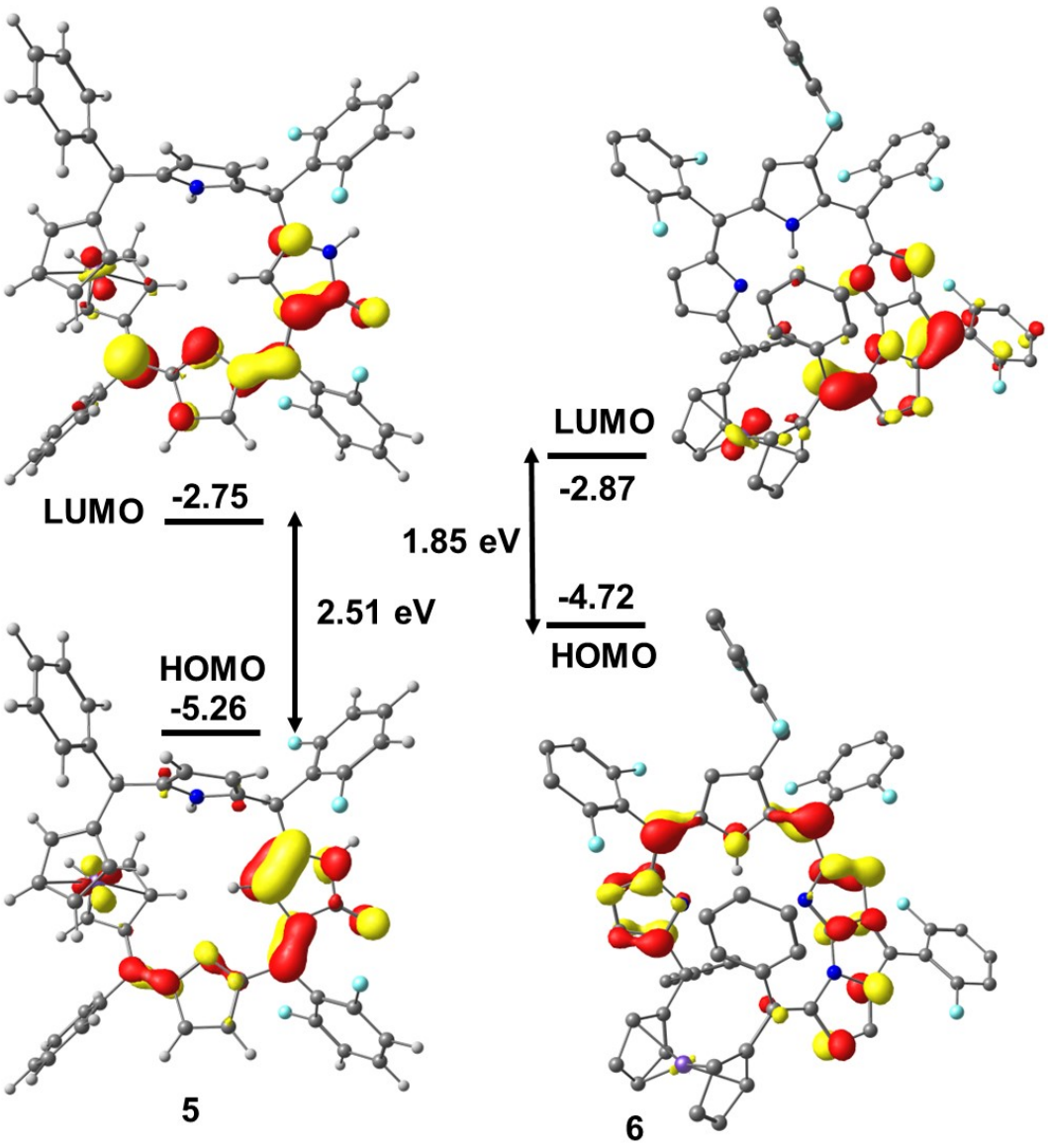


Fig. S58: HOMO-LUMO gap of DFT optimized structures of **5** and **6**.

Table 12: HOMO-LUMO Gap (eV) of isomers of **7** at uB3LYP/LanL2DZ(Fe) and 6-31G** (for rest of the atoms) level of theory.

S.No	Isomers	HOMO (eV)	LUMO (eV)	HOMO-LUMO gap (eV)
1	**7a**	-4.51	-3.18	1.34
2	**7b**	-4.54	-3.28	1.26
3	**7c**	-4.58	-3.20	1.38
4	**7d**	-4.27	-3.34	0.92
5	**7e**	-4.19	-3.38	0.81
6	**7f**	-4.21	-3.41	0.81
7	**7g**	-4.22	-3.40	0.82

Table 13: Total electronic energy (E), zero point energy (ZPE), free energy (G) in hartree of **5**, **6**, deprotonated **6** and isomers of **7a-7g** at uB3LYP/LANL2DZ (Fe) and 6-31G** (for rest of the atoms) level of theory. Relative energies of isomers of **7** are given in kcal/mol.

	E	E+ZPE	G	ΔE	ΔE+ZPE	ΔG
5	-2687.429556	-2686.729981	-2686.814487			
6	-3756.401141	-3755.502144	-3755.608186			
[6]$^{-1}$	-3755.822907	-3754.939911	-3755.045953			
7	-2819.959645	-2819.224889	-2819.311229	0.0	0.0	0.0
7b	-2819.933375	-2819.199346	-2819.28591	16.48	16.03	15.89
7c	-2819.916055	-2819.182523	-2819.26865	27.35	26.59	26.72
7d	-2819.881366	-2819.149068	-2819.233544	49.12	47.58	48.75
7e	-2819.882653	-2819.149738	-2819.234266	48.31	47.16	48.30
7f	-2819.87675	-2819.143636	-2819.228661	52.02	50.99	51.81
7g	-2819.873341	-2819.140538	-2819.225326	54.16	52.93	53.90

Cartesian Coordinates

5

E=-2687.429555, NImag =0

26	-2.425901	-2.274255	-0.867697
9	-0.309113	5.302817	-2.569528
9	1.094789	4.496902	1.858379
7	-1.844225	1.871450	-0.618060
1	-1.638507	1.449214	-1.510475
6	3.737647	2.200152	-0.125176
6	-3.650816	-0.872129	0.100072
6	-6.175527	1.807073	-0.575706
6	-1.729292	-3.748267	-2.127285
6	-1.616855	3.035597	1.257990
6	-2.936316	1.553084	0.162285
6	-2.442163	-2.782096	-2.885502
6	-3.983195	0.561110	-0.291511
6	-7.427257	2.227738	-0.125981
6	-1.027782	2.773287	0.036732
6	-2.612677	-1.309504	0.980388
6	-2.725629	-2.723051	1.138860
6	-1.790333	-1.522336	-2.716949
6	0.368338	-3.753036	-0.619501
6	-5.368791	0.978080	0.213802
6	-0.600677	-3.097499	-1.494330
6	1.469233	2.524404	-0.306650
6	0.662158	7.604040	0.050642
6	1.457007	-3.123151	-0.043698
6	-0.671557	-1.703507	-1.861444
6	0.104968	5.756079	-1.364708
6	0.217990	3.321618	-0.621320
6	0.230337	7.128876	-1.187261
6	-2.814966	2.275523	1.333910
7	2.730891	3.100420	-0.471053
6	0.813250	5.352270	0.852584
6	0.958894	6.714785	1.083952
6	-3.834052	-3.170220	0.360075
6	1.596589	1.213040	0.033607
6	2.923442	-1.574650	0.384011
6	-5.845682	0.576027	1.467964
6	3.630999	-0.294686	0.378805
6	3.003960	0.904361	0.149157
6	0.386878	4.817150	-0.367320
6	-7.096031	0.999398	1.922854
6	-4.400615	-2.030292	-0.285471
6	-0.015148	-5.703136	0.925941
6	-7.891634	1.825836	1.127931
6	0.187041	-5.215195	-0.375574
6	0.227076	-6.135236	-1.437291
6	0.071145	-7.500862	-1.202330
6	-0.181045	-7.069174	1.158835
6	-0.138484	-7.972401	0.095723
6	5.099566	-0.362839	0.621837
6	7.878746	-0.579914	1.108289
6	7.083048	0.189044	1.958150
9	4.965222	1.025249	2.524931
6	5.723298	0.285676	1.695687
6	7.314348	-1.242016	0.018635
6	5.946982	-1.119094	-0.197052
9	5.406719	-1.756619	-1.255931
7	1.746674	-1.768526	-0.194671
6	2.532630	-3.774818	0.706413
6	3.450735	-2.811843	0.966705
8	4.927217	2.467601	-0.108442
1	2.913716	4.084810	-0.589389
1	-4.027453	0.603892	-1.388003
1	0.072097	3.237839	-1.706887

6

Energy = -3756.401141, NImag =0.0

26	0.081765	5.958271	0.059765
9	-0.253828	-0.007730	6.654541
9	2.826296	2.771063	8.940319
9	2.155224	12.982884	6.580534
9	-1.122581	6.204661	10.466390
9	-1.425422	12.160472	3.622897
9	2.865921	8.558704	9.592612
9	-3.416792	10.176717	9.251335
9	0.250843	12.485291	11.086501
7	0.017947	3.942382	5.180663
7	1.376829	9.047770	3.907185
7	0.592185	9.014494	6.601522
7	0.192892	6.103697	6.429129
6	-0.336052	3.927931	3.810315
6	0.278275	4.817806	6.220413
6	0.822509	2.629126	6.937168
6	0.751224	4.011626	7.354038
6	1.856706	8.843465	2.699447
6	2.119045	7.442444	2.185896
1	1.565077	6.779483	2.857784
6	-0.888055	4.960713	3.073741
6	0.362485	10.345748	6.366288
6	-1.619112	6.068712	3.741458
6	1.200848	10.431618	4.021288
6	-0.922898	4.861706	1.609457
6	0.571901	6.214327	7.791294
6	3.603119	7.098679	2.348092
6	1.255945	1.476429	7.725344
6	0.551461	7.403703	8.485708
6	0.934125	4.914328	8.361668
1	1.305292	4.746412	9.359797
6	0.392059	2.640792	5.611307
6	1.634909	11.086074	2.798296
1	1.629845	12.150901	2.610347
6	0.308272	8.704825	7.904202
6	1.605275	7.262181	0.761309
6	-1.506063	7.407841	3.333188
1	-0.814582	7.662469	2.542028
6	-0.167681	9.893350	8.531007
6	-0.133190	10.896408	7.565792
1	-0.437517	11.923222	7.700540
6	-2.245946	8.412740	3.954453
1	-2.111458	9.446651	3.649985
6	2.079466	-0.746567	9.317036
1	2.394011	-1.591823	9.920102
6	0.714951	0.184818	7.579800
6	2.062457	10.092018	1.971142
1	2.460025	10.188021	0.969945
6	-0.661317	13.014618	4.334392
6	-0.136842	2.543979	3.412951
1	-0.387799	2.167246	2.433866
6	0.669223	11.028104	5.146614

6	2.111548	6.345046	-0.212005
1	2.905959	5.631850	-0.044400
6	0.383694	12.493160	5.106119
6	-2.525484	5.766490	4.776078
1	-2.650424	4.734557	5.089045
6	2.236848	1.573731	8.731465
6	2.651440	0.509124	9.519317
1	3.419054	0.679325	10.265710
6	-1.540451	11.271167	10.152685
6	-1.862351	5.524963	0.742200
1	-2.599181	6.246605	1.062405
6	1.133813	13.429184	5.827571
6	0.260669	1.783831	4.476596
1	0.411490	0.715888	4.486773
6	1.102076	-0.912175	8.335889
1	0.624103	-1.868098	8.154003
6	-0.105969	4.029764	0.756464
1	0.750238	3.451636	1.068743
6	0.421458	7.552953	-1.217828
1	-0.302900	7.907176	-1.938498
6	-0.680286	10.045136	9.948354
1	-1.270905	9.163946	10.213676
1	0.154252	10.091843	10.654368
6	0.543410	7.994670	0.133092
1	-0.053967	8.765176	0.598779
6	-3.277178	6.766682	5.385954
1	-3.972333	6.507879	6.179562
6	-3.168003	13.551234	10.543909
1	-3.792731	14.425790	10.695054
6	-1.675966	5.054037	-0.586335
1	-2.231169	5.378596	-1.455809
6	-3.714757	12.399138	9.976201
1	-4.755106	12.342623	9.676943
6	0.878868	14.795496	5.794712
1	1.504578	15.464827	6.373850
6	2.028479	7.955237	10.455273
6	-1.048305	12.450330	10.715430
6	0.862702	7.367904	9.945391
6	0.032386	6.751963	10.889733
6	-3.135678	8.095616	4.982370
1	-3.710640	8.878370	5.468856
6	4.009391	6.288070	3.415245
1	3.261822	5.893322	4.098136
6	1.392523	6.529861	-1.431462
1	1.535149	5.965693	-2.343107
6	-2.890981	11.294882	9.794078
6	-1.825581	13.585757	10.920824
1	-1.374900	14.465116	11.366570
6	-0.956667	14.371553	4.270462
1	-1.783548	14.705726	3.654437
6	-0.175438	15.260826	5.008568
1	-0.389484	16.324139	4.970323
6	6.325234	6.507953	2.751279
1	7.375922	6.278677	2.904903
6	0.324886	6.707733	12.248313
1	-0.368511	6.219210	12.923224
6	5.359010	5.992199	3.615751
1	5.652797	5.359014	4.448266
6	-0.597359	4.119157	-0.578020
1	-0.182231	3.616331	-1.440743
6	4.582776	7.615703	1.487989
1	4.288342	8.244687	0.652897
6	2.365506	7.936124	11.803485
1	3.288719	8.403959	12.125530
6	1.501942	7.304845	12.699590
1	1.747627	7.279385	13.756404
6	5.931800	7.322050	1.686651
1	6.676760	7.730495	1.009181
1	0.873737	8.363481	5.867897

Deprotonated 6 [6]$^{-1}$

E= -3755.8229067, NImag =0.0

26	-0.353860	6.214215	0.355504
9	0.383225	-0.049585	6.756627
9	3.005580	2.994424	9.275916
9	2.935202	12.445407	7.154934
9	-1.389364	6.248239	10.506267
9	-0.315532	12.592041	3.734328
9	2.567572	8.792023	10.077110
9	-3.499068	9.839578	8.118877
9	-1.070744	12.618705	11.050373
7	0.177169	3.938878	5.444014
7	1.669972	9.001845	3.873810
7	0.965611	8.949200	6.822255
7	0.125368	6.083246	6.718726
6	-0.098227	3.952636	4.061878
6	0.328736	4.818509	6.514013
6	1.097236	2.698153	7.184635
6	0.863600	4.055901	7.637563
6	2.267560	8.857478	2.705915
6	2.167310	7.519595	1.986835
1	1.754755	6.842037	2.739780
6	-0.784745	4.913585	3.356130
6	0.766757	10.263988	6.527876
6	-1.646235	5.936187	4.037687
6	1.820176	10.342971	4.222151
6	-0.876237	4.819130	1.893232
6	0.502255	6.241741	8.067215
6	3.523276	6.958026	1.575439
6	1.648845	1.577590	7.940363
6	0.463090	7.473781	8.700856
6	0.937516	4.976765	8.657116
1	1.322626	4.847816	9.657139
6	0.700039	2.692804	5.842117
6	2.558218	11.031881	3.182376
1	2.848920	12.074588	3.189356
6	0.361002	8.739572	8.010932
6	1.153188	7.614569	0.849498
6	-1.211559	7.232091	4.344324
1	-0.184447	7.539585	4.173995
6	-0.289863	9.947928	8.501740
6	-0.021352	10.907398	7.556787
1	-0.376902	11.929827	7.549508
6	-2.083509	8.136652	4.954091
1	-1.714403	9.122749	5.218332
6	2.696449	-0.600218	9.480793
1	3.095524	-1.425131	10.062273
6	1.286952	0.232169	7.726051
6	2.858217	10.091433	2.231188
1	3.414966	10.239213	1.314857
6	0.505181	13.205357	4.607721
6	0.324698	2.629504	3.605644
1	0.197084	2.283356	2.591267
6	1.306761	10.923023	5.384052

6	1.275649	7.176725	-0.506853
1	2.124532	6.654908	-0.924527
6	1.314019	12.420347	5.438361
6	-2.961599	5.564654	4.366632
1	-3.298377	4.553528	4.150078
6	2.573902	1.748194	8.991773
6	3.092065	0.709062	9.753310
1	3.804406	0.945386	10.536079
6	-2.221126	11.168418	9.583406
6	-2.016157	5.205947	1.102114
1	-2.903363	5.682110	1.493252
6	2.121180	13.132564	6.334312
6	0.755127	1.880003	4.661832
1	1.062042	0.845601	4.636653
6	1.784714	-0.840396	8.452683
1	1.437594	-1.838972	8.210771
6	0.094203	4.281921	0.974284
1	1.097057	3.973951	1.232981
6	-0.808556	8.141135	-0.273328
1	-1.815653	8.480153	-0.476321
6	-1.178217	10.082202	9.720923
1	-1.698030	9.133262	9.890440
1	-0.591258	10.282630	10.624166
6	-0.145499	8.202017	0.985986
1	-0.549508	8.600544	1.905166
6	-3.829816	6.472538	4.975035
1	-4.840857	6.163644	5.230214
6	-4.176783	13.200094	9.282471
1	-4.924330	13.978750	9.165255
6	-1.777517	4.841918	-0.254403
1	-2.448470	5.017035	-1.084980
6	-4.322411	11.988800	8.603929
1	-5.166661	11.790542	7.953136
6	2.143233	14.522150	6.408435
1	2.802124	15.001372	7.123918
6	1.642053	8.174401	10.828534
6	-2.130813	12.398016	10.237343
6	0.591625	7.500430	10.186371
6	-0.322231	6.870217	11.043066
6	-3.390318	7.765010	5.269457
1	-4.048002	8.469413	5.771871
6	4.058244	5.867522	2.275523
1	3.487866	5.434043	3.092775
6	0.069001	7.502371	-1.200866
1	-0.150800	7.271007	-2.234932
6	-3.347580	11.011752	8.768494
6	-3.075336	13.413077	10.110083
1	-2.931675	14.341533	10.651493
6	0.486861	14.596878	4.647587
1	-0.173185	15.134819	3.976229
6	1.315952	15.253256	5.556316
1	1.316989	16.338313	5.601298
6	6.056413	5.900195	0.911016
1	7.031493	5.493953	0.654823
6	-0.215593	6.889038	12.430288
1	-0.970313	6.384971	13.023557
6	5.310115	5.342036	1.949533
1	5.701046	4.497466	2.511026
6	-0.470455	4.271242	-0.335783
1	0.028374	3.945205	-1.238807
6	4.287457	7.510992	0.535385
1	3.896415	8.353667	-0.026281
6	1.792813	8.218432	12.211142
1	2.638801	8.751103	12.630822
6	0.854238	7.568122	13.012007
1	0.955810	7.592860	14.092847
6	5.538816	6.988851	0.205743
1	6.111616	7.435659	-0.603300

7a

E= -2819.9596452, NImag =0.0

26	-0.523470	2.801568	0.860124
9	4.375813	8.011740	1.405638
9	6.449034	5.013988	4.394744
7	1.967176	4.790502	2.821486
7	6.376479	2.889652	0.794448
6	-0.599033	3.300459	2.919562
6	-1.843288	6.636434	3.936617
1	-1.236599	7.196412	3.231699
6	-1.535317	3.296571	-0.866317
1	-2.604193	3.186124	-0.969169
6	2.609250	6.638750	3.936995
1	3.245678	7.414365	4.337031
6	0.846558	5.245962	3.514684
6	-0.862585	4.449024	-0.379422
1	-1.332547	5.362342	-0.042113
6	-0.383031	4.622576	3.526219
6	-2.923703	7.254836	4.566266
1	-3.141014	8.298634	4.357138
6	3.065229	5.605976	3.028097
6	0.359103	2.246408	2.683791
1	1.406984	2.263304	2.944495
6	-0.314103	1.136617	2.100253
1	0.151433	0.210005	1.793240
6	0.532711	4.164571	-0.357967
1	1.315273	4.840284	-0.042249
6	-0.889467	0.945026	-1.682553
6	-1.537929	5.283464	4.180262
6	-0.556829	2.276957	-1.174183
6	4.765159	4.277692	1.744674
6	7.272563	8.430784	3.533321
1	8.007164	9.189407	3.783941
6	-0.005911	-0.110349	-1.779829
6	0.728636	2.836996	-0.831854
1	1.698319	2.376006	-0.943186
6	5.342920	7.726169	2.300737
6	4.342498	5.408294	2.526344
6	6.269565	8.716935	2.607299
1	6.195677	9.681822	2.118684
6	1.297991	6.424634	4.229747
1	0.684171	6.988882	4.915747
6	6.183662	4.008724	1.426445
6	6.383738	6.222698	3.803029
6	7.337677	7.176224	4.140286
1	8.103008	6.926816	4.866370
6	-1.690251	1.480158	1.955234
1	-2.456736	0.868133	1.500472
6	4.090926	3.193708	1.181814
6	1.920067	-1.327943	-1.729848
6	-2.371569	4.568537	5.063409
1	-2.155506	3.524204	5.266963
6	3.275718	-1.615548	-1.547137
6	5.085742	2.346452	0.604697
6	5.358154	6.449409	2.876366
6	-3.450395	5.186949	5.690643

1	-4.070672	4.617240	6.377001
6	-1.864427	2.806105	2.442252
1	-2.787723	3.367245	2.438725
6	-3.082156	-0.294604	-1.590804
1	-2.663885	-0.923086	-0.810177
6	-3.731391	6.534297	5.447275
1	-4.574742	7.014456	5.934915
6	-2.289935	0.726447	-2.144756
6	-2.855674	1.540704	-3.142860
1	-2.256915	2.330839	-3.585860
6	-4.163218	1.332643	-3.577902
1	-4.576669	1.964907	-4.358508
6	-4.393198	-0.499566	-2.023982
1	-4.988947	-1.291374	-1.578735
6	-4.938141	0.312611	-3.019271
1	-5.958178	0.154175	-3.356835
6	3.778203	-2.932622	-2.029463
6	4.717353	-5.448482	-2.935419
1	5.079097	-6.411570	-3.281098
6	3.840487	-5.385459	-1.852442
1	3.503448	-6.274682	-1.332005
9	2.546551	-4.086963	-0.380493
6	3.395769	-4.138870	-1.426783
6	5.130766	-4.281489	-3.578263
1	5.805066	-4.299740	-4.426880
6	4.651293	-3.060202	-3.118443
9	5.047086	-1.939450	-3.752839
1	3.038888	2.955881	1.164437
7	1.316061	-0.161248	-1.341892
6	-0.232074	-1.378267	-2.454609
6	0.915939	-2.105803	-2.421460
1	-1.159807	-1.648557	-2.935548
1	1.090586	-3.075255	-2.863962
1	1.869609	0.515154	-0.814786
6	4.969123	1.126801	-0.053829
6	6.128635	0.296169	-0.380580
6	5.637107	-0.843004	-0.917372
6	4.177590	-0.678368	-0.969726
7	3.801922	0.507267	-0.432820
1	7.150966	0.579223	-0.179912
1	6.187377	-1.707703	-1.258948
1	7.014025	4.655578	1.688481
1	1.902706	4.100404	2.092990

7b

Energy = -2819.933375, NImag=0.0

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F, 4.346750, 8.129516, 1.912799
F, 6.780228, 4.870992, 4.305252
N, 2.094751, 4.797151, 2.859213
N, 6.438746, 3.021163, 0.685305
C, -0.550773, 3.343706, 2.841528
C, -1.738477, 6.725367, 3.693965
H, -1.100370, 7.232645, 2.976795
C, -1.724546, 3.162900, -0.892483
H, -2.793013, 3.012746, -0.933333
C, 2.692051, 6.599041, 4.079208
H, 3.314643, 7.339818, 4.558770
C, 0.934678, 5.261968, 3.485728
C, -1.069137, 4.353338, -0.474085
H, -1.554210, 5.258041, -0.134980
C, -0.309838, 4.668619, 3.426185
C, -2.820060, 7.399797, 4.261636
H, -3.011045, 8.434007, 3.989299
C, 3.189173, 5.591095, 3.168128
C, 0.393191, 2.281400, 2.588277
H, 1.447604, 2.303629, 2.816793
C, -0.310614, 1.150841, 2.084595
H, 0.132909, 0.209022, 1.791562
C, 0.334103, 4.116669, -0.518958
H, 1.111292, 4.822448, -0.259019
C, -1.062543, 0.816119, -1.714846
C, -1.468903, 5.383235, 4.020816
C, -0.735260, 2.166604, -1.231746
C, 4.918261, 4.275355, 1.939077
C, 7.436380, 8.389331, 3.777780
H, 8.177575, 9.137080, 4.040941
C, -0.171343, -0.235758, -1.769253
C, 0.545392, 2.782277, -0.971343
H, 1.527998, 2.367173, -1.138804
C, 5.402202, 7.771082, 2.672842
C, 4.491971, 5.401142, 2.720299
C, 6.335401, 8.748081, 3.000122
H, 6.192201, 9.759501, 2.637235
C, 1.358023, 6.407512, 4.266554
H, 0.708616, 6.961310, 4.927877
C, 6.271189, 4.128356, 1.346405
C, 6.626993, 6.136373, 3.869542
C, 7.590775, 7.074755, 4.218679
H, 8.433004, 6.766670, 4.827599
C, -1.692017, 1.490508, 2.002182
H, -2.481115, 0.861310, 1.614565
C, 4.266077, 3.112890, 1.547752
C, 1.809254, -1.396233, -1.632145
C, -2.331251, 4.736736, 4.927657
H, -2.138952, 3.702916, 5.197696
C, 3.169579, -1.619903, -1.458088
C, 5.196113, 2.352562, 0.773331
C, 5.500426, 6.435431, 3.088938
C, -3.409767, 5.411568, 5.494871
H, -4.053923, 4.896125, 6.201676
C, -1.840295, 2.834129, 2.446618
H, -2.763692, 3.393839, 2.472123
C, -3.237700, -0.456205, -1.657771
H, -2.820308, -1.084680, -0.876616
C, -3.659601, 6.746583, 5.164882
H, -4.503062, 7.270110, 5.605367
C, -2.454371, 0.583456, -2.190848
C, -3.025211, 1.400668, -3.184624
H, -2.435387, 2.205880, -3.612352
C, -4.324718, 1.177669, -3.635338
H, -4.740557, 1.813727, -4.411673
C, -4.539685, -0.678589, -2.108953
H, -5.126897, -1.485402, -1.679414
C, -5.088216, 0.136851, -3.099589
H, -6.101719, -0.034388, -3.450332
C, 3.757257, -2.873983, -2.014021
C, 4.900619, -5.250886, -3.028357
H, 5.342001, -6.162894, -3.417829
C, 4.186635, -5.284680, -1.830788
H, 4.055030, -6.198918, -1.263332
F, 2.945762, -4.134334, -0.193376
C, 3.637336, -4.099927, -1.352638
C, 5.049626, -4.055041, -3.731356
H, 5.596232, -4.001976, -4.665968

C, 4.476073, -2.898893, -3.214676
F, 4.600378, -1.755632, -3.908901
H, 3.276369, 2.766890, 1.795432
N, 1.134294, -0.240527, -1.285234
C, -0.339606, -1.539133, -2.391702
C, 0.832797, -2.224814, -2.306996
H, -1.248690, -1.864474, -2.874586
H, 1.044171, -3.209498, -2.697522
H, 1.607617, 0.561467, -0.910157
C, 4.966491, 1.157615, 0.111693
C, 5.949765, 0.385043, -0.665777
N, 5.433095, -0.677317, -1.203972
C, 4.041674, -0.653801, -0.862614
C, 3.755700, 0.425164, -0.028802
H, 2.062401, 4.202826, 2.045413
H, 2.837035, 0.635511, 0.499404
H, 6.994112, 0.652970, -0.780109
H, 7.065338, 4.864007, 1.424552

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Fe, -0.152975, 2.453861, -0.145605
F, -5.393634, -1.899205, 2.343623
F, -4.409901, -5.071204, -1.021428
N, -3.268806, -0.191756, -0.623320
N, -0.511184, -4.068869, 0.266572
C, -1.844630, 2.386621, -1.437291
C, -4.792187, 3.865837, 0.109667
H, -4.720593, 3.246068, 0.998534
C, 0.597093, 3.615214, 1.398607
H, 0.843241, 4.661967, 1.296108
C, -5.471121, -0.517026, -0.250038
H, -6.408698, -1.022473, -0.070973
C, -3.878680, 1.054243, -0.755184
C, -0.676804, 3.090263, 1.754441
H, -1.569338, 3.669024, 1.947718
C, -3.259937, 2.246740, -1.069898
C, -5.570293, 5.024740, 0.129316
H, -6.106266, 5.297100, 1.034250
C, -4.183584, -1.178792, -0.274286
C, -0.875861, 1.376677, -1.792989
H, -1.037609, 0.312918, -1.853601
C, 0.357611, 2.011564, -2.118419
H, 1.263591, 1.503957, -2.416639
C, -0.583168, 1.667868, 1.736068
H, -1.385674, 0.972046, 1.940172
C, 2.962351, 2.675537, 0.958921
C, -4.083327, 3.489025, -1.044945
C, 1.517293, 2.524745, 1.189196
C, -2.515537, -2.993333, -0.259634
C, -6.694810, -5.225804, 1.776682
H, -7.401914, -5.916833, 2.223972
C, 3.775695, 1.659021, 0.497408
C, 0.749437, 1.315717, 1.377975
H, 1.121418, 0.302777, 1.330533
C, -5.586681, -3.099814, 1.757326
C, -3.855585, -2.500576, -0.010579
C, -6.500261, -3.966533, 2.344245
H, -7.027697, -3.650232, 3.236996
C, -5.294227, 0.799242, -0.541990
H, -6.063580, 1.550382, -0.641150
C, -1.768312, -3.956719, 0.584580
C, -5.083441, -4.698299, 0.083866
C, -5.980846, -5.601440, 0.638590
H, -6.109611, -6.571220, 0.171684
C, 0.189204, 3.416443, -1.954394
H, 0.951626, 4.171353, -2.087466
C, -1.595813, -2.595965, -1.202290
C, 4.398557, -0.457546, -0.171147
C, -4.172189, 4.320014, -2.177438
H, -3.635755, 4.044247, -3.080459
C, 4.221052, -1.759630, -0.601408
C, -0.339425, -3.212183, -0.841532
C, -4.847396, -3.412353, 0.602993
C, -4.949132, 5.476647, -2.157818
H, -5.011688, 6.097128, -3.047429
C, -1.144883, 3.647335, -1.518976
H, -1.569462, 4.608880, -1.271868
C, 4.470921, 4.625614, 0.462610
H, 4.654369, 4.196701, -0.517986
C, -5.651953, 5.834531, -1.003998
H, -6.255395, 6.737464, -0.989360
C, 3.596443, 3.963293, 1.344547
C, 3.349271, 4.555919, 2.598226
H, 2.684576, 4.059088, 3.298073
C, 3.961474, 5.754641, 2.957117
H, 3.764463, 6.186274, 3.934483
C, 5.084404, 5.825859, 0.823218
H, 5.751620, 6.320101, 0.122534
C, 4.832542, 6.395812, 2.071832
H, 5.306681, 7.331801, 2.352467
C, 5.225138, -2.818510, -0.423092
C, 7.093397, -4.941353, -0.133484
H, 7.806836, -5.751337, -0.021754
C, 6.375304, -4.805530, -1.322300
H, 6.506614, -5.485679, -2.156015
F, 4.795154, -3.630918, -2.599143
C, 5.469545, -3.761479, -1.438713
C, 6.893579, -4.041699, 0.913160
H, 7.422762, -4.128668, 1.855307
C, 5.970949, -3.015781, 0.752363
F, 5.777749, -2.177672, 1.792620
H, -1.760531, -1.924746, -2.031797
N, 3.352585, 0.448885, -0.036491
C, 5.219455, 1.522623, 0.624628
C, 5.579939, 0.262386, 0.264517
H, 5.866427, 2.298162, 1.006710
H, 6.573401, -0.160145, 0.282865
H, 2.394291, 0.234739, -0.260161
C, 1.037241, -1.801657, -2.394811
C, 0.887192, -2.805365, -1.332795
N, 2.093179, -3.004598, -0.670814
C, 2.907910, -2.086301, -1.160589
C, 2.296364, -1.323437, -2.267562
H, -2.278817, -0.317709, -0.478740
H, 2.802821, -0.579913, -2.869835
H, -2.191655, -4.504855, 1.422252
H, 0.284809, -1.516507, -3.117397

7d
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F, 3.679331, 1.763148, 2.975491

N, 1.310304, 4.456802, 2.061433
N, 3.759873, 4.653816, -2.302820
C, -1.554615, 3.933325, 2.421593
C, -0.992576, 7.099423, 4.391198
H, -0.080451, 7.420319, 3.898735
C, -2.228257, 3.230368, -1.663919
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C, -0.813627, 4.904392, 3.194133
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C, 7.248306, 2.331699, 2.900303
H, 8.158923, 1.899194, 3.302027
C, 0.750307, 0.741185, -1.472865
C, -0.093769, 3.821902, -1.025286
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C, 3.626270, 4.055906, 1.325683
C, 7.322728, 3.453743, 2.074186
H, 8.267539, 3.922307, 1.824771
C, 1.579752, 5.183629, 4.157491
H, 1.352222, 5.549649, 5.147889
C, 2.901930, 5.628894, -1.834014
C, 4.866179, 2.328067, 2.680082
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C, -2.725496, 5.449124, 4.734033
H, -3.136084, 4.460803, 4.556940
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C, 4.879087, 3.447079, 1.831140
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H, -4.303335, 6.006843, 6.077698
C, -2.892729, 4.065609, 1.891308
H, -3.480509, 4.972327, 1.915467
C, -2.158353, -0.566767, -1.467066
H, -1.804277, -0.722473, -0.452530
C, -2.844382, 7.582520, 5.872900
H, -3.355854, 8.260055, 6.550143
C, -1.578581, 0.445121, -2.249543
C, -2.046892, 0.621472, -3.562454
H, -1.603862, 1.394627, -4.183371
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C, -3.173761, -1.376128, -1.979104
H, -3.609141, -2.151634, -1.355213
C, -3.629849, -1.188490, -3.285017
H, -4.419524, -1.818242, -3.684137
C, 4.985167, -0.882234, -0.389288
C, 6.140928, -3.372126, 0.278525
H, 6.586717, -4.328241, 0.534106
C, 5.519660, -2.610860, 1.267338
H, 5.463060, -2.939935, 2.298727
F, 4.349296, -0.658514, 1.870850
C, 4.956548, -1.390185, 0.909640
C, 6.190624, -2.914210, -1.039067
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C, 5.616276, -1.686051, -1.343242
F, 5.645192, -1.262320, -2.617810
N, 1.971564, 1.316453, -1.098205
C, 0.992709, -0.667684, -1.522428
C, 2.291163, -0.905194, -1.153214
H, 0.259065, -1.405298, -1.804231
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H, 2.192222, 2.303555, -1.115447
C, 5.134634, 2.901697, -1.357895
C, 5.264995, 1.486713, -0.921649
N, 6.601297, 1.095782, -1.031860
C, 7.225972, 2.101028, -1.610467
C, 6.373979, 3.224314, -1.865113
H, 2.525933, 6.384725, -2.515158
H, 0.872103, 4.163974, 1.198661
H, 8.289763, 2.042340, -1.825546
H, 2.052436, 6.182540, 0.125070
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7e

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N, 1.357919, 4.480254, 2.123036
C, 3.595556, 4.586649, -2.155069
C, -1.515349, 3.943009, 2.430706
C, -0.999746, 7.197919, 4.258514
H, -0.062725, 7.482627, 3.791318
C, -2.123913, 3.219529, -1.663653
H, -2.993194, 2.675934, -2.001429
C, 2.831704, 4.903586, 3.746184
H, 3.768386, 5.002151, 4.276263
C, 0.623544, 4.939525, 3.185400
C, -2.079505, 4.604206, -1.345388
H, -2.916215, 5.288372, -1.370826
C, -0.803834, 4.943599, 3.180312
C, -1.677995, 8.114183, 5.056670
H, -1.253722, 9.101382, 5.217233
C, 2.705309, 4.449347, 2.410712
C, -1.069450, 2.589885, 2.141963
H, -0.110759, 2.177248, 2.422770
C, -2.143734, 1.870288, 1.561916
H, -2.119661, 0.830475, 1.268348
C, -0.750852, 4.918279, -0.939879
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C, -0.457781, 1.279487, -1.714103
C, -1.526201, 5.907957, 4.014958
C, -0.787013, 2.657605, -1.526463

C, 2.674108, 5.460081, -0.412083
C, 7.278295, 2.299985, 3.016456
H, 8.182504, 1.852078, 3.415825
C, 0.785049, 0.650241, -1.459932
C, 0.022942, 3.729579, -0.994283
H, 1.073271, 3.681159, -0.765643
C, 6.202080, 3.984783, 1.696227
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C, 7.368554, 3.436658, 2.212270
H, 8.319309, 3.900482, 1.977031
C, 1.567844, 5.249895, 4.206459
H, 1.312070, 5.632691, 5.183606
N, 2.765755, 5.612288, -1.715112
C, 4.897527, 2.319612, 2.781422
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H, -4.179205, 2.532173, 0.894847
C, 3.469079, 4.342252, 0.080584
C, 2.973660, 0.236790, -0.939567
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H, -3.440800, 4.945905, 1.847676
C, -2.181614, -0.572417, -1.452640
H, -1.853559, -0.717311, -0.427928
C, -2.905067, 7.777374, 5.634381
H, -3.434562, 8.494317, 6.254805
C, -1.555963, 0.404859, -2.243650
C, -1.996672, 0.570484, -3.567458
H, -1.519599, 1.318135, -4.194391
C, -3.028155, -0.215288, -4.082680
H, -3.349050, -0.073396, -5.110743
C, -3.212699, -1.359855, -1.967571
H, -3.683396, -2.108717, -1.336760
C, -3.640523, -1.183353, -3.284524
H, -4.442922, -1.795610, -3.685506
C, 5.028385, -0.987523, -0.428088
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F, 4.504447, -0.691974, 1.852137
C, 5.059497, -1.457249, 0.884894
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H, 6.626381, -3.637022, -1.873707
C, 5.610168, -1.818222, -1.388358
F, 5.591716, -1.419147, -2.671944
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C, 0.987527, -0.760184, -1.411746
C, 2.294117, -1.004602, -1.058224
H, 0.224754, -1.496850, -1.605240
H, 2.754512, -1.970596, -0.927428
H, 2.276924, 2.194416, -1.293846
C, 5.174069, 2.823332, -1.249397
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H, 8.362890, 2.020873, -1.652418
H, 3.823499, 4.484077, -3.209872
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H, -0.089914, 7.508231, 3.740166
C, -2.111882, 3.209044, -1.636217
H, -2.987646, 2.674132, -1.971314
C, 2.827621, 4.965856, 3.781851
H, 3.759348, 5.089428, 4.315354
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C, -2.054662, 4.592345, -1.311725
H, -2.885403, 5.283992, -1.329533
C, -0.807222, 4.948807, 3.189018
C, -1.721006, 8.159490, 4.975111
H, -1.306962, 9.154428, 5.112468
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H, -0.071822, 2.185721, 2.459195
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H, -2.054508, 0.804025, 1.304829
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H, -0.351088, 5.856406, -0.592171
C, -0.461366, 1.260612, -1.727034
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C, -0.778141, 2.636296, -1.517979
C, 2.679615, 5.464648, -0.370089
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H, 1.094274, 3.636851, -0.759099
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H, -4.138987, 2.472324, 0.914720
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C, 4.084320, 3.780130, -1.071918
C, 4.944027, 3.482959, 2.014290

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H, -1.889602, -0.713686, -0.441322
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H, -1.514224, 1.307134, -4.211161
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C, -3.672966, -1.162489, -3.302912
H, -4.482566, -1.764437, -3.705102
C, 5.014542, -1.045820, -0.485687
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C, 5.742266, -2.689721, 1.182154
H, 5.830515, -2.957574, 2.228840
F, 4.726259, -0.664549, 1.823314
C, 5.166898, -1.471886, 0.836177
C, 6.055262, -3.156382, -1.175019
H, 6.393863, -3.789980, -1.986745
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N, 2.026323, 1.178203, -1.206762
C, 0.967574, -0.793188, -1.430354
C, 2.276125, -1.049262, -1.090182
H, 0.193122, -1.522285, -1.605312
H, 2.721497, -2.021174, -0.949687
H, 2.284855, 2.148887, -1.343088
C, 5.172862, 2.795288, -1.184195
C, 5.275301, 1.352512, -0.937263
C, 6.721368, 1.097712, -1.074440
N, 7.400279, 2.157112, -1.416066
C, 6.456257, 3.189232, -1.473648
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H, 3.790200, 4.421308, -3.157703
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7g

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7	1.369213	4.430563	2.139370
6	3.634166	4.555598	-2.135109
6	-1.512599	3.915774	2.437594
6	-0.991085	7.181271	4.234620
1	-0.056025	7.461239	3.760816
6	-2.122994	3.223975	-1.660769
1	-2.993310	2.685035	-2.003553
6	2.841063	4.899986	3.750946
1	3.777706	5.018358	4.276852
6	0.631729	4.905821	3.193721
6	-2.076167	4.606156	-1.330129
1	-2.911403	5.292321	-1.350004
6	-0.796115	4.912802	3.184921
6	-1.669046	8.106864	5.022229
1	-1.246774	9.097155	5.167950
6	2.716187	4.422350	2.425007
6	-1.071313	2.562343	2.140141
1	-0.114498	2.144109	2.418850
6	-2.148248	1.850640	1.556352
1	-2.127679	0.812688	1.256046
6	-0.747148	4.913466	-0.921437
1	-0.387146	5.876300	-0.587027
6	-0.460201	1.282446	-1.732006
6	-1.516384	5.887621	4.010170
6	-0.787348	2.658490	-1.530935
6	2.679784	5.414721	-0.401205
6	7.342570	2.389121	3.036631
1	8.261024	1.976265	3.441766
6	0.778610	0.647234	-1.470115
6	0.023747	3.722780	-0.986553
1	1.073943	3.668385	-0.760012
6	6.212959	4.020469	1.691561
6	3.699623	4.048202	1.453368
6	7.397118	3.510740	2.209306
1	8.332469	3.997068	1.958735
6	1.573178	5.239791	4.208273
1	1.315386	5.637114	5.179043
7	2.793027	5.576892	-1.699029
6	4.961078	2.336753	2.815573
6	6.121310	1.789329	3.345114
1	6.052007	0.906168	3.968589
6	-3.236982	2.755604	1.366081
1	-4.181536	2.523739	0.893868
6	3.474193	4.293808	0.095402
6	2.961170	0.218962	-0.928602
6	-2.754262	5.570843	4.616214
1	-3.166481	4.575491	4.489790
6	4.378928	0.308749	-0.739446
6	4.092183	3.748656	-1.114082
6	4.955823	3.456860	1.970345
6	-3.429833	6.500988	5.399925
1	-4.374001	6.226543	5.862098
6	-2.839329	4.027510	1.866655
1	-3.436262	4.928333	1.862753
6	-2.204536	-0.555519	-1.496685
1	-1.893736	-0.703642	-0.467042
6	-2.893162	7.774614	5.608789
1	-3.422008	8.498628	6.221508
6	-1.557692	0.416260	-2.277412
6	-1.977836	0.586674	-3.607302
1	-1.484967	1.330708	-4.226311
6	-3.009103	-0.188879	-4.138314
1	-3.313981	-0.042790	-5.170677
6	-3.234827	-1.333589	-2.027418
1	-3.721637	-2.078571	-1.404214
6	-3.641734	-1.152214	-3.350305
1	-4.443755	-1.756790	-3.763567
6	4.984061	-1.031233	-0.398940
6	6.136414	-3.521431	0.272281
1	6.580714	-4.477479	0.530087
6	5.673737	-2.678144	1.282374
1	5.739471	-2.945954	2.330753
9	4.652858	-0.650068	1.904030
6	5.109187	-1.458194	0.925104
6	6.030495	-3.146191	-1.067693
1	6.379717	-3.782234	-1.873045

6	5.457901	-1.916044	-1.371977
9	5.349488	-1.556578	-2.664368
7	2.019977	1.210089	-1.168573
6	0.967769	-0.764414	-1.406688
6	2.268340	-1.016784	-1.038957
1	0.198911	-1.495941	-1.595466
1	2.711616	-1.987823	-0.888060
1	2.284853	2.178458	-1.313739
6	5.204427	2.793225	-1.226670
6	5.303215	1.339437	-0.902826
6	6.728140	1.071388	-1.032278
6	7.296623	2.221645	-1.481665
7	6.377308	3.269934	-1.589487
1	0.959007	4.094331	1.278276
1	8.335162	2.396488	-1.737842
1	3.892761	4.472114	-3.183636
1	2.132128	6.117754	0.217306
1	7.215785	0.121685	-0.874938