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Electronic Supplementary Information

Solvent-Promoted Catalyst-Free Regioselective *N*-incorporation Multicomponent Domino Reaction: Rapid Assembly of π-Functionalized [60]Fullerene-Fused Dihydrocarbolines

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1. General Information

Reagents were purchased as reagent grade and used without further purification. 1,2-Dichlorobenzene (ODCB) and dimethyl sulfoxide (DMSO) were treated with CaH_2. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 and 150 MHz) were registered on Bruker 400 and 600 M spectrometers with tetramethylsilane (TMS) as internal standard. HRMS were measured on Bru ker Ultraflex II MALDI-TOF/TOF.

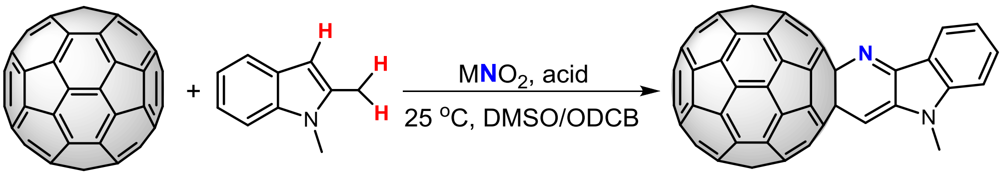
All of the DFT calculations were performed with the Gaussian 09 program.[1] The geometries optimizations were performed at the (U)B3LYP[2]/6-311++G(d,p) level. The vibrational frequencies were computed at the same level to check whether each optimized structure is an energy minimum or a transition state and to evaluate its thermal corrections at 298 K. Solvation energies were evaluated by a self-consistent reaction field (SCRF) using the SMD model[3] in dimethylsulfoxide (DMSO) at (U)M06[4]/6-311++G(d,p) level based on the structures in gas phase at the same basis set. The Gibbs free energies (ΔG) in DMSO solution are used to discuss the reaction.

2. Experimental Procedures and Control Experiments

*General Procedure for the Synthesis of Products **2**:* A dry 15-mL tube equipped with a magnetic stirrer was charged with C_{60} (36.0 mg, 0.05 mmol), **1a** (**1b**−**1ff**, 0.10 mmol), $NaNO_2$ (6.9 mg, 0.10 mmol) and CF_3CO_2H (0.10 mmol for **1a**−**1c**, **1e**, **1m**, **1o**, **1q**, **1s** and **1aa**; 0.15 mmol for **1d**, **1f**−**1l**, **1n**, **1p**, **1r**, **1t**−**1z**, **1bb** and **1cc**; 0.25 mmol for **1dd**−**1ff**). After dissolving the solids in a mixture of anhydrous ODCB (4 mL) and DMSO (1 mL) by sonication, the sealed tube was stirred under room temperature or designated temperature for 1 h. The reaction mixture was filtered through a silica gel plug to remove any insoluble material. After the solvent had been evaporated under vacuum, the residue was separated on a silica gel column with CS_2 as the eluent to recover unreacted C_{60}, and then the eluent was switched to CS_2/DCM to give product **2a** (**2b**−**2ff**, for **2h** with CS_2/EtOAc/CH_3OH as eluent).

3. Screening of the Reaction Conditions

Table S1. Optimization of the reaction conditions [a]



entry	"N" source	acid	additive	solvent (1:4)	yield (%)[b]
1	$AgNO_2$	TFA	—	DMSO/ODCB	31 (97)
2	$NaNO_2$	TFA	—	DMSO/ODCB	64 (88)
3	KNO_2	TFA	—	DMSO/ODCB	65 (87)
4	*t*-BuONO	TFA	—	DMSO/ODCB	38 (81)
5	Isopentylnitrite	TFA	—	DMSO/ODCB	49 (86)
6	$NaNO_2$	—	—	DMSO/ODCB	nr
7	$NaNO_2$	HOAc	—	DMSO/ODCB	nr
8	$NaNO_2$	TfOH	—	DMSO/ODCB	18 (60)
9	$NaNO_2$	PTSA	—	DMSO/ODCB	20 (74)
10[c]	$NaNO_2$	TFA	—	DMSO/ODCB	63 (71)
11[d]	$NaNO_2$	TFA	—	DMSO/ODCB	26 (84)
12[e]	$NaNO_2$	TFA	—	DMSO/ODCB	60 (89)
13	$NaNO_2$	TFA	—	ODCB	nr
14	$NaNO_2$	TFA	—	DMF/ODCB	61 (88)
15	$NaNO_2$	TFA	—	CH_3CN/ODCB	nr
16	$NaNO_2$	TFA	—	DCE/ODCB	trace
17	$NaNO_2$	TFA	—	MeOH/ODCB	trace
18	$NaNO_2$	TFA	—	CH_3NO_2/ODCB	< 5
19	$NaNO_2$	TFA	—	1,4-dioxane/ODCB	< 5
20	$NaNO_2$	TFA	—	actone/ODCB	13 (84)
21	$NaNO_2$	$AlCl_3$	—	DMSO/ODCB	trace
22	$NaNO_2$	$Cu(OTf)_2$	—	DMSO/ODCB	nr
23	$NaNO_2$	$Sc(OTf)_3$	—	DMSO/ODCB	nr

24[f]	$NaNO_2$	TFA	LiBr	DMSO/ODCB	7 (90)
25[f]	$NaNO_2$	TFA	KBr	DMSO/ODCB	40 (81)
26[f]	$NaNO_2$	TFA	TBAB	DMSO/ODCB	33 (73)
27[f]	$NaNO_2$	TFA	TBAI	DMSO/ODCB	< 5
28[f]	$NaNO_2$	TFA	NHPI	DMSO/ODCB	15 (85)
29	NaN_3	TFA	—	DMSO/ODCB	nr
30	$TMSN_3$	TFA	—	DMSO/ODCB	nr
31	$AgNO_3$	TFA	—	DMSO/ODCB	nr
32	$Fe(NO_3)•9H_2O$	TFA	—	DMSO/ODCB	nr

[a] All reactions were carried out with C_{60}/**1a**/“N” source /acid = 1:2:2:2 in a designated molar ratio in a mixture of anhydrous ODCB (4 mL) and DMSO (1 mL) for 1 h at 25 ^{o}C in air unless specified otherwise. [b] Isolated yield; that in parentheses was based on consumed C_{60}. [c] 3 equiv of TFA was used. [d] 1 equiv of TFA was used. [e] Under a nitrogen atmosphere. [f] 0.1 equiv of additive was employed.

4. Mechanism Studies

***[Na^15^NO~2~]-Labeled Experiment*:** A mixture of C_{60} (36.0 mg, 0.05 mmol), **1a** (14.5 mg, 0.10 mmol), $Na^{15}NO_2$ (98% ^{15}N specified by Sigma-Aldrich) (7.0 mg, 0.10 mmol) and CF_3CO_2H (7.4 μL, 0.10 mmol) was dissolved in co-solvent of anhydrous ODCB (4 mL) and DMSO (1 mL) by sonication, and then the sealed mixture was stirred under room temperature for 1 h. The reaction mixture was filtered through a silica gel plug to remove any insoluble material. After the solvent was evaporated in vacuo, the residue was separated on a silica gel column with carbon disulfide as the eluent to give unreacted C_{60} (8.7 mg, 24%), then with CS_2/DCM as the eluent to give product **2a** (28.4 mg, 65%).The ^{15}N was determined in product **2a** by HRMS. HRMS m/z (ESI) calcd. for $C_{70}H_9N^{15}N$ $[M]^+$ 878.0731, found 878.0712.

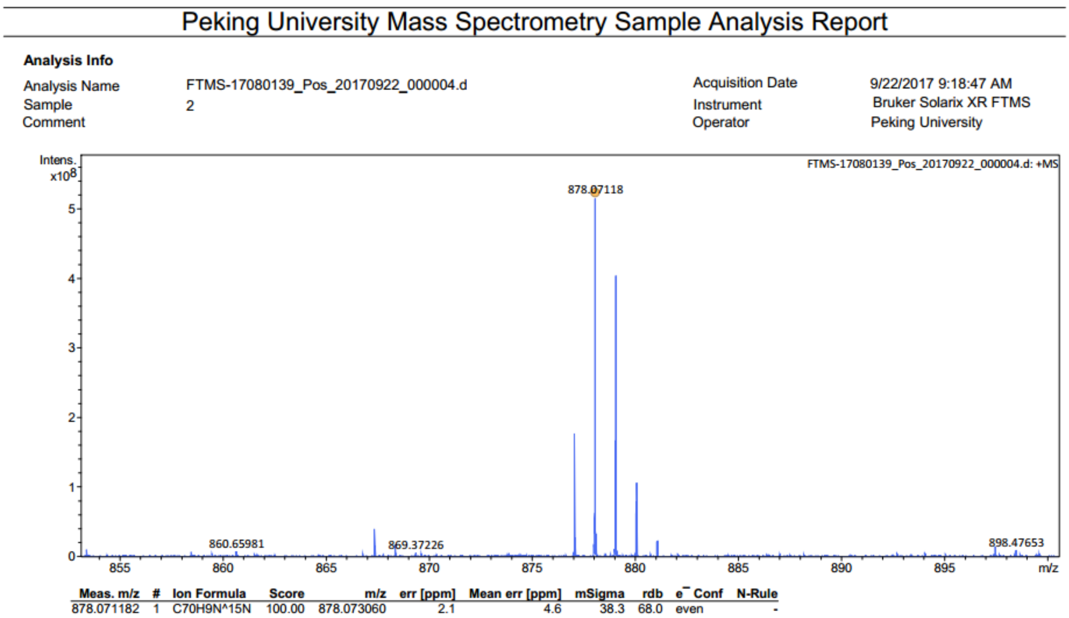
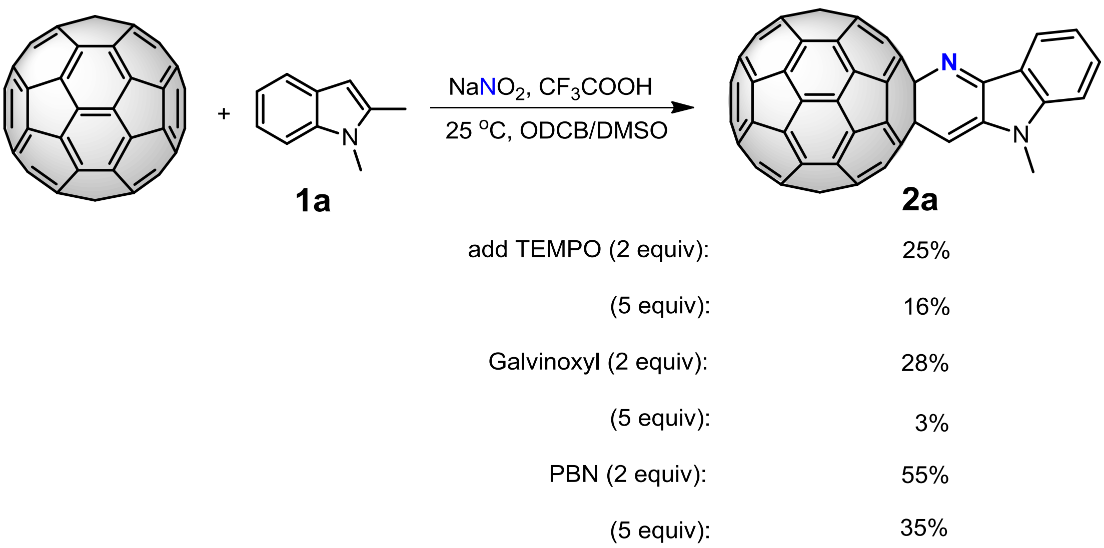


Figure S1. ^{15}N-Labeled mass spectra of **2a**

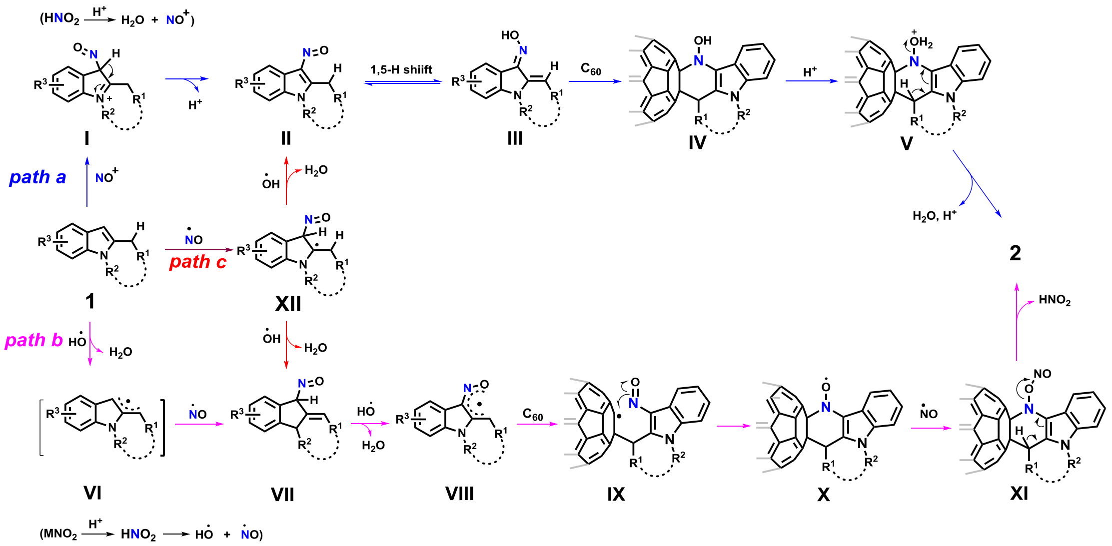
***Radical-Trapping Experiments*:** A mixture of C_{60} (36.0 mg, 0.05 mmol), **1a** (14.5 mg, 0.10 mmol), $NaNO_2$ (6.9 mg, 0.10 mmol), CF_3CO_2H (7.4 μL, 0.10 mmol) and 2,2,6,6-tetramethylpiperidine-1-oxy (TEMPO) [2,6-ditert-butyl-α-(3,5-di-tert-butyl-4-oxo-2,5-cyclohexadiene-1-ylidene)-p-tolyloxy (Galvinoxyl) or N-tert-butyl-α-phenylnitrone (PBN)] (0.10 or 0.25 mmol) was dissolved in a mixture solvent of anhydrous *o*-dichlorobenzene (4 mL) and dimethyl sulfoxide (1 mL) by sonication. The sealed tube was stirred under room temperature for 1 h. The reaction mixture was filtered through a silica gel plug to remove any insoluble material. After the solvent had been evaporated under vacuum, the residue was separated on a silica gel column with CS_2 as the eluent to recover unreacted C_{60}, and then the eluent was switched to CS_2/DCM to give product **2a**. The results confirmed that TEMPO, Galvinoxyl and PBN all could retarded the formation of **2a**. Several attempts were made to trap the radical intermediates formed during this transformation, but all of these failed.



Scheme S1. Radical-trapping experiments

Possible reaction pathways

On the basis of experimental observations and literature survey, a possible mechanism involving different pathways for the formation of C_{60}-fused dihydrocarbolines **2** is depicted in Scheme S2. Under the applied reaction conditions, the unstable nitrous acid generated *in situ* could decompose into a nitrosonium ion[5] or a nitro radical.[6] In proposed reaction **path a**, the reaction is triggered by electrophilic addition of the nitrosonium ion to indole **1**, and the corresponding intermediate **I** is generated. Then, **I** aromatized into the species **II**, which further undergoes 1,5-hydrogen migration to form the key intermediate **III**. The subsequent electrocyclic reaction of **III** with C_{60} affords the cyclic intermediate **IV**,[7] followed by an elimination process access to the final product **2**. Different from reaction **path a**, the reaction **path b** involves a free radical process. Indole **1** first undergoes a hydrogen-atom abstraction from the hydroxyl radical to generate radical species **VI**.[8] Species **VI** then reacts with a nitroso radical to form intermediate **VII**, which further converts into the active radical **VIII** through a hydrogen-atom abstraction process. Radical **VIII** is next captured by C_{60} to produce fullerenyl radical **IX**, followed by a rapid intramolecular radical cyclization to give intermediate **X**. Coupling of the nitroso radical with **X** results in the unstable species **XI**, which undergoes elimination process to afford product **2**. Compared with reaction **path b**, in reaction **path c**, indole **1** encounters the direct attack from nitroso radical to generate the corresponding radical **XII**, which further transforms into intermediate **II** or **VI** via hydrogen-atom abstraction and thus leads to the final product.



Scheme S2. Possible reaction pathways

Theoretical calculation

To better understand the mechanism of this transformation, the nitrogen incorporation reaction of indole **1a** with C_{60}, as a model reaction, was studied by density functional theory (DFT) calculations. The free energy profiles of three paths are presented in Figure S2. In reaction **path a**, a π-complex **I** was initially formed from the electrophilic addition of nitrosonium ion to indole **1a**, which is an exothermic process by 30.0 kcal/mol. The subsequent aromatization from **I** to species **II** readily proceeds by requiring 5.3 kcal/mol. Before the formation of the key intermediate **III** through 1,5-hydrogen migration, species **II** first undergoes a N=O group rotating by overcoming 20.9 kcal/mol. Then, the 1,5-hydrogen migration climbs free energy barriers of 24.4 kcal/mol access to **III**. In radical **path b**, indole **1a** undergoes a hydrogen-atom abstraction from the hydroxyl radical to generate radical species **VI** by requiring 1.6 kcal/mol. Moreover, the next coupling of species **I** with nitroso radical delivers nitrosomethyl intermediate **VII'** rather than **VII** due to 9.2 kcal/mol priority. In another reaction **path c**, the direct addition of nitroso radical to indole **1a** forms the radical species **XII** and is endothermic by 6.5 kcal/mol. And then hydroxyl radical abstracts a hydrogen-atom of **XII** to form **II'** or **VII** by overcoming 31.3 and 22.0 kcal/mol, respectively.

Thus, in proposed three reaction paths, the reaction is most likely to happen via reaction **path a**. However, the energy barrier of 33.0 kcal/mol seems to be high in room temperature. On the other hand, based on the results of the optimization experiment, we think that the solvent DMSO may also play a crucial role in this transformation.

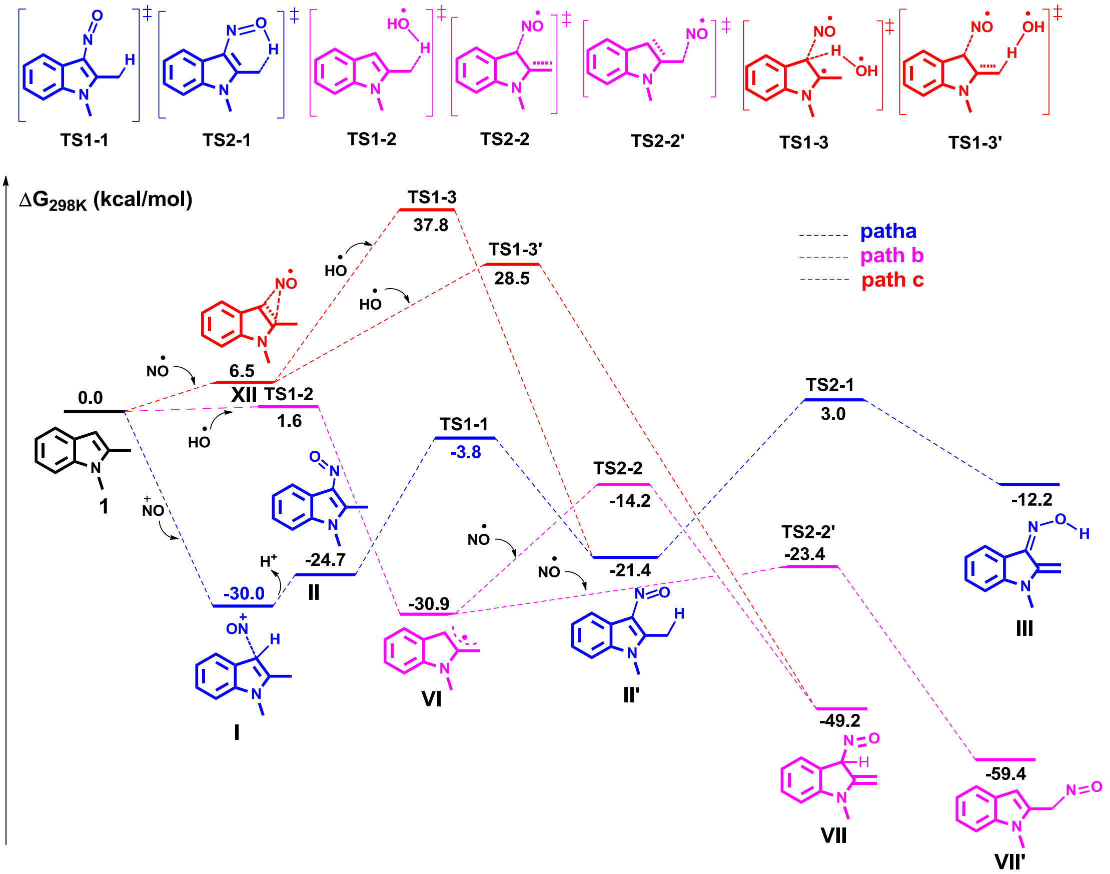


Figure S2. Energy profile of proposed mechanism

DFT energy profiles for DMF-promoted nitrogen incorporation reaction (from I to I-D2)

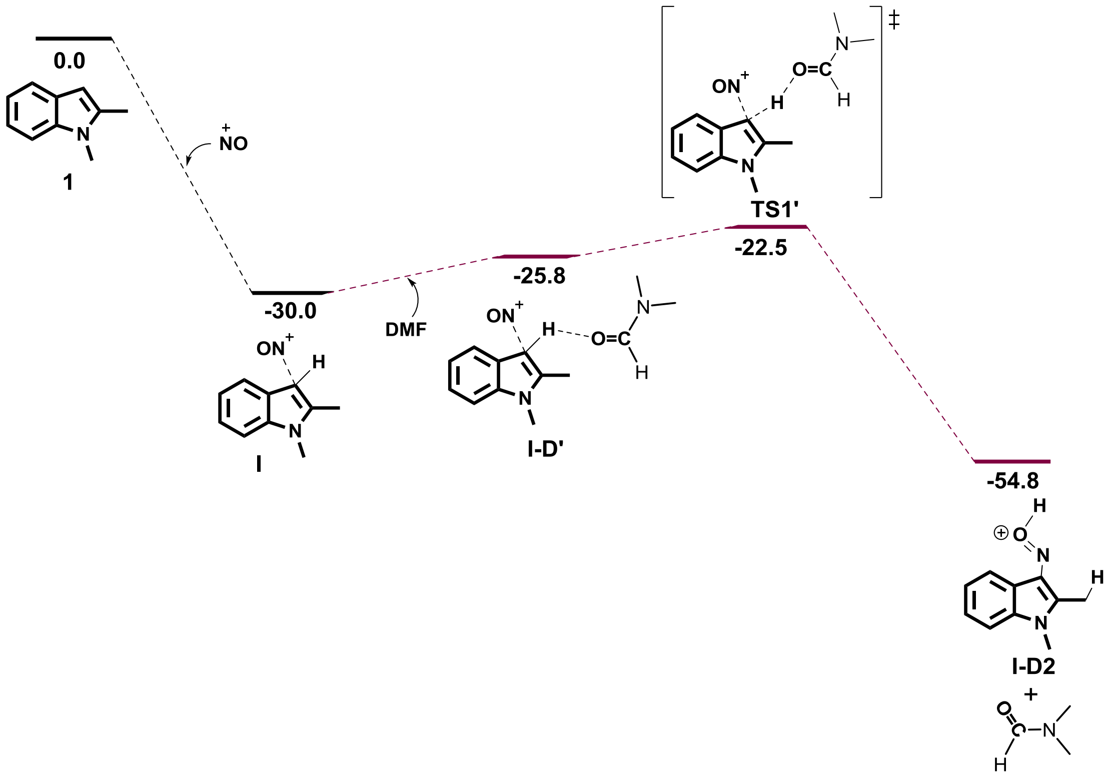
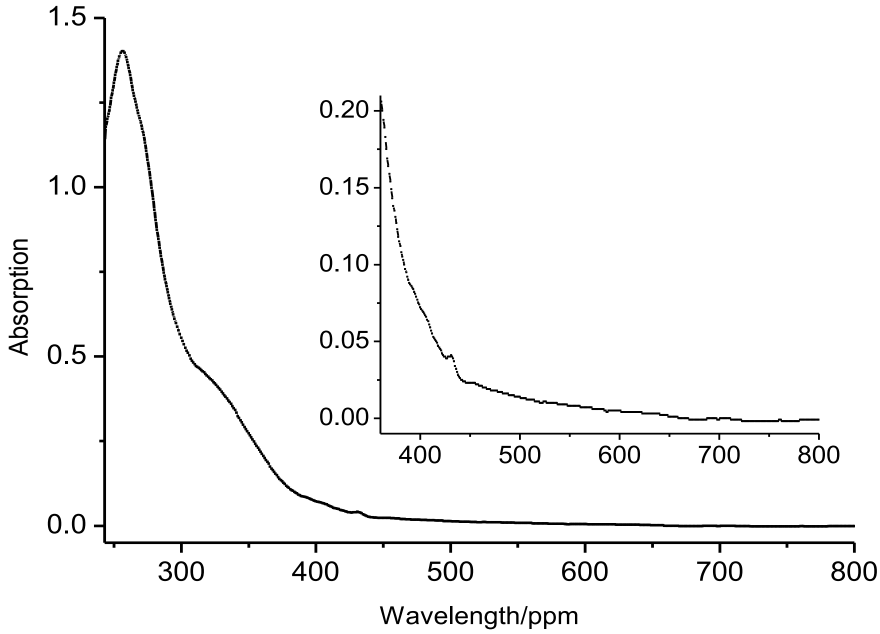


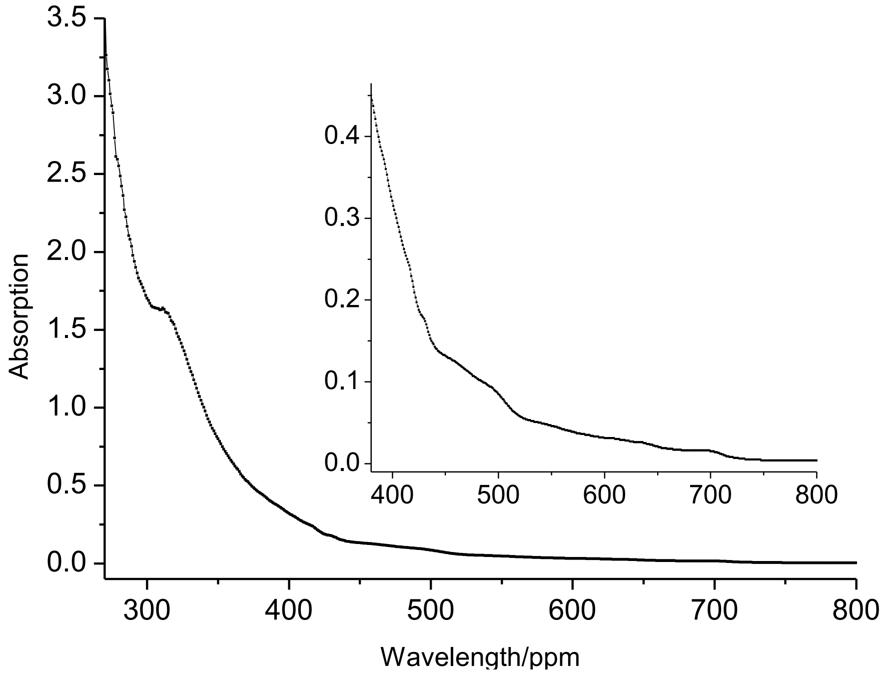
Figure S3. DMF-promoted DFT energy profiles for from **I** to **I-D2**

Seen from energy profiles for from **I** to **I-D2**: 1) like DMSO, DMF-aided deprotonation could also occur; 2) **I** could very readily proceed through **TS1′** with an activation free energy of only 7.5 kcal/mol to produce **I-D2** at room temperature. The above all indicates that **DMF** and **DMSO** play the same role in this nitrogen incorporation transformation.

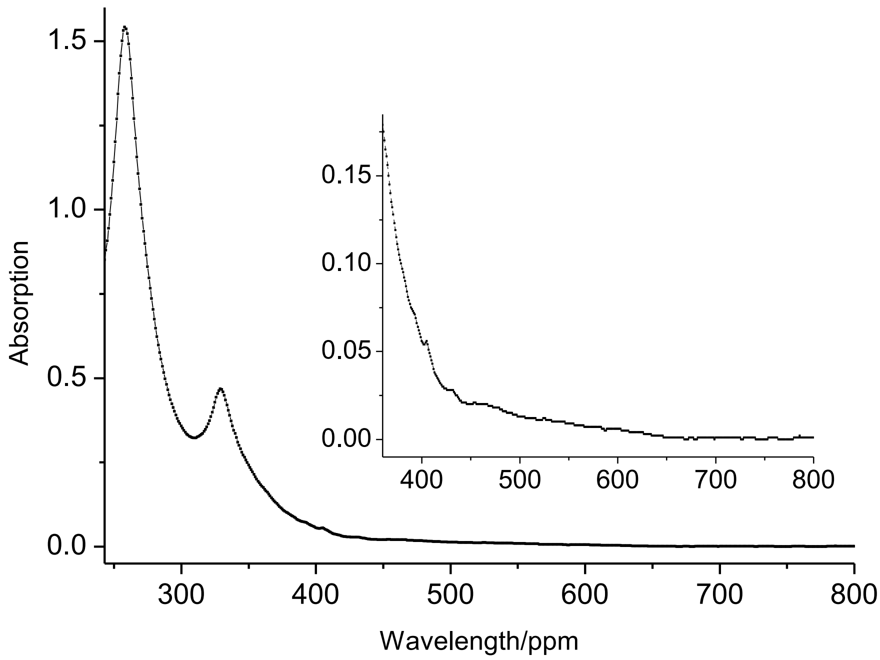
5. UV–vis Spectra of Representative Compounds



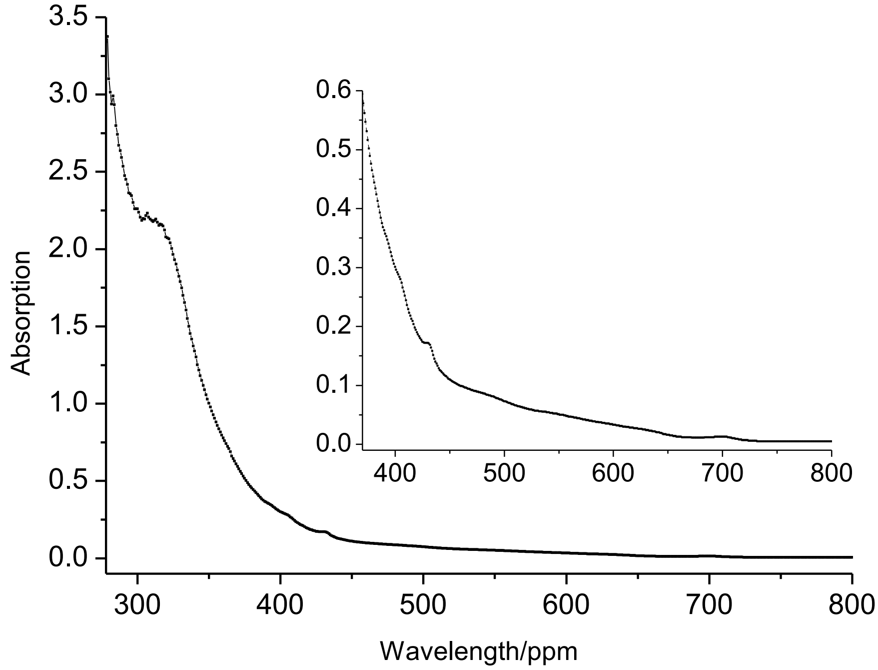
UV–vis spectrum of compound **2a** in $CHCl_3$ (1.4×10^{-5} mol/L)



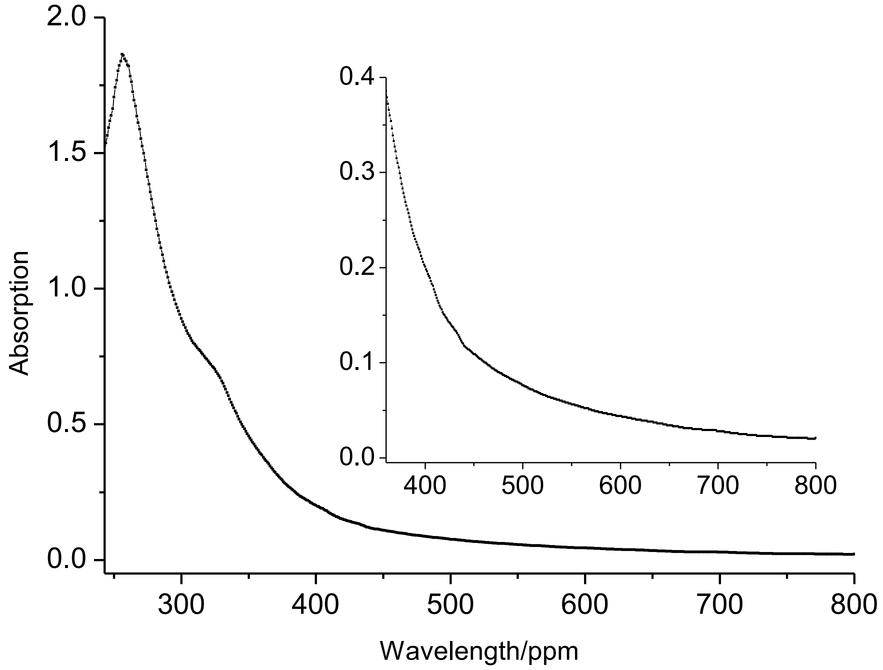
UV–vis spectrum of compound **2e** in $CHCl_3$ (1.8×10^{-5} mol/L)



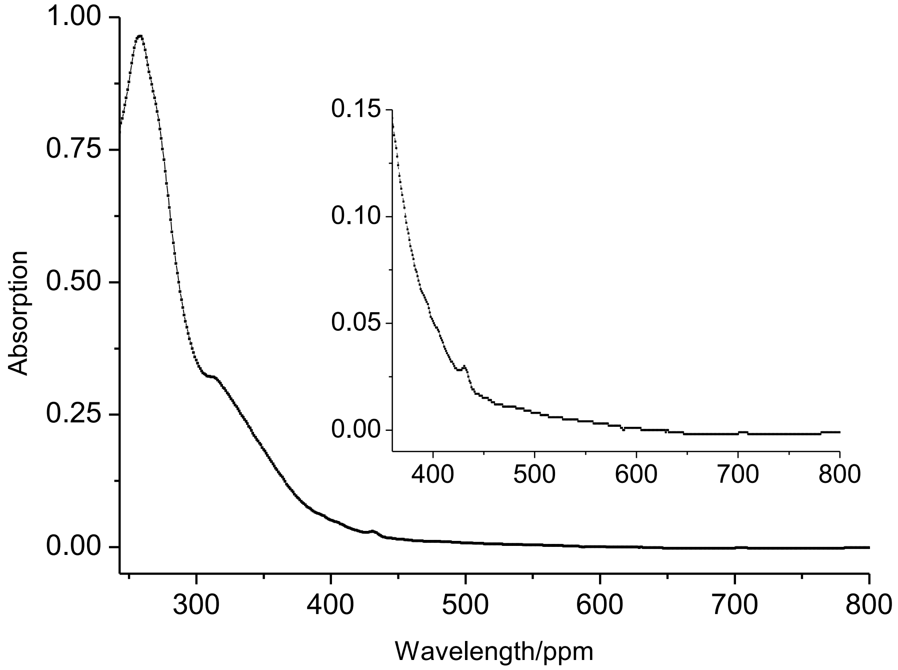
UV–vis spectrum of compound **2m** in $CHCl_3$ (1.4×10^{-5} mol/L)



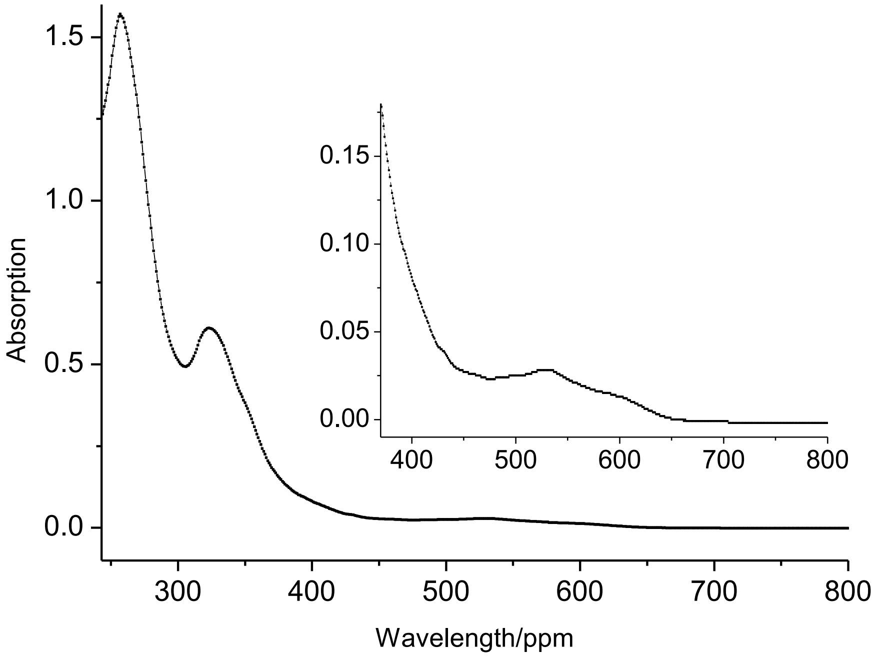
UV–vis spectrum of compound **2s** in $CHCl_3$ (1.8×10^{-5} mol/L)



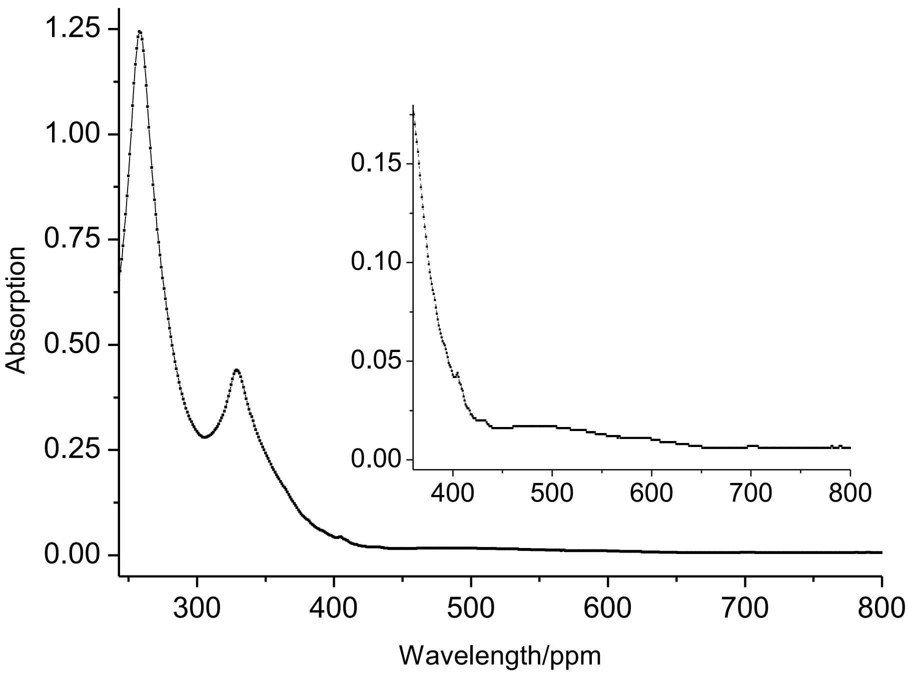
UV–vis spectrum of compound **2t** in $CHCl_3$ (1.5×10^{-5} mol/L)



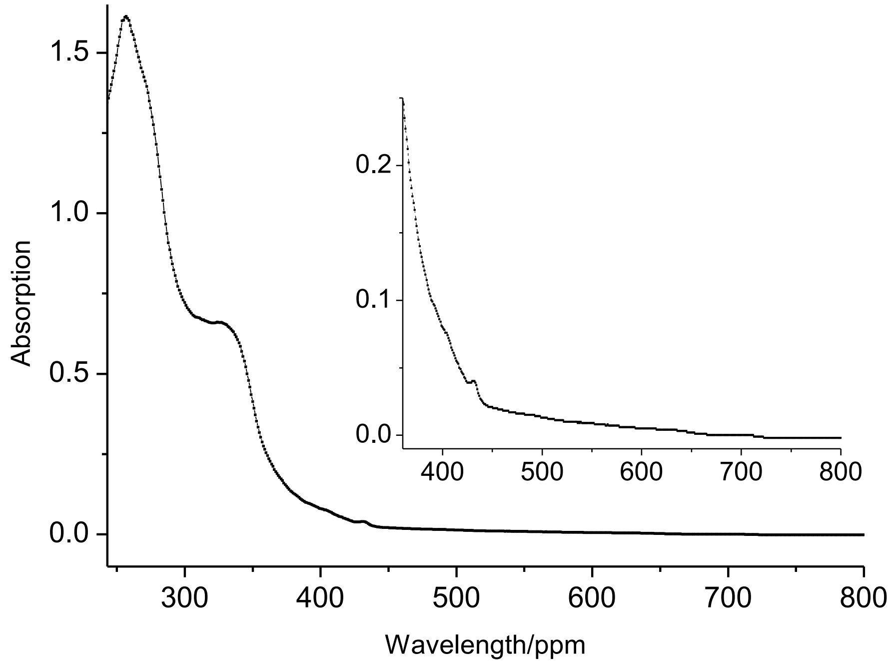
UV–vis spectrum of compound **2y** in $CHCl_3$ (1.2×10^{-5} mol/L)



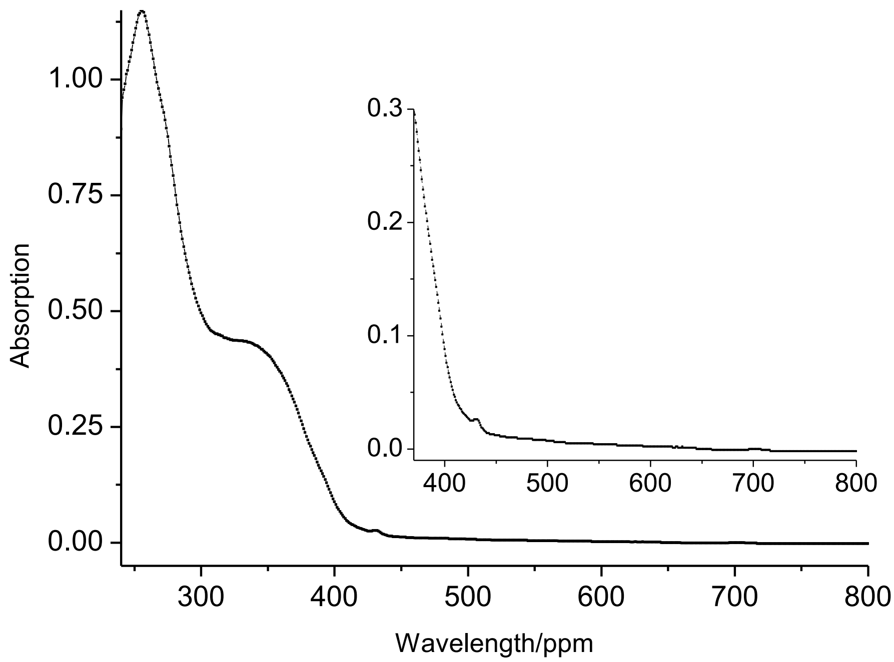
UV–vis spectrum of compound **2z** in $CHCl_3$ (1.3×10^{-5} mol/L)



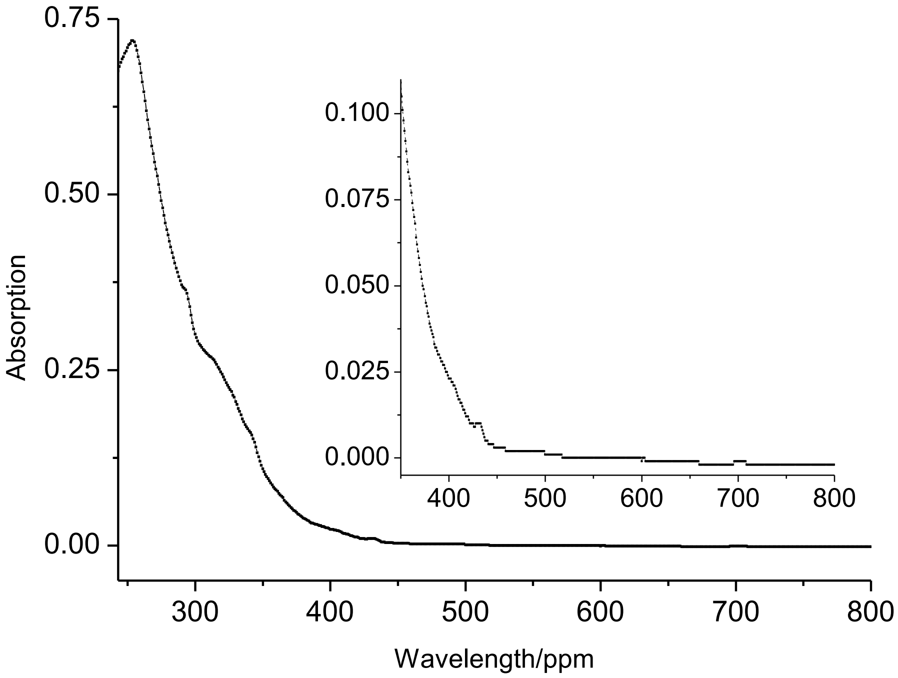
UV–vis spectrum of compound **2cc** in $CHCl_3$ (1.2×10^{-5} mol/L)



UV–vis spectrum of compound **2dd** in $CHCl_3$ (1.3×10^{-5} mol/L)



UV–vis spectrum of compound **2ee** in $CHCl_3$ (1.2×10^{-5} mol/L)



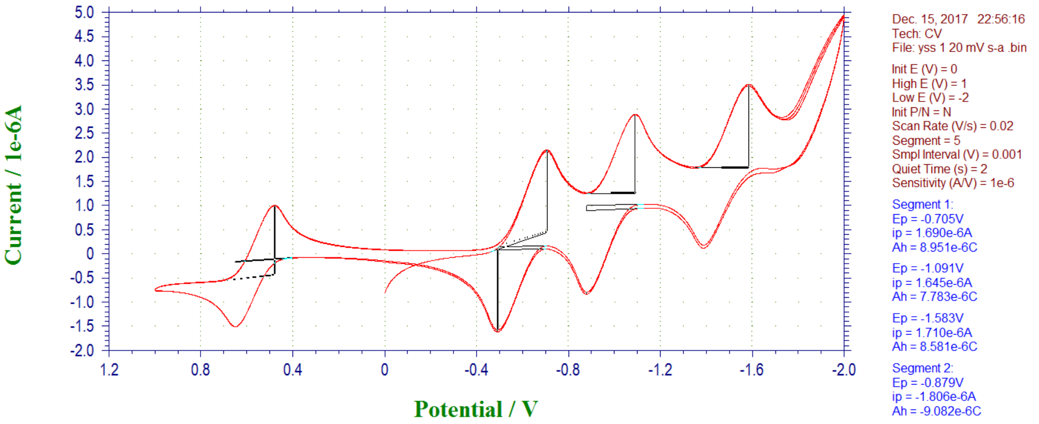
UV–vis spectrum of compound **2ff** in $CHCl_3$ (1.2×10^{-5} mol/L)

6. Table S2. Half-Wave Reduction Potentials (V) and Related Parameters of Selected Compounds, PCBM and C_{60}[a]

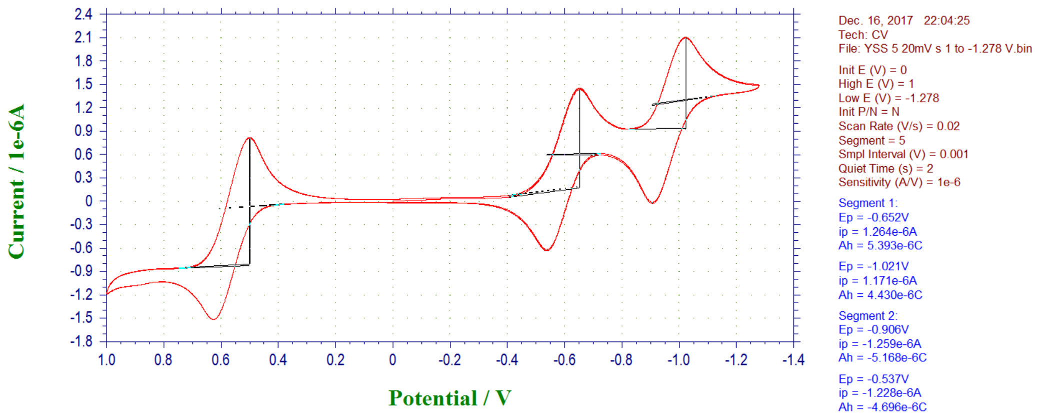
compound	$\Delta E_{(Fc/Fc+)}$[b]	E_1	ΔE_1[b]	E_2	ΔE_2[b]	E_3	ΔE_3[b]
2a	0.17	–1.17	0.22	–1.56	0.21	–2.06	0.19
2e	0.12	–1.16	0.12	–1.53	0.12	—	—
2m	0.12	–1.16	0.12	–1.53	0.12	—	—
2o	0.13	–1.17	0.12	–1.55	0.14	—	—
2r	0.12	–1.16	0.11	–1.53	0.12	—	—
2x	0.12	–1.16	0.13	–1.53	0.13	—	—
2y	0.13	–1.19	0.14	–1.59	0.14	—	—
2z	0.13	–1.18	0.13	–1.56	0.14	—	—
PCBM	0.13	–1.18	0.17	–1.58	0.17	–2.10	0.15
C_{60}	0.13	–1.08	0.15	–1.47	0.14	–1.94	0.14

[a] Versus ferrocene/ferrocenium; experimental conditions: 1 mM of compound **2** and 0.1 M of $(n\text{-Bu})_4NClO_4$ in anhydrous *o*-dichlorobenzene; reference electrode: SCE; working electrode: Pt; auxiliary electrode: Pt wire; scanning rate: 20 mV s^{-1}. [b] The distance between anodic and cathodic peaks.

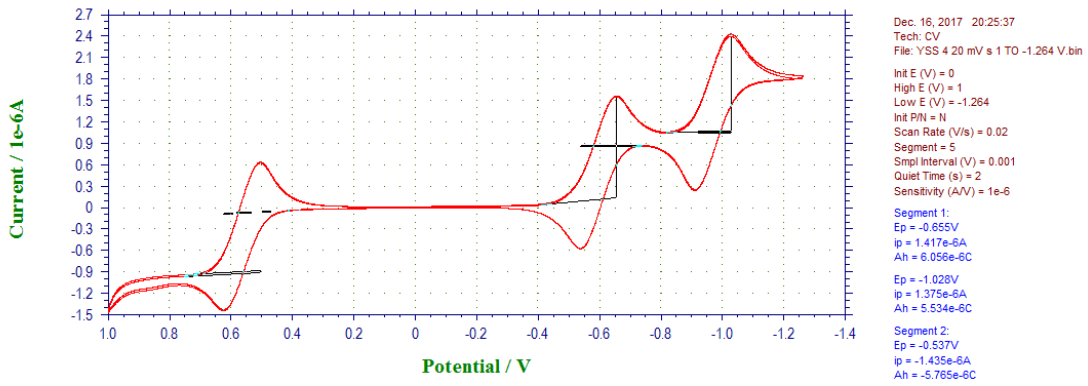
CVs of Representative Compounds



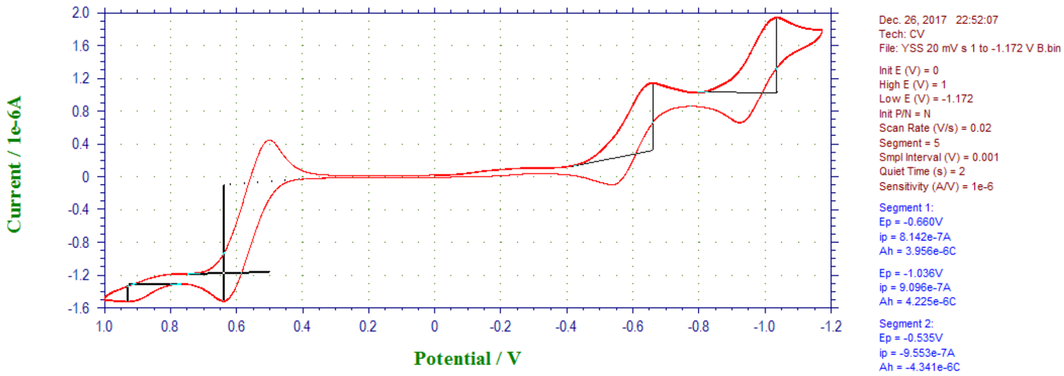
Cyclic voltammogram of compound **2a** (scanning rate: 20 mV s^{-1})



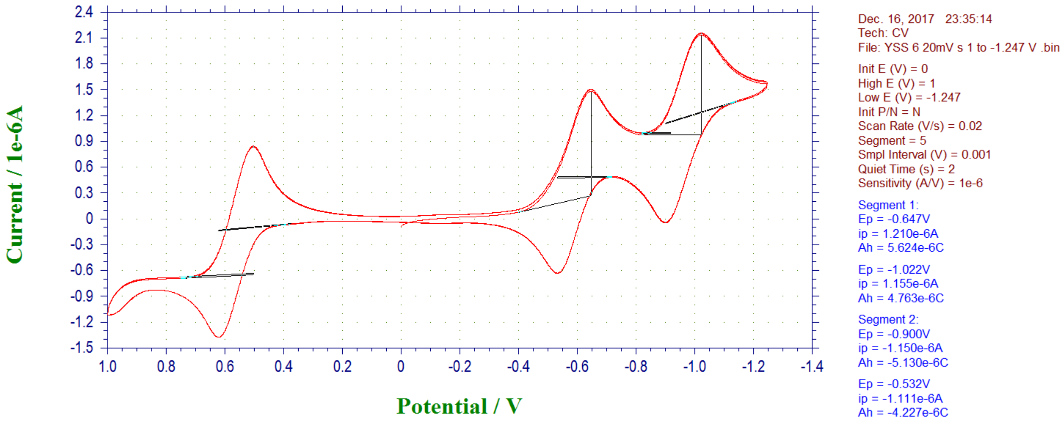
Cyclic voltammogram of compound **2e** (scanning rate: 20 mV s^{-1})



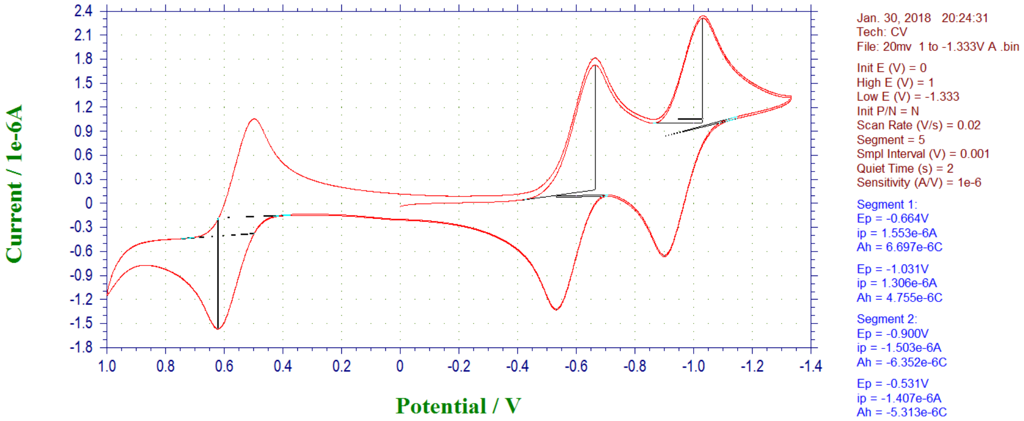
Cyclic voltammogram of compound **2m** (scanning rate: 20 mV s^{-1})



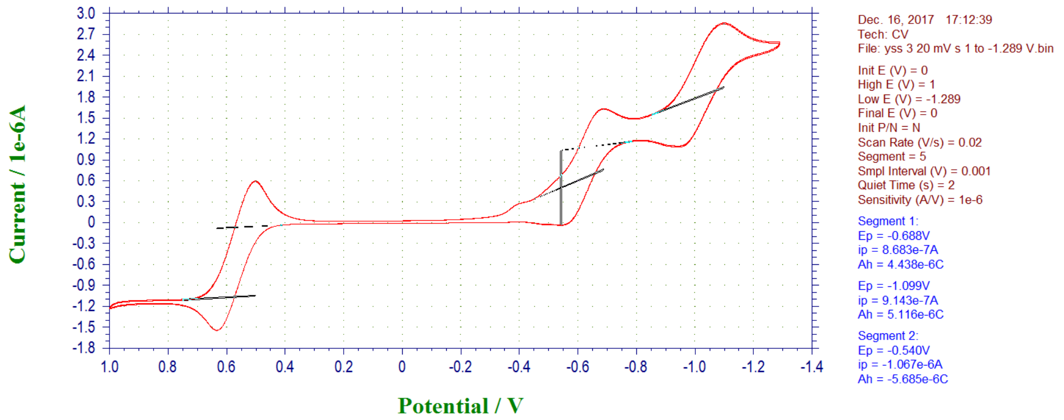
Cyclic voltammogram of compound **2o** (scanning rate: 20 mV s^{-1})



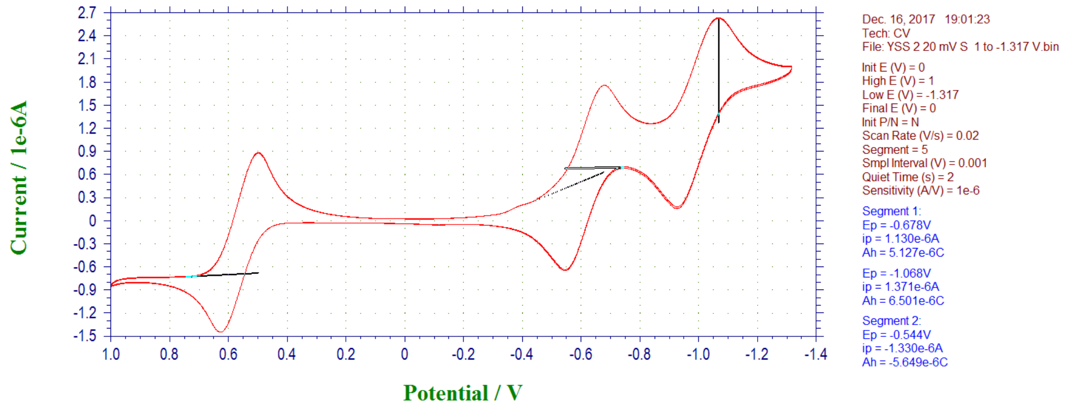
Cyclic voltammogram of compound **2r** (scanning rate: 20 mV s^{-1})



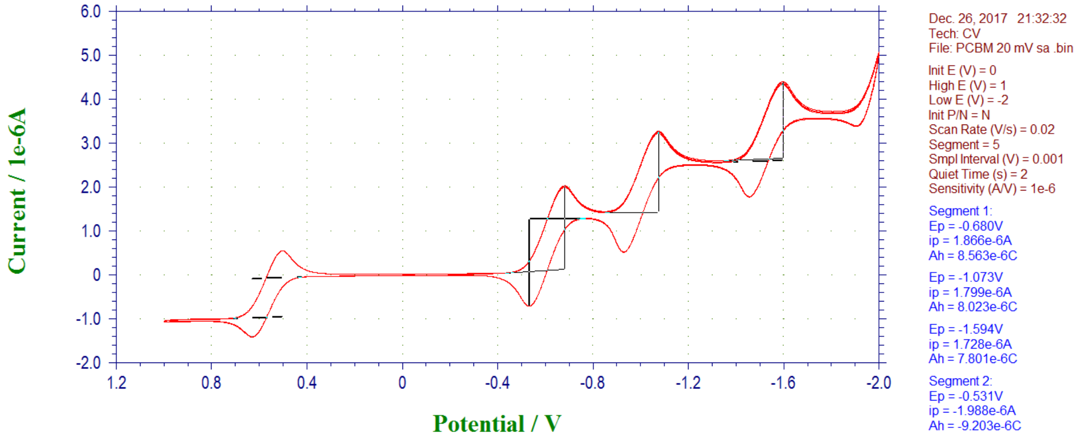
Cyclic voltammogram of compound **2x** (scanning rate: 20 mV s^{-1})



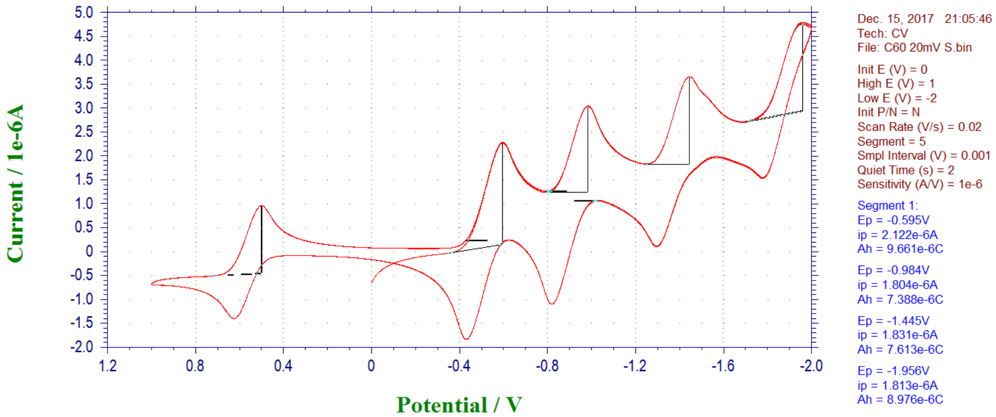
Cyclic voltammogram of compound **2y** (scanning rate: 20 mV s^{-1})



Cyclic voltammogram of compound **2z** (scanning rate: 20 mV s^{-1})

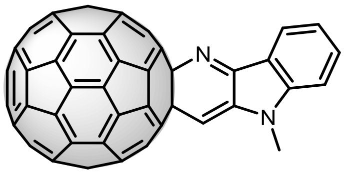


Cyclic voltammogram of compound **PCBM** (scanning rate: 20 mV s^{-1})



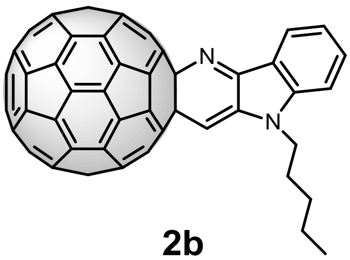
Cyclic voltammogram of compound **C_{60}** (scanning rate: 20 mV s^{-1})

7. Spectral data for Compounds 2



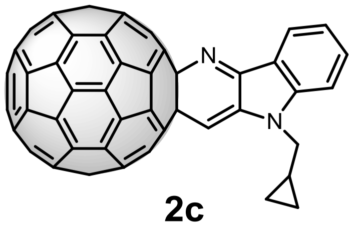
2a

Spectral data of **2a**: ^{1}H NMR (400 MHz, CD_2Cl_2/CS_2) δ 7.88 (d, J = 7.2 Hz, 1H), 7.50 (t, J = 7.6 Hz, 1H), 6.98 (t, J = 7.6 Hz, 1H), 6.91 (d, J = 8.0 Hz, 1H), 5.90 (s, 1H), 3.45 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6/CS_2 with $Cr(acac)_3$ as relaxation reagent, all 2C unless indicated) δ 158.51 (1C), 151.27 (1C), 150.34, 148.68, 148.33 (1C), 148.08 (1C), 146.62, 146.61, 146.46, 146.44, 146.38, 146.30, 145.57, 145.52, 145.41, 145.05, 144.75(4C), 144.50, 143.27, 143.21, 142.81, 142.69, 142.63, 142.27 (4C), 141.67, 141.32, 140.60, 140.54, 134.53, 134.46, 134.38 (1C), 133.44 (1C), 124.15 (1C), 123.28 (1C), 120.51 (1C), 108.26 (1C), 99.22 (1C), 84.16 (1C), 58.41 (1C), 29.06 (1C); FT-IR ν/cm^{-1} (KBr) 1632, 1605, 1510, 1469, 1427, 1383, 1331, 1258, 1137, 1108, 851, 806, 768, 742, 698, 648, 551, 525; UV-vis ($CHCl_3$) λ_{max}/nm 256, 431, 702; MALDI-TOF MS m/z calcd for $C_{70}H_8N_2$ $[M]^+$ 876.0682, found 876.0676.



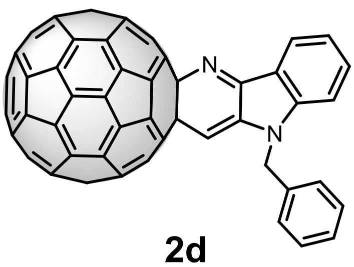
2b

Spectral data of **2b**: ^{1}H NMR (600 MHz, $CDCl_3/CS_2$) δ 7.94 (d, J = 6.6 Hz, 1H), 7.46 (t, J = 7.8 Hz, 1H), 6.96 (t, J = 6.6 Hz, 1H), 6.88 (d, J = 7.8 Hz, 1H), 5.84 (s, 1H), 3.82 (t, J = 7.2 Hz, 2H), 1.92 (t, J = 7.2 Hz, 2H), 1.53−1.49 (m, 4H), 0.99 (t, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 2C unless indicated) δ 158.73 (1C), 150.68 (1C), 149.83, 148.16, 148.11 (1C), 147.88 (1C), 146.38, 146.21 (6C), 146.15, 146.07, 145.34, 145.29, 145.21, 144.81, 144.49, 144.27, 144.23, 143.02, 142.92, 142.57, 142.45, 142.37, 142.00, 141.97, 141.41, 141.06, 140.45, 140.31, 134.43, 134.30, 133.96 (1C), 132.47 (1C), 124.07 (1C), 122.95 (1C), 119.97 (1C), 107.66 (1C), 98.78 (1C), 83.84 (1C), 58.11 (1C), 42.91 (1C), 29.68 (1C), 27.40 (1C), 22.86 (1C), 14.23 (1C); FT-IR ν/cm^{-1} (KBr) 2923, 2865, 1633, 1605, 1511, 1466, 1428, 1350, 1311, 1188, 1140, 1107, 807, 768, 742, 526; UV-vis ($CHCl_3$) λ_{max}/nm 206, 256, 431, 705; MALDI-TOF MS *m/z* calcd for $C_{74}H_{16}N_2$ $[M]^+$ 932.1308, found 932.1319.



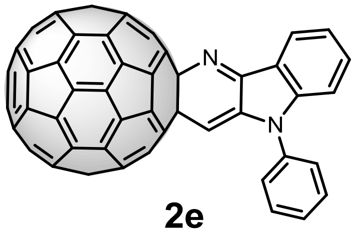
2c

Spectral data of **2c**: ^{1}H NMR (600 MHz, $CDCl_3/CS_2$) δ 7.98 (d, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 7.8 Hz, 1H), 6.99 (t, *J* = 7.2 Hz, 1H), 6.92 (d, *J* = 7.8 Hz, 1H), 5.92 (s, 1H), 3.79 (d, *J* = 6.0 Hz, 2H), 1.40 (br, 1H), 0.72 (d, *J* = 4.2 Hz, 2H), 0.50 (d, *J* = 4.2 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 2C unless indicated) δ 158.66 (1C), 150.82 (1C), 149.83, 148.17, 148.12 (1C), 147.89 (1C), 146.40, 146.24 (6C), 146.17, 146.08, 145.35, 145.31, 145.24, 144.84, 144.52, 144.27, 144.24, 143.04, 142.93, 142.59, 142.46, 142.39, 142.00 (4C), 141.43, 141.08, 140.47, 140.35, 134.43, 134.36, 133.95 (1C), 132.81 (1C), 124.11 (1C), 123.05 (1C), 120.11 (1C), 107.92 (1C), 99.23 (1C), 83.86 (1C), 58.11 (1C), 46.99 (1C), 9.98 (1C), 4.46; FT-IR ν/cm^{-1} (KBr) 1632, 1605, 1511, 1466, 1426, 1381, 1346, 1215, 1107, 1017, 807, 768, 742, 526; UV-vis ($CHCl_3$) λ_{max}/nm 256, 431, 697; MALDI-TOF MS *m/z* calcd for $C_{73}H_{12}N_2$ $[M]^+$ 916.0995, found 916.0987.



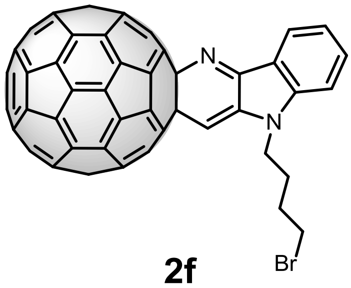
2d

Spectral data of **2d**: ^{1}H NMR (600 MHz, $CDCl_3/CS_2$) δ 7.98 (d, *J* = 7.8 Hz, 1H), 7.46−7.40 (m, 5H), 7.33−7.32 (m, 1H), 7.01 (t, *J* = 7.2 Hz, 1H), 6.84 (d, *J* = 8.4 Hz, 1H), 5.88 (s, 1H), 5.06 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 2C unless indicated) δ 158.52 (1C), 150.65 (1C), 149.71, 148.13, 148.10 (1C), 147.85 (1C), 146.38, 146.20, 146.18 (4C), 146.14, 146.06, 145.33, 145.28, 145.22, 144.82, 144.46, 144.22, 144.20, 143.00, 142.85, 142.55, 142.42, 142.34, 141.98, 141.94, 141.40, 141.03, 140.44, 140.27, 135.94 (1C), 134.43, 134.28, 134.07 (1C), 132.86 (1C), 129.07, 127.78 (1C), 126.46, 124.07 (1C), 123.00 (1C), 120.50 (1C), 108.14 (1C), 99.69 (1C), 83.85 (1C), 58.04 (1C), 46.69 (1C); FT-IR ν/cm^{-1} (KBr) 1633, 1607, 1511, 1466, 1384, 1346, 1196, 1008, 845, 808, 768, 744, 693, 526; UV-vis ($CHCl_3$) λ_{max}/nm 220, 256, 431, 706; MALDI-TOF MS *m/z* calcd for $C_{76}H_{12}N_2$ $[M]^+$ 952.0995, found 952.0985.



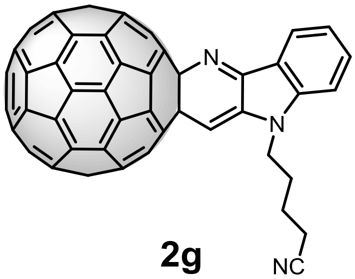
2e

Spectral data of **2e**: ^{1}H NMR (600 MHz, $CDCl_3/CS_2$) δ 8.01 (d, *J* = 7.2 Hz, 1H), 7.64 (d, *J* = 7.8 Hz, 2H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.60 (t, *J* = 7.8 Hz, 1H), 7.43−7.41 (m, 2H), 7.06 (t, *J* = 7.8 Hz, 1H), 6.95 (d, *J* = 8.4 Hz, 1H), 6.04 (s, 1H); ^{13}C NMR (150 MHz, DMSO-d_6/CS_2 with $Cr(acac)_3$ as relaxation reagent, all 2C unless indicated) δ 158.19 (1C), 150.53 (1C), 149.96, 148.60, 148.32 (1C), 148.08 (1C), 146.62, 146.60, 146.46, 146.42, 146.38, 146.31, 145.57, 145.55, 145.46, 145.14, 144.74, 144.63, 144.48, 143.27, 143.12, 142.83, 142.68, 142.63, 142.29, 142.26, 141.69, 141.31, 140.63, 140.54, 136.99 (1C), 134.56, 134.49, 134.28 (1C), 133.03 (1C), 130.64, 127.92 (1C), 126.66, 124.41(1C), 123.61 (1C), 121.73 (1C), 109.43 (1C), 100.92 (1C), 84.03 (1C), 58.24 (1C); FT-IR ν/cm^{-1} (KBr) 1670, 1609, 1593, 1498, 1463, 1398, 1314, 1209, 1093, 1029, 936, 748, 695, 551, 527; UV-vis ($CHCl_3$) λ_{max}/nm 249, 262, 431, 690; MALDI-TOF MS *m/z* calcd for $C_{75}H_{10}N_2$ $[M]^+$ 938.0838, found 938.0836.



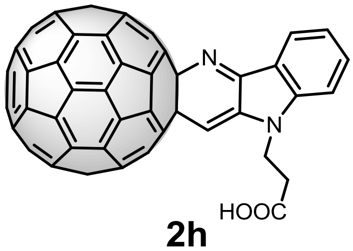
2f

Spectral data of **2f**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.97 (d, J = 7.2 Hz, 1H), 7.51−7.47 (m, 1H), 7.00 (t, J = 7.6 Hz, 1H), 6.90 (d, J = 8.0 Hz, 1H), 5.88 (s, 1H), 3.90 (t, J = 6.0 Hz, 2H), 3.54 (t, J = 6.0 Hz, 2H), 2.13−2.11 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 2C unless indicated) δ 158.54 (1C), 150.45 (1C), 149.75, 148.14, 148.10 (1C), 147.91 (1C), 146.42, 146.25, 146.21 (4C), 146.19, 146.11, 145.38, 145.33, 145.26, 144.88, 144.51, 144.25 (4C), 143.06, 142.91, 142.60, 142.48, 142.39, 142.03, 141.98, 141.44, 141.10, 140.48, 140.36, 134.46, 134.35, 134.09 (1C), 132.39 (1C), 124.21 (1C), 123.04 (1C), 120.30 (1C), 107.65 (1C), 99.10 (1C), 83.86 (1C), 58.04 (1C), 42.17 (1C), 32.97 (1C), 30.44 (1C), 26.44 (1C); FT-IR ν/cm^{-1} (KBr) 2944, 1634, 1606, 1510, 1467, 1428, 1350, 1311, 1181, 1108, 847, 807, 768, 741, 699, 526; UV-vis ($CHCl_3$) λ_{max}/nm 256, 431, 704; MALDI-TOF MS *m/z* calcd for $C_{73}H_{13}BrN_2$ $[M]^+$ 996.0257, found 998.0234.



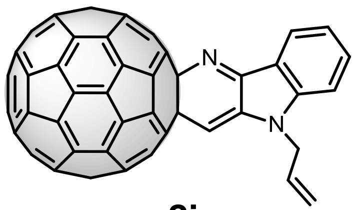
2g

Spectral data of **2g**: ^{1}H NMR (600 MHz, $CDCl_3/CS_2$) δ 7.95 (d, J = 6.6 Hz, 1H), 7.48 (t, J = 7.2 Hz, 1H), 7.00 (t, J = 7.2 Hz, 1H), 6.89 (d, J = 7.8 Hz, 1H), 5.87 (s, 1H), 3.93 (t, J = 6.0 Hz, 2H), 2.51 (t, J = 6.6 Hz, 2H), 2.15−2.11 (m, 2H), 1.95−1.84 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 2C unless indicated) δ 158.10 (1C), 150.13 (1C), 149.57, 148.00, 147.94 (1C), 147.78 (1C), 146.29, 146.14, 146.07 (6C), 145.99, 145.25, 145.21, 145.14, 144.77, 144.39, 144.11, 144.07, 142.94, 142.77, 142.49, 142.37, 142.28, 141.89, 141.86, 141.32, 140.97, 140.36, 140.23, 134.20 (4C), 133.96 (1C), 132.22 (1C), 124.15 (1C), 122.96 (1C), 120.43 (1C), 118.15 (1C), 107.43 (1C), 99.02 (1C), 83.73 (1C), 57.78 (1C), 42.06 (1C), 26.98 (1C), 23.56 (1C), 17.24 (1C); FT-IR ν/cm^{-1} (KBr) 1633, 1605, 1510, 1466, 1426, 1348, 1312, 1173, 1108, 807, 768, 742, 526; UV-vis ($CHCl_3$) λ_{max}/nm 231, 256, 431, 703; MALDI-TOF MS *m/z* calcd for $C_{74}H_{13}N_3$ $[M]^+$ 943.1104, found 943.1095.



2h

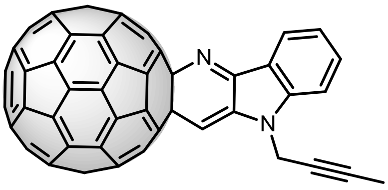
Spectral data of **2h**: ^{1}H NMR (400 MHz, DMSO-d_6/CS_2) δ 12.23 (s, 1H), 7.76 (d, J = 7.6 Hz, 1H), 7.42 (t, J = 7.6 Hz, 1H), 7.03 (d, J = 8.0 Hz, 1H), 6.91 (t, J = 7.6 Hz, 1H), 6.17 (s, 1H), 4.09 (t, J = 6.8 Hz, 2H), 2.73 (t, J = 6.8 Hz, 2H); the ^{13}C NMR spectrum of **2h** could not be obtained because of poor solubility of the product; FT-IR ν/cm^{-1} (KBr) 1711, 1633, 1607, 1512, 1468, 1428, 1388, 1351, 1313, 1182, 1110, 810, 769, 745, 526; UV-vis ($CHCl_3$) λ_{max}/nm 215, 224, 257, 431, 702; MALDI-TOF MS *m/z* calcd for $C_{72}H_{10}N_2O_2$ $[M]^+$ 934.0737, found 934.0739.



2i

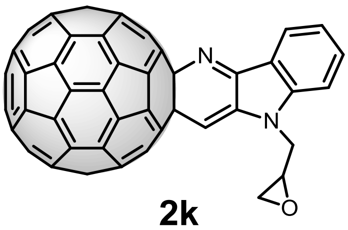
Spectral data of **2i**: ^{1}H NMR (600 MHz, $CDCl_3$/CS_2) δ 7.98 (d, J = 7.2 Hz, 1H), 7.47 (t, J = 7.8 Hz, 1H), 7.00 (t, J = 7.2 Hz, 1H), 6.89 (d, J = 8.4 Hz, 1H), 6.08−6.05 (m, 1H), 5.89 (s, 1H), 5.49 (d, J = 17.4 Hz, 1H), 5.38 (d, J = 10.2 Hz, 1H), 4.47 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$/CS_2 with Cr(acac)$_3$ as relaxation reagent, all 2C unless indicated) δ 158.56 (1C), 150.40 (1C), 149.76, 148.12, 148.08 (1C), 147.84 (1C), 146.36, 146.19, 146.17 (4C), 146.12, 146.04, 145.31, 145.26, 145.20, 144.80, 144.45, 144.24, 144.20, 143.00, 142.85, 142.53, 142.41, 142.33, 141.97, 141.92, 141.38, 141.02, 140.42, 140.28, 134.43, 134.29, 133.99 (1C), 132.41 (1C), 131.18

(1C), 124.05 (1C), 122.97 (1C), 120.30 (1C), 117.57 (1C), 108.02 (1C), 99.54 (1C), 83.79 (1C), 58.06 (1C), 45.24 (1C); FT-IR *ν*/cm^{-1} (KBr) 3051, 1632, 1605, 1511, 1466, 1428, 1381, 1345, 1198, 1108, 922, 845, 807, 768, 742, 700, 526; UV-vis ($CHCl_3$) λ_{max}/nm 225, 257, 431, 703; MALDI-TOF MS *m/z* calcd for $C_{72}H_{10}N_2$ $[M]^+$ 902.0838, found 902.0831.



2j

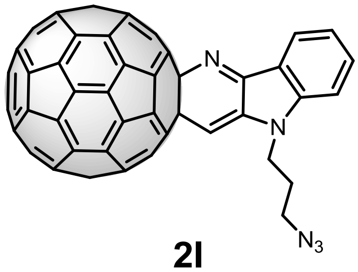
Spectral data of **2j**: ^{1}H NMR (600 MHz, $CDCl_3/CS_2$) δ 7.93 (d, *J* = 7.2 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 1H), 7.01 (t, *J* = 7.2 Hz, 1H), 6.98 (d, *J* = 8.4 Hz, 1H), 5.99 (s, 1H), 4.53 (s, 2H), 1.88 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6/CS_2 with Cr(acac)$_3$ as relaxation reagent, all 2C unless indicated) δ 158.33 (1C), 150.26, 150.01 (1C), 148.73, 148.33 (1C), 148.09 (1C), 146.64, 146.61, 146.46 (4C), 146.38, 146.31, 145.57, 145.53, 145.44, 145.10, 144.76 (4C), 144.50, 143.28, 143.20, 142.82, 142.70, 142.64, 142.29 (4C), 141.69, 141.34, 140.61, 140.55, 134.54, 134.52, 134.19 (1C), 131.18 (1C), 124.15 (1C), 123.56 (1C), 120.98 (1C), 109.07 (1C), 100.21 (1C), 84.05 (1C), 80.72 (1C), 73.96 (1C), 58.35 (1C), 32.74 (1C), 4.15 (1C); FT-IR *ν*/cm^{-1} (KBr) 2960, 2923, 2853, 1636, 1607, 1466, 1428, 1352, 1261, 1200, 1104, 1021, 806, 744, 699, 660, 526; UV-vis ($CHCl_3$) λ_{max}/nm 209, 222, 257, 431, 703; MALDI-TOF MS *m/z* calcd for $C_{73}H_{10}N_2$ $[M]^+$ 914.0838, found 914.0836.



2k

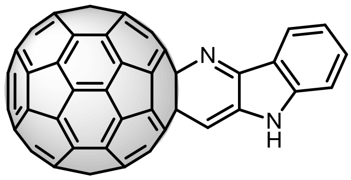
Spectral data of **2k**: ^{1}H NMR (600 MHz, $CDCl_3/CS_2$) δ 7.97 (d, *J* = 7.2 Hz, 1H), 7.51−7.48 (m, 1H), 7.03 (t, *J* = 7.2 Hz, 1H), 6.99 (d, *J* = 7.8 Hz, 1H), 6.05 (s, 1H), 4.28 (dd, *J* = 16.2, 1.6 Hz, 1H), 3.83 (dd, *J* = 16.2, 4.8 Hz, 1H), 3.42−3.40 (m, 1H), 2.95 (t, *J* = 4.8 Hz, 1H), 2.81 (dd, *J* = 4.8, 1.6 Hz, 1H); ^{13}C NMR (150 MHz,

$CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 2C unless indicated) δ 157.95 (1C), 150.36 (1C), 149.69 (1C), 149.64 (1C), 148.08, 148.00 (1C), 147.77 (1C), 146.29, 146.14 (4C), 146.06 (4C), 145.98, 145.25, 145.21, 145.14, 144.79 (1C), 144.78 (1C), 144.40, 144.15, 144.12, 142.94, 142.78, 142.48, 142.36, 142.28, 141.91, 141.89, 141.33, 140.98, 140.34, 140.24, 134.21, 134.19, 133.89 (1C), 132.84 (1C), 123.98 (1C), 123.01 (1C), 120.70 (1C), 108.08 (1C), 100.00 (1C), 83.70 (1C), 57.86 (1C), 49.97 (1C), 45.22 (1C), 44.68 (1C); FT-IR ν/cm^{-1} (KBr) 2920, 1635, 1605, 1467, 1429, 1387, 1348, 1312, 1203, 1109, 1055, 851, 809, 769, 745, 699, 668, 526; UV-vis ($CHCl_3$) λ_{max}/nm 207, 225, 256, 431, 699; MALDI-TOF MS *m/z* calcd for $C_{72}H_{10}N_2O$ $[M]^+$ 918.0788, found 918.0792.



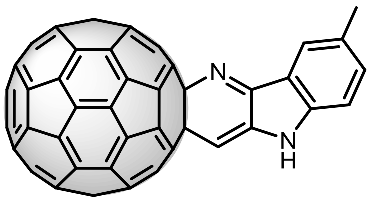
2l

Spectral data of **2l**: ^1H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.93 (d, *J* = 7.2 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.00 (t, *J* = 7.2 Hz, 1H), 6.94 (d, *J* = 8.4 Hz, 1H), 5.92 (s, 1H), 3.97 (t, *J* = 6.4 Hz, 2H), 3.61 (t, *J* = 6.4 Hz, 2H), 2.19−2.13 (m, 2H); ^{13}C NMR (150 MHz, DMSO-d_6/CS_2 with $Cr(acac)_3$ as relaxation reagent, all 2C unless indicated) δ 158.47 (1C), 150.74 (1C), 150.26, 148.63, 148.32 (1C), 148.08 (1C), 146.62, 146.61, 146.46 (4C), 146.37, 146.30, 145.56, 145.52, 145.41, 145.06, 144.82, 144.74, 144.50, 143.27, 143.19, 142.81, 142.70, 142.63, 142.27 (4C), 141.67, 141.32, 140.60, 140.49, 134.53, 134.49, 134.44 (1C), 132.56 (1C), 124.23 (1C), 123.30 (1C), 120.62 (1C), 108.40 (1C), 99.29 (1C), 84.02 (1C), 58.36 (1C), 49.24 (1C), 40.02 (1C), 27.52 (1C); FT-IR ν/cm^{-1} (KBr) 2925, 1635, 1608, 1467, 1429, 1350, 1312, 1259, 1187, 1145, 1109, 808, 769, 744, 526; UV-vis ($CHCl_3$) λ_{max}/nm 255, 426, 568, 700; MALDI-TOF MS *m/z* calcd for $C_{72}H_{11}N_5$ $[M]^-$ 945.1020, found 945.1048.



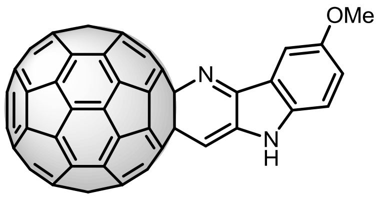
2m

Spectral data of **2m**: ^{1}H NMR (400 MHz, DMSO-d_6/CS_2) δ 9.46 (s, 1H), 7.71 (d, J = 7.2 Hz, 1H), 7.31 (t, J = 7.2 Hz, 1H), 6.85 (d, J = 8.0 Hz, 1H), 6.83 (t, J = 7.2 Hz, 1H), 5.93 (s, 1H); ^{13}C NMR (150 MHz, DMSO-d_6/CS_2 with Cr(acac)$_3$ as relaxation reagent, all 2C unless indicated) δ 159.67 (1C), 151.12 (1C), 150.40, 148.98, 148.31 (1C), 148.06 (1C), 146.74, 146.57, 146.52, 146.41, 146.34, 146.26, 145.52, 145.48, 145.35, 144.98, 144.80, 144.77, 144.50, 143.26 (4C), 142.78, 142.66, 142.63, 142.33, 142.26, 141.67, 141.30, 140.57, 140.54, 134.51 (4C), 134.08 (1C), 132.06 (1C), 124.14 (1C), 123.10 (1C), 119.86 (1C), 110.93 (1C), 100.39 (1C), 83.95 (1C), 58.57 (1C); FT-IR ν/cm^{-1} (KBr) 1610, 1509, 1460, 1428, 1337, 1253, 1215, 1182, 1047, 1025, 1005, 819, 744, 707, 576, 526; UV-vis ($CHCl_3$) λ_{max}/nm 212, 258, 329, 454, 786; MALDI-TOF MS m/z calcd for $C_{69}H_6N_2$ $[M]^+$ 862.0525, found 862.0516.



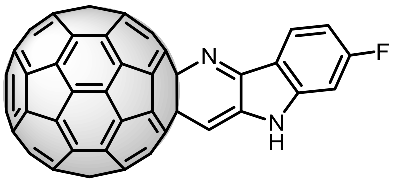
2n

Spectral data of **2n**: ^{1}H NMR (400 MHz, DMSO-d_6/CS_2) δ 9.28 (s, 1H), 7.54 (s, 1H), 7.12 (d, J = 7.2 Hz, 1H), 6.75 (d, J = 8.0 Hz, 1H), 5.88 (s, 1H), 2.36 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6/CS_2 with Cr(acac)$_3$ as relaxation reagent, all 2C unless indicated) δ 159.73 (1C), 150.41, 149.25 (1C), 148.99, 148.29 (1C), 148.04 (1C), 146.70, 146.55, 146.52, 146.38, 146.32, 146.24, 145.50, 145.46, 145.31, 144.94, 144.79, 144.74, 144.50, 143.26, 143.24, 142.76, 142.64, 142.61, 142.32, 142.25, 141.64, 141.28, 140.55, 140.52, 135.02 (1C), 134.53, 134.49, 132.40 (1C), 128.58 (1C), 124.42 (1C), 123.27 (1C), 110.74 (1C), 100.03 (1C), 83.93 (1C), 58.61 (1C), 21.38 (1C); FT-IR ν/cm^{-1} (KBr) 1699, 1617, 1511, 1486, 1428, 1327, 1289, 1208, 1187, 1130, 839, 807, 767, 552, 526; UV-vis ($CHCl_3$) λ_{max}/nm 205, 214, 257, 435, 699; MALDI-TOF MS *m/z* calcd for $C_{70}H_8N_2$ $[M]^+$ 876.0682, found 876.0671.



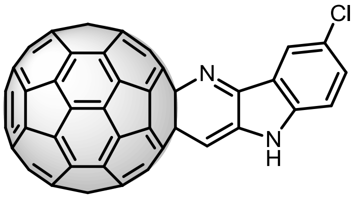
2o

Spectral data of **2o**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.44 (d, J = 2.0 Hz, 1H), 7.01 (dd, J = 8.4, 2.4 Hz, 1H), 6.85 (d, J = 8.4 Hz, 1H), 6.36 (s, 1H), 6.02 (s, 1H), 3.82 (s, 3H); the ^{13}C NMR spectrum of **2o** could not be obtained because of poor solubility of the product; FT-IR ν/cm^{-1} (KBr) 1616, 1510, 1485, 1434, 1330, 1292, 1273, 1199, 1171, 1151, 1029, 840, 812, 768, 747, 552, 526; UV-vis ($CHCl_3$) λ_{max}/nm 258, 329, 786; MALDI-TOF MS *m/z* calcd for $C_{70}H_8N_2O$ $[M]^+$ 892.0631, found 892.0619.



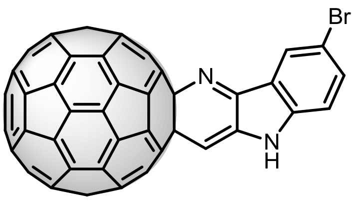
2p

Spectral data of **2p**: ^{1}H NMR (400 MHz, DMSO-d_6/CS_2) δ 9.70 (s, 1H), 7.71 (dd, J = 8.4, 6.0 Hz, 1H), 6.59 (dd, J = 9.6, 2.0 Hz, 1H), 6.55−6.50 (m, 1H), 5.98 (s, 1H); ^{13}C NMR (150 MHz, DMSO-d_6/CS_2 with Cr(acac)$_3$ as relaxation reagent, all 2C unless indicated) δ 158.36 (1C), 152.84 (1C), 152.76 (1C), 150.32, 148.97, 148.31 (1C), 148.06 (1C), 146.67, 146.57, 146.49, 146.42, 146.34, 146.27, 145.52, 145.49, 145.36, 145.01, 144.79, 144.75, 144.49, 143.25, 143.20, 142.78, 142.66, 142.61, 142.32, 142.25, 141.66, 141.29, 140.56, 140.52, 134.52, 134.44, 132.30 (1C), 125.63 (1C), 119.32 (1C), 107.17 (1C), 101.12 (1C), 98.51 (1C), 83.79 (1C), 58.35 (1C); FT-IR ν/cm^{-1} (KBr) 1612, 1596, 1496, 1451, 1320, 1282, 1211, 1143, 1099, 956, 840, 807, 766, 526; UV-vis ($CHCl_3$) λ_{max}/nm 256, 314, 430, 698; MALDI-TOF MS *m/z* calcd for $C_{69}H_5FN_2$ $[M]^+$ 880.0431, found 880.0439.



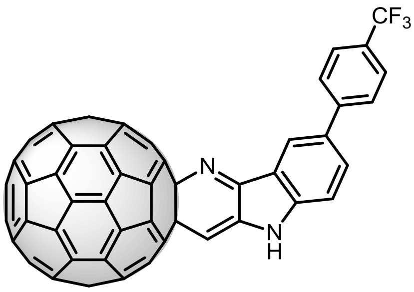
2q

Spectral data of **2q**: ^{1}H NMR (400 MHz, DMSO-d_6/CS_2) δ 9.63 (s, 1H), 7.67 (d, J = 3.6 Hz, 1H), 7.26 (dd, J = 8.4, 2.0 Hz, 1H), 6.86 (d, J = 8.4 Hz, 1H), 5.98 (s, 1H); ^{13}C NMR (150 MHz, DMSO-d_6/CS_2 with Cr(acac)$_3$ as relaxation reagent, all 2C unless indicated) δ 159.00 (1C), 150.05, 149.64 (1C), 148.59, 148.31 (1C), 148.07 (1C), 146.65, 146.58, 146.48, 146.42, 146.36, 146.27, 145.55, 145.49, 145.39, 145.01, 144.76, 144.74, 144.48, 143.26, 143.23, 142.79, 142.67, 142.63, 142.27, 142.25, 141.66, 141.29, 140.59, 140.54, 134.54, 134.48, 133.78 (1C), 132.09 (1C), 124.98 (1C), 124.51 (1C), 123.73 (1C), 112.07 (1C), 101.20 (1C), 83.94 (1C), 58.52 (1C); FT-IR ν/cm^{-1} (KBr) 1610, 1513, 1462, 1326, 1271, 1215, 1049, 1024, 1006, 814, 767, 704, 672, 552, 526; UV-vis ($CHCl_3$) λ_{max}/nm 257, 314, 698; MALDI-TOF MS *m/z* calcd for $C_{69}H_5N_2Cl$ $[M]^+$ 896.0136, found 896.0141.



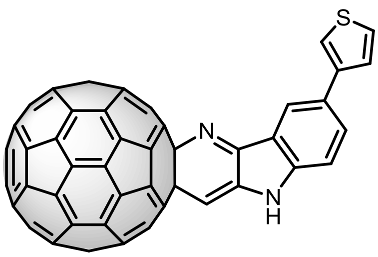
2r

Spectral data of **2r**: ^{1}H NMR (400 MHz, DMSO-d_6/CS_2) δ 9.65 (s, 1H), 7.82 (d, J = 2.0 Hz, 1H), 7.39 (dd, J = 8.4, 2.1 Hz, 1H), 6.82 (d, J = 8.4 Hz, 1H), 5.98 (s, 1H); ^{13}C NMR (150 MHz, DMSO-d_6/CS_2 with Cr(acac)$_3$ as relaxation reagent, all 2C unless indicated) δ 158.83 (1C), 150.04, 149.97 (1C), 148.58, 148.30 (1C), 148.07 (1C), 146.65, 146.58, 146.47, 146.42, 146.36, 146.27, 145.55, 145.49, 145.39, 145.01, 144.74 (4C), 144.47, 143.21 (4C), 142.79, 142.67, 142.63, 142.27, 142.24, 141.66, 141.28, 140.60, 140.54, 136.49 (1C), 134.52, 134.48, 131.93 (1C), 126.72 (1C), 125.06 (1C), 112.59 (1C), 112.33 (1C), 101.28 (1C), 83.94 (1C), 58.50 (1C); FT-IR ν/cm^{-1} (KBr) 1700, 1608, 1460, 1443, 1358, 1325, 1274, 1214, 814, 552, 526; UV-vis ($CHCl_3$) λ_{max}/nm 213, 256, 430, 698; MALDI-TOF MS *m/z* calcd for $C_{69}H_5N_2Br$ $[M]^+$ 936.9631, found 936.9637.



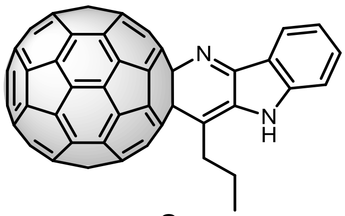
2s

Spectral data of **2s**: ^{1}H NMR (600 MHz, DMSO-d_6/CS_2) δ 9.75 (s, 1H), 8.06 (s, 1H), 7.73 (d, J = 8.4 Hz, 2H), 7.65 (d, J = 8.4 Hz, 1H), 7.61 (d, J = 8.4 Hz, 2H), 7.00 (d, J = 8.4 Hz, 1H), 6.02 (s, 1H); ^{13}C NMR (150 MHz, DMSO-d_6/CS_2 with Cr(acac)$_3$ as relaxation reagent, all 2C unless indicated) δ 159.43 (1C), 151.20 (1C), 150.16, 148.76, 148.31 (1C), 148.06 (1C), 146.62, 146.58, 146.48, 146.42, 146.35, 146.28, 145.54, 145.49, 145.36, 145.01, 144.77, 144.74, 144.49, 144.44 (1C), 143.26, 143.23, 142.79, 142.67, 142.61, 142.29, 142.26, 141.66, 141.30, 140.60, 140.55, 134.54, 134.50, 133.30 (1C), 132.21 (1C), 130.95 (1C), 126.93 (3C), 126.03, 123.96 (1C), 122.70 (1C), 111.54 (1C), 101.25 (1C), 83.96 (1C), 58.57 (1C); FT-IR ν/cm^{-1} (KBr) 1611, 1477, 1428, 1324, 1263, 1211, 1165, 1125, 1069, 1016, 843, 814, 526; UV-vis ($CHCl_3$) λ_{max}/nm 216, 256, 434, 698; MALDI-TOF MS m/z calcd for $C_{76}H_9F_3N_2$ [M]$^+$ 1006.0712, found 1006.0715.



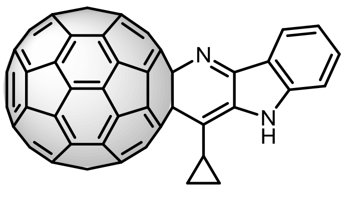
2t

Spectral data of **2t**: ^{1}H NMR (600 MHz, $CDCl_3$/CS_2) δ 8.20 (s, 1H), 7.70 (d, J = 8.4 Hz, 1H), 7.41−7.39 (m, 2H), 7.36−7.35 (m, 1H), 6.99 (d, J = 8.4 Hz, 1H), 6.62 (s, 1H), 6.10 (s, 1H); ^{13}C NMR (150 MHz, DMSO-d_6/CS_2 with Cr(acac)$_3$ as relaxation reagent, all 2C unless indicated) δ 159.64 (1C), 150.29, 150.23 (1C), 148.89, 148.31 (1C), 148.06 (1C), 146.68, 146.57, 146.51, 146.41, 146.35, 146.27, 145.53, 145.49, 145.35, 144.99, 144.80, 144.76, 144.50, 143.26 (4C), 142.79, 142.66, 142.63, 142.32, 142.26, 142.06 (1C), 141.67, 141.30, 140.59, 140.55, 134.54, 134.51, 132.60 (1C), 132.33 (1C), 127.94 (1C), 126.68 (1C), 126.36 (1C), 125.10 (1C), 121.81 (1C), 119.36 (1C), 111.18 (1C), 100.74 (1C), 83.97 (1C), 58.60 (1C); FT-IR *ν*/cm^{-1} (KBr) 1700, 1615, 1481, 1456, 1429, 1361, 1329, 1262, 1210, 1187, 1099, 1025, 815, 775, 526; UV-vis ($CHCl_3$) λ_{max}/nm 210, 225, 257, 433, 692; MALDI-TOF MS *m/z* calcd for $C_{73}H_8N_2S$ $[M]^+$ 944.0403, found 944.0404.



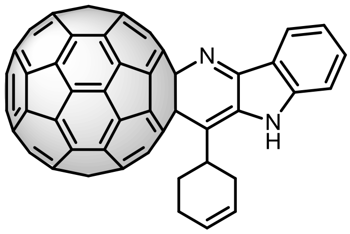
2u

Spectral data of **2u**: ^{1}H NMR (400 MHz, DMSO-*d*$_6$/CS_2) δ 9.37 (s, 1H), 7.70 (d, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 7.2Hz, 1H), 6.90 (d, *J* = 8.0 Hz, 1H), 6.82 (t, *J* = 7.6 Hz, 1H), 2.83 (t, *J* = 8.0 Hz, 2H), 1.74−1.68 (m, 2H), 1.01 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (150 MHz, DMSO-*d*$_6$/CS_2 with Cr(acac)$_3$ as relaxation reagent, all 2C unless indicated) δ 158.71 (1C), 151.81, 150.90 (1C), 148.26 (1C), 148.08 (1C), 147.79, 146.73, 146.55 (6C), 146.28, 146.27, 146.21, 145.48, 145.44, 145.26, 145.14, 144.97, 144.42, 143.26, 142.90, 142.86, 142.70 (4C), 142.39, 142.24, 141.79, 140.97, 140.57, 139.16, 134.85, 133.93, 133.74 (1C), 130.55 (1C), 123.98 (1C), 123.60 (1C), 119.61 (1C), 110.99 (1C), 108.15 (1C), 84.75 (1C), 61.60 (1C), 30.37 (1C), 22.80 (1C), 15.21 (1C); FT-IR *ν*/cm^{-1} (KBr) 2957, 1636, 1614, 1464, 1430, 1335, 1307, 1232, 1146, 1049, 1024, 1005, 814, 747, 715, 574, 552, 526; UV-vis ($CHCl_3$) λ_{max}/nm 218, 259, 431, 699; MALDI-TOF MS *m/z* calcd for $C_{72}H_{12}N_2$ $[M]^+$ 904.0995, found 904.0987.



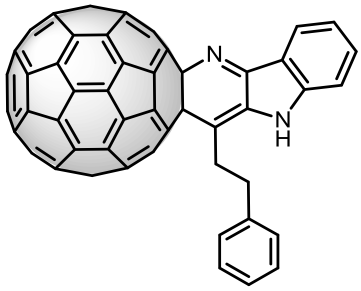
2v

Spectral data of **2v**: ^{1}H NMR (600 MHz, DMSO-*d*$_6$/CS_2) δ 9.09 (s, 1H), 7.73 (d, *J* = 7.2 Hz, 1H), 7.32 (t, *J* = 7.8 Hz, 1H), 7.02 (d, *J* = 7.8 Hz, 1H), 6.85 (t, *J* = 7.2 Hz, 1H), 1.80−1.76 (m, 1H), 1.07−1.05 (m, 2H), 1.03−1.01 (m, 2H); ^{13}C NMR (150 MHz, DMSO-d_6/CS_2 with Cr(acac)$_3$ as relaxation reagent, all 2C unless indicated) δ 159.13 (1C), 152.98, 152.36 (1C), 148.71, 148.24 (1C), 148.07 (1C), 146.95, 146.87, 146.59, 146.55, 146.41 146.29, 146.28, 145.45 (4C), 145.39, 145.23, 144.91, 144.50, 143.20, 142.84, 142.82, 142.73, 142.59, 142.48, 141.18, 141.90, 141.03, 140.63, 138.82, 134.11, 134.03, 133.73 (1C), 130.67 (1C), 123.82 (1C), 123.21 (1C), 119.81 (1C), 111.56 (1C), 107.16 (1C), 84.38 (1C), 62.66 (1C), 13.19 (1C), 10.56; FT-IR ν/cm^{-1} (KBr) 2960, 2923, 1630, 1611, 1514, 1464, 1328, 1262, 1230, 1099, 1027, 868, 803, 742, 526; UV-vis ($CHCl_3$) λ_{max}/nm 257, 323, 518; MALDI-TOF MS *m/z* calcd for $C_{72}H_{10}N_2$ [M]$^+$ 902.0838, found 902.0845.



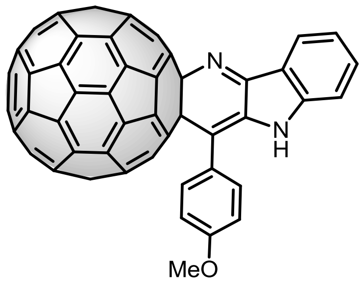
2w

Spectral data of **2w**: ^{1}H NMR (600 MHz, $CDCl_3$/CS_2) δ 7.93 (d, J = 7.8 Hz, 1H), 7.44 (t, J = 7.8 Hz, 1H), 7.01 (t, J = 7.2 Hz, 1H), 6.98 (d, J = 7.8 Hz, 1H), 6.55 (s, 1H), 5.81 (s, 2H), 3.94−3.89 (m, 1H), 2.80−2.75 (m, 1H), 2.36−2.33 (m, 1H), 2.25 (d, J = 16.2 Hz, 1H), 2.21−2.09 (m, 2H), 2.07−2.05 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$/CS_2 with Cr(acac)$_3$ as relaxation reagent, all 2C unless indicated) δ 158.44 (1C), 151.08, 148.62 (1C), 148.00 (1C), 147.89 (1C), 146.58 (1C), 146.41 (5C), 146.26, 146.06 (5C), 145.96, 145.93 (1C), 145.29, 145.22, 145.06 (3C), 145.02 (1C), 144.76, 144.06, 143.03, 142.67, 142.50, 142.46 (4C), 142.10, 141.84, 141.47, 140.53, 140.46, 138.56, 135.07 (1C), 135.00 (1C), 133.74 (1C), 133.61 (1C), 133.59 (1C), 129.00 (1C), 127.44 (1C), 126.17 (1C), 123.87 (1C), 120.58 (1C), 113.06 (1C), 110.40 (1C), 84.47 (1C), 61.13 (1C), 33.58 (1C), 28.27 (1C), 26.54 (1C), 25.78 (1C); FT-IR ν/cm^{-1} (KBr) 2922, 1707, 1636, 1613, 1466, 1433, 1330, 1260, 1227, 1097, 1027, 802, 745, 669, 650, 526; UV-vis ($CHCl_3$) λ_{max}/nm 218, 257, 431, 698; MALDI-TOF MS *m/z* calcd for $C_{75}H_{14}N_2$ [M]$^+$ 942.1151, found 942.1152.



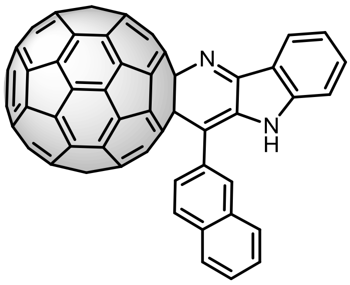
2x

Spectral data of **2x**: ^{1}H NMR (400 MHz, $CDCl_3/CS_2$) δ 7.90 (d, J = 7.2 Hz, 1H), 7.40−7.36 (m, 1H), 7.32 (d, J = 4.0 Hz, 4H), 7.23−7.19 (m, 1H), 6.98 (t, J = 7.2 Hz, 1H), 6.76 (d, J = 8.0 Hz, 1H), 5.65 (s, 1H), 3.29 (t, J = 7.6 Hz, 2H), 3.06 (t, J = 7.6 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 2C unless indicated) δ 157.74 (1C), 151.14, 149.27 (1C), 148.01 (1C), 147.88 (1C), 147.10, 146.37, 146.34, 146.16 (4C), 146.09, 146.06, 145.64, 145.29, 145.24, 145.14, 145.04, 144.70, 144.09, 143.02, 142.64, 142.56, 142.48, 142.43, 142.08, 141.85, 141.54, 141.03 (1C), 140.73, 140.46, 138.96, 134.62, 133.60, 133.56 (1C), 130.94 (1C), 128.91, 128.68, 126.79 (1C), 123.86 (1C), 123.63 (1C), 120.74 (1C), 110.95 (1C), 108.22 (1C), 84.50 (1C), 60.92 (1C), 58.44 (1C), 34.98 (1C); FT-IR ν/cm^{-1} (KBr) 2960, 2921, 2851, 1701, 1637, 1613, 1493, 1464, 1333, 1261, 1231, 1187, 1096, 1027, 802, 746, 698, 526; UV-vis ($CHCl_3$) λ_{max}/nm 232, 257, 315, 429; MALDI-TOF MS m/z calcd for $C_{77}H_{14}N_2$ $[M]^+$ 966.1151, found 966.1149.



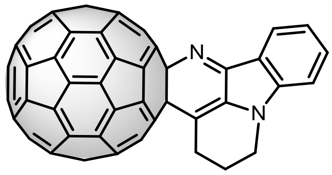
2y

Spectral data of **2y**: ^{1}H NMR (400 MHz, DMSO-d_6/CS_2) δ 8.77 (s, 1H), 7.21 (d, J = 7.2 Hz, 1H), 7.29−7.23 (m, 3H), 6.88 (d, J = 8.0 Hz, 2H), 6.83−6.81 (m, 2H), 3.73 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6/CS_2 with $Cr(acac)_3$ as relaxation reagent, all 2C unless indicated) δ 159.55, 151.24, 148.36 (1C), 148.15 (1C), 148.00, 146.72 (4C), 146.61 (6C), 146.39 (4C), 145.57 (4C), 145.45, 145.23, 144.97, 144.54, 143.31, 143.17 (4C), 142.95, 142.81, 142.74, 142.42 (4C), 141.94, 141.07, 140.68, 139.01, 134.69, 134.34, 134.08, 133.27, 130.97 (1C), 126.52 (1C), 124.01 (1C), 123.35 (1C), 119.94 (1C), 114.70, 111.63 (1C), 108.69 (1C), 85.10 (1C), 62.01 (1C), 55.35 (1C); FT-IR *ν*/cm^{-1} (KBr) 1605, 1508, 1463, 1334, 1285, 1245, 1173, 1052, 1027, 1006, 834, 747, 526; UV-vis ($CHCl_3$) λ_{max}/nm 258, 431, 702; MALDI-TOF MS *m/z* calcd for $C_{76}H_{12}N_2O$ $[M]^+$ 968.0944, found 968.0936.



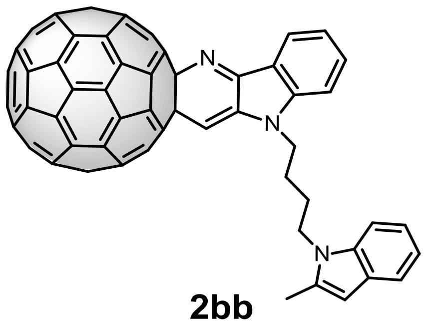
2z

Spectral data of **2z**: ^{1}H NMR (400 MHz, DMSO-d_6/CS_2) δ 8.88 (s, 1H), 7.89 (s, 1H), 7.84−7.73 (m, 4H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.43−7.41 (m, 2H), 7.24 (t, *J* = 7.2 Hz, 1H), 6.82 (t, *J* = 7.2 Hz, 1H), 6.75 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (150 MHz, DMSO-d_6/CS_2 with Cr(acac)$_3$ as relaxation reagent, all 2C unless indicated) δ 159.53 (1C), 151.19, 150.93 (1C), 148.24 (1C), 148.03 (1C), 147.78, 146.74 (1C), 146.61, 146.51 (4C), 146.27 (5C), 146.17 (1C), 145.49, 145.43, 145.15, 144.86, 144.40, 143.19 (3C), 142.85 (4C), 142.68, 142.59, 142.30 (4C), 141.87, 140.91, 140.61, 138.98 (1C), 138.86 (1C), 134.61, 134.32 (1C), 134.22 (1C), 133.98, 133.63 (1C), 133.08 (1C), 132.31 (1C), 131.64 (1C), 130.83 (1C), 129.56 (1C), 128.67 (1C), 128.64 (1C), 128.09 (1C), 126.94 (1C), 126.51 (1C), 123.92 (1C), 123.17 (1C), 119.89 (1C), 111.42 (1C), 108.54 (1C), 85.05 (1C), 61.62 (1C), 30.39 (1C); FT-IR *ν*/cm^{-1} (KBr) 1615, 1464, 1431, 1334, 1262, 1230, 1097, 1033, 857, 799, 745, 699, 526; UV-vis ($CHCl_3$) λ_{max}/nm 231, 257, 323, 527; MALDI-TOF MS *m/z* calcd for $C_{79}H_{12}N_2$ $[M]^+$ 988.0995, found 988.0993.



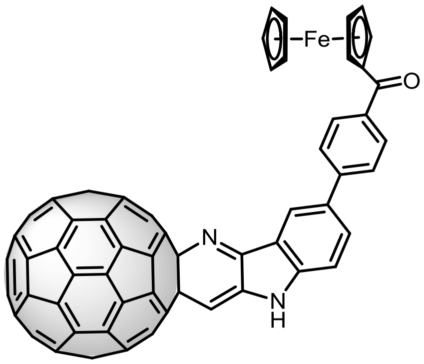
2aa

Spectral data of **2aa**: ^{1}H NMR (600 MHz, DMSO-d_6/CS_2) δ 7.81 (d, J = 7.2 Hz, 1H), 7.44 (t, J = 7.8 Hz, 1H), 6.93−6.89 (m, 2H), 3.87 (t, J = 6.0 Hz, 2H), 2.90 (t, J = 6.0 Hz, 2H), 2.46−2.42 (m, 2H); the ^{13}C NMR spectrum of **2aa** could not be obtained because of poor solubility of the product; FT-IR ν/cm^{-1} (KBr) 2925, 1710, 1637, 1610, 1509, 1471, 1456, 1423, 1389, 1367, 1323, 1279, 1247, 1200, 1144, 969, 839, 742, 551, 526; UV-vis ($CHCl_3$) λ_{max}/nm 226, 259, 431, 464; MALDI-TOF MS *m/z* calcd for $C_{72}H_{10}N_2$ $[M]^+$ 902.0838, found 902.0837.



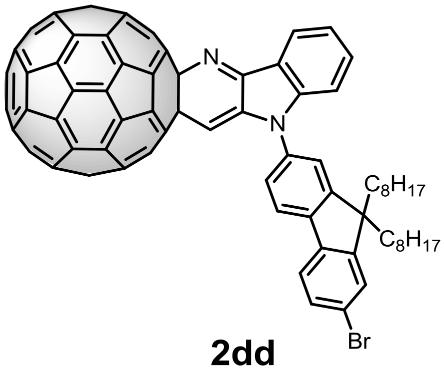
2bb

Spectral data of **2bb**: ^{1}H NMR (400 MHz, $CDCl_3$/CS_2) δ 7.97 (d, J = 7.2 Hz, 1H), 7.48 (d, J = 7.6 Hz, 1H), 7.46 (d, J = 8.0 Hz, 1H), 7.29 (d, J = 8.0 Hz, 1H), 7.12 (t, J = 8.0 Hz, 1H), 7.05−7.01 (m, 1H), 6.98 (t, J = 7.6 Hz, 1H), 6.74 (d, J = 8.0 Hz, 1H), 4.22 (t, J = 6.8 Hz, 2H), 3.74 (t, J = 6.8 Hz, 2H), 2.47 (s, 3H), 2.05−2.02 (m, 2H), 1.99−1.94 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$/CS_2 with $Cr(acac)_3$ as relaxation reagent, all 2C unless indicated) δ 158.61 (1C), 150.44 (1C), 149.57, 148.04 (1C), 147.97, 147.79 (1C), 146.30, 146.14 (4C), 146.08 (4C), 146.00, 145.26, 145.20, 145.15, 144.76, 144.39, 144.25, 144.15, 142.96, 142.79, 142.48, 142.37, 142.26, 141.92, 141.84, 141.31, 140.98, 140.37, 140.20, 136.44 (1C), 135.74 (1C), 134.49, 134.31, 134.10 (1C), 132.26 (1C), 128.03 (1C), 124.07 (1C), 122.86 (1C), 120.60 (1C), 120.09 (1C), 119.87 (1C), 119.41 (1C), 108.72 (1C), 107.67 (1C), 100.65 (1C), 98.94 (1C), 83.71 (1C), 57.99 (1C), 42.74 (1C), 42.66 (1C), 28.01 (1C), 25.20 (1C), 12.97 (1C); FT-IR ν/cm^{-1} (KBr) 2924, 1708, 1634, 1606, 1466, 1397, 1349, 1311, 1217, 1184, 808, 769, 744, 526; UV-vis ($CHCl_3$) λ_{max}/nm 226, 259, 431, 464; MALDI-TOF MS *m/z* calcd for $C_{82}H_{21}N_3$ $[M]^+$ 1047.1730, found 1047.1736.



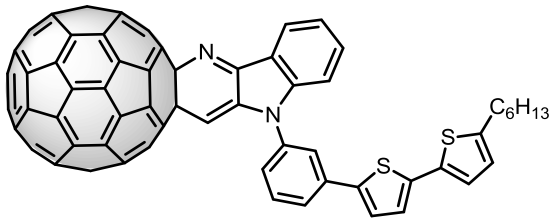
2cc

Spectral data of **2cc**: ^{1}H NMR (400 MHz, DMSO-d_6/CS_2) δ 9.75 (s, 1H), 8.10 (s, 1H), 7.88 (d, J = 8.0 Hz, 2H), 7.70 (d, J = 8.0 Hz, 1H), 7.68 (d, J = 8.0 Hz, 2H), 7.02 (d, J = 8.0 Hz, 1H), 6.02 (s, 1H), 4.78 (s, 2H), 4.47 (s, 2H), 4.10 (s, 5H); the ^{13}C NMR spectrum of **2cc** could not be obtained because of poor solubility of the product; FT-IR ν/cm^{-1} (KBr) 1617, 1599, 1512, 1475, 1444, 1375, 1333, 1284, 1212, 1134, 1026, 817, 770, 669, 526; UV-vis ($CHCl_3$) λ_{max}/nm 258, 329, 430, 482, 702; MALDI-TOF MS *m/z* calcd for $C_{86}H_{18}N_2OFe$ $[M]^+$ 1150.0763, found 1150.0789.



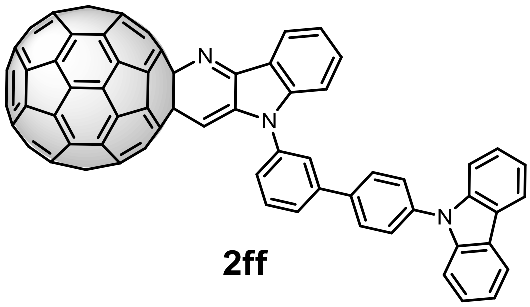
2dd

Spectral data of **2dd**: ^{1}H NMR (400 MHz, $CDCl_3$/CS_2) δ 8.07 (d, J = 7.6 Hz, 1H), 7.86 (d, J = 8.0 Hz, 1H), 7.63−7.57 (m, 3H), 7.48−7.42 (m, 3H), 7.09 (t, J = 7.6 Hz, 1H), 7.00 (d, J = 8.4 Hz, 1H), 6.06 (s, 1H), 2.01 (t, J = 6.8 Hz, 2H), 1.98 (t, J = 6.8 Hz, 2H), 1.18−1.03 (m, 20H), 0.80 (t, J = 7.2 Hz, 6H), 0.72 (br, 4H); ^{13}C NMR (100 MHz, $CDCl_3$/CS_2 with $Cr(acac)_3$ as relaxation reagent, all 2C unless indicated) δ 158.31 (1C), 152.89 (1C), 152.36 (1C), 150.33 (1C), 149.58, 148.13, 147.89 (1C), 146.42, 146.26, 146.22, 146.18 (5C), 146.10, 145.37, 145.34, 145.29, 144.88, 144.51, 144.21, 144.09, 143.05, 142.86, 142.61, 142.47, 142.40, 142.02, 141.96, 141.45, 141.02, 140.51, 140.32, 139.21 (1C), 138.88 (1C), 135.78 (1C), 134.37, 134.34, 133.83 (1C), 132.85 (1C), 130.24 (1C), 126.20 (1C), 124.89 (1C), 124.24 (1C), 123.36 (1C), 121.92 (1C), 121.29 (1C), 121.25 (1C), 121.17 (1C), 120.77 (1C), 108.97 (1C), 101.27 (1C), 83.86 (1C), 58.04 (1C), 55.48 (1C), 40.35, 31.96, 30.28, 29.56, 29.48, 24.18, 22.90, 14.30; FT-IR ν/cm^{-1} (KBr) 2921, 2849, 1634, 1607, 1490, 1462, 1429, 1377, 1314, 1214, 1062, 1007, 813, 745, 526; UV-vis ($CHCl_3$) λ_{max}/nm 209, 257, 324, 432; MALDI-TOF MS *m/z* calcd for $C_{86}H_{45}N_2Br$ $[M]^+$ 1328.2761, found 1328.2768.



2ee

Spectral data of **2ee**: ^{1}H NMR (600 MHz, $CDCl_3/CS_2$) δ 8.03 (d, *J* = 7.8 Hz, 1H), 7.83 (s, 1H), 7.60−7.58 (m, 2H), 7.54−7.53 (m, 1H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.25 (d, *J* = 4.2 Hz, 1H), 7.08 (t, *J* = 7.8 Hz, 1H), 7.04 (d, *J* = 3.6 Hz, 1H), 6.99 (d, *J* = 7.8 Hz, 1H), 6.96 (d, *J* = 3.6 Hz, 1H), 6.65 (d, *J* = 3.6 Hz, 1H), 6.08 (s, 1H), 2.78 (t, *J* = 7.8 Hz, 2H), 1.70−1.65 (m, 2H), 1.39−1.37 (m, 2H), 1.32−1.31 (m, 4H), 0.89 (t, *J* = 6.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 2C unless indicated) δ 158.21 (1C), 150.27 (1C), 149.52, 148.12, 148.08 (1C), 147.82 (1C), 146.37, 146.19 (4C), 146.15, 146.13, 146.05, 145.68 (1C), 145.31, 145.29, 145.24, 144.88, 144.45, 144.26, 144.19, 143.14, 142.99, 142.80, 142.54, 142.40, 142.34, 141.97 (4C), 141.39, 141.02, 140.59 (1C), 140.44, 140.28, 138.42 (1C), 137.49 (1C), 136.45 (1C), 134.38, 134.34, 133.97 (1C), 132.82 (1C), 130.78 (1C), 125.14 (1C), 124.88 (1C), 124.57 (1C), 124.53 (1C), 124.19 (1C), 123.87 (1C), 123.69 (1C), 123.23 (1C), 121.32 (1C), 109.09 (1C), 101.17 (1C), 83.76 (1C), 58.00 (1C), 31.73 (1C), 31.70 (1C), 30.31 (1C), 28.95 (1C), 22.85 (1C), 14.26 (1C); FT-IR ν/cm^{-1} (KBr) 2921, 1710, 1634, 1606, 1491, 1462, 1429, 1378, 1315, 1245, 1213, 1102, 787, 744, 690, 551, 526; UV-vis ($CHCl_3$) λ_{max}/nm 216, 255, 331, 431; MALDI-TOF MS *m/z* calcd for $C_{89}H_{26}N_2S_2$ $[M]^+$ 1186.1532, found 1186.1529.



2ff

Spectral data of **2ff**: ^{1}H NMR (600 MHz, $CDCl_3/CS_2$) δ 8.09 (d, J = 7.8 Hz, 2H), 8.06 (d, J = 7.8 Hz, 1H), 7.97 (s, 1H), 7.88 (d, J = 7.2 Hz, 2H), 7.74 (d, J = 4.2 Hz, 2H), 7.68 (d, J = 7.2 Hz, 3H), 7.47 (t, J = 7.8 Hz, 1H), 7.44 (d, J = 7.8 Hz, 1H), 7.38 (t, J = 7.8 Hz, 2H), 7.26 (t, J = 7.8 Hz, 2H), 7.09 (t, J = 7.2 Hz, 1H), 7.05 (d, J = 8.4 Hz, 1H), 6.13 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3/CS_2$ with $Cr(acac)_3$ as relaxation reagent, all 2C unless indicated) δ 158.31 (1C), 150.40 (1C), 149.55, 148.15, 148.12 (1C), 147.88 (1C), 146.41, 146.25, 146.18 (6C), 146.09, 145.35, 145.32, 145.29, 144.92, 144.49, 144.28, 144.21, 143.04, 142.84, 142.59 (3C), 142.45, 142.37, 141.99 (4C), 141.43, 141.04, 140.49, 140.48, 140.29, 138.69 (1C), 137.57 (1C), 137.55 (1C), 134.43, 134.40, 134.00 (1C), 132.93 (1C), 130.89 (1C), 128.58, 127.37, 126.29 (1C), 126.02, 125.65 (1C), 125.06 (1C), 124.26 (1C), 123.44, 123.34 (1C), 121.35 (1C), 120.35, 120.20, 109.63, 109.09 (1C), 101.14 (1C), 83.82 (1C), 58.07 (1C); FT-IR ν/cm^{-1} (KBr) 1634, 1607, 1519, 1489, 1463, 1451, 1378, 1316, 1227, 1102, 1017, 794, 747, 723, 526; UV-vis ($CHCl_3$) λ_{max}/nm 222, 254, 432; MALDI-TOF MS m/z calcd for $C_{93}H_{21}N_3$ $[M]^+$ 1179.1735, found 1179.1732.

8. Single-Crystal X-Ray Crystallography of 2f

Black block crystals of **2f** was obtained from slow evaporation of *n*-hexane into a saturated solution in carbon disulfide at 10 ^{o}C. Single-crystal X-ray diffraction data were collected on a diffractometer (Gemini S Ultra, Agilent Technologies) equipped with a CCD area detector using graphite-monochromated Cu Kα radiation (λ = 1.54184 Å). The structure was solved with direct methods using SHELXS-97 and refined with full-matrix least-squares refinement using the SHELXL-97 program within OLEX2. Crystallographic data have been deposited in the Cambridge Crystallographic Data Centre as deposition number CCDC 1835479.

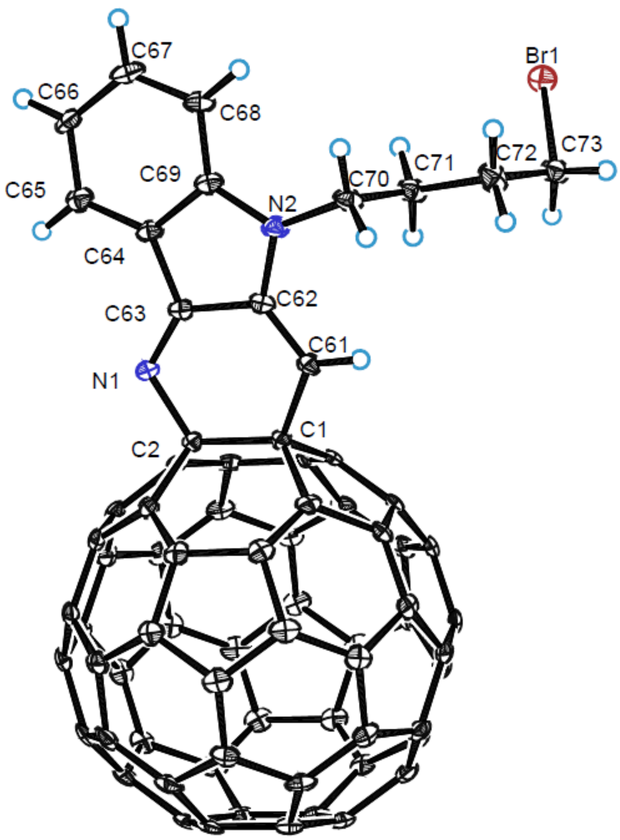


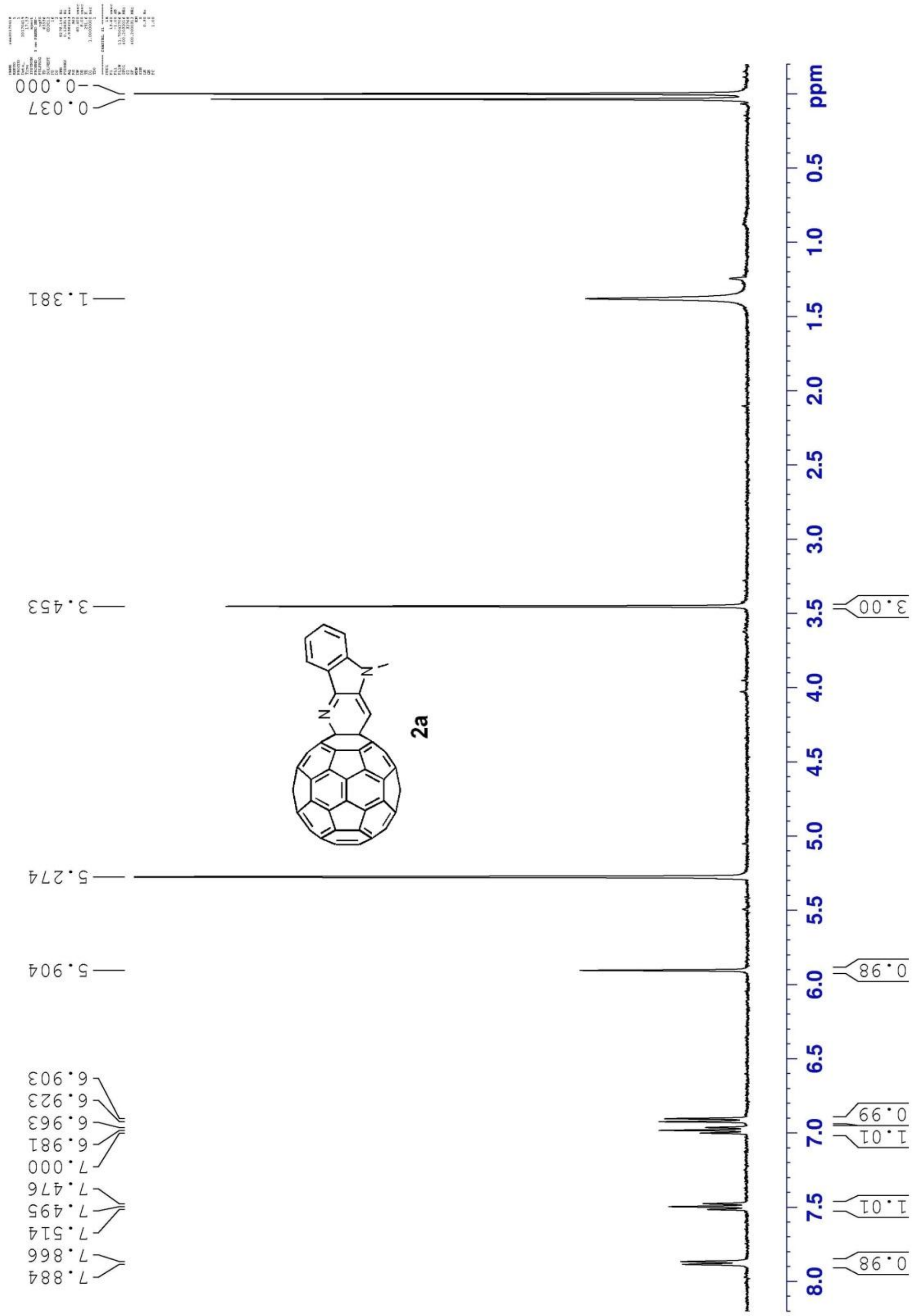
Figure S4. ORTEP Diagrams of **2f** with 50% Thermal Ellipsoids. The Carbon Disulfide Molecule is Omitted for Clarity

Crystal data and structure refinement for compound 2f.

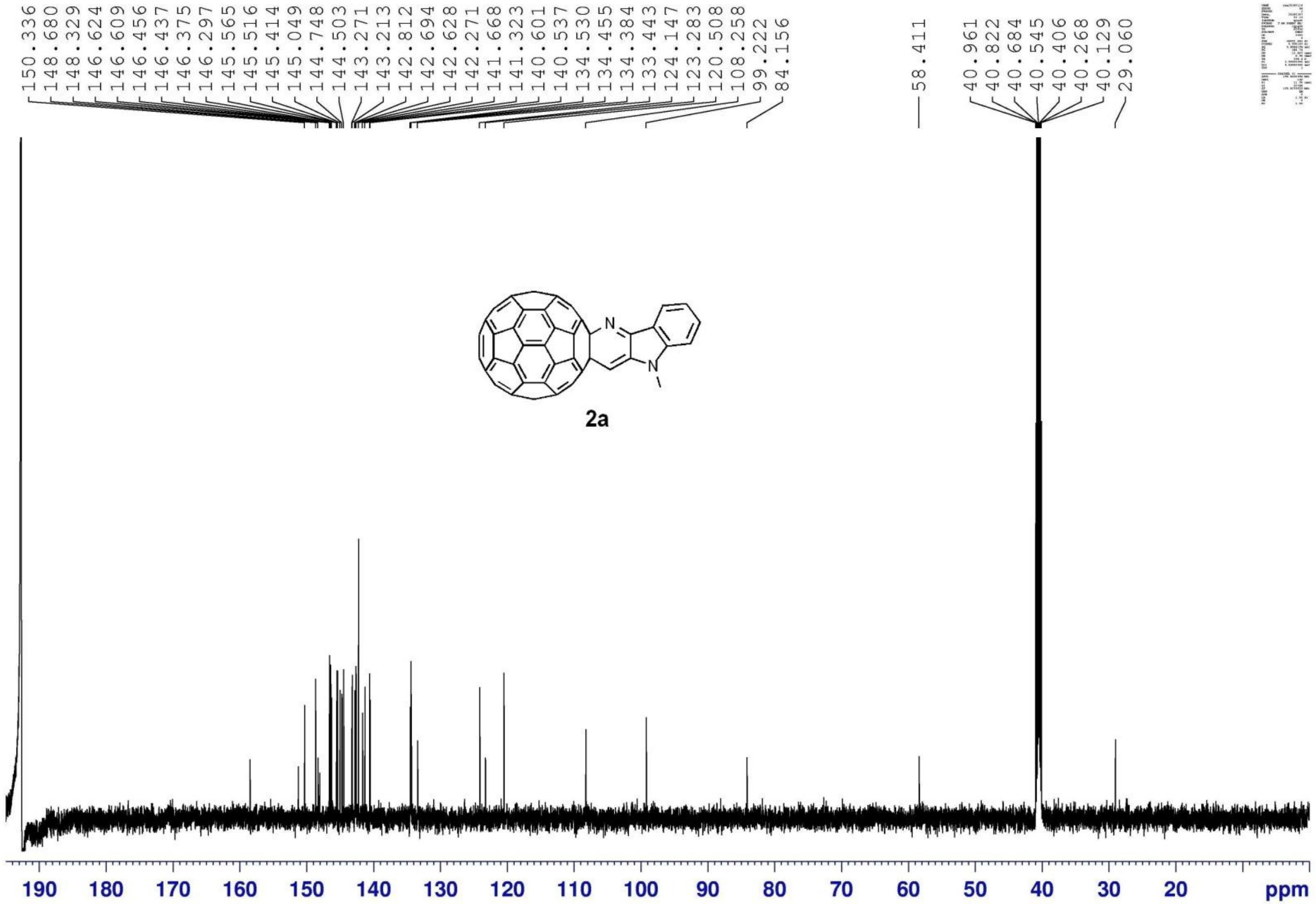
Empirical formula	$C_{295}H_{52}Br_4N_8S_6$
Formula weight	4219.44
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1
a/Å	14.3499(3)
b/Å	16.3659(3)
c/Å	18.7206(3)
α/°	112.433(2)
β/°	94.237(2)
γ/°	102.687(2)
Volume/$Å^3$	3903.50(14)
Z	1
$\rho_{calc}g/cm^3$	1.795
μ/mm^{-1}	2.689
F(000)	2114.0
Crystal size/mm^3	0.250 × 0.220 × 0.200
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.512 to 142.71
Index ranges	$-17 \leq h \leq 17$, $-20 \leq k \leq 15$, $-23 \leq l \leq 21$
Reflections collected	26998
Independent reflections	14646 [R_{int} = 0.0194, R_{sigma} = 0.0255]
Data/restraints/parameters	14646/0/1411
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0536, wR_2 = 0.1581
Final R indexes [all data]	R_1 = 0.0560, wR_2 = 0.1606
Largest diff. peak/hole / e $Å^{-3}$	1.74/-1.72

9. ^{1}H NMR and ^{13}C NMR Spectra of Compounds 2

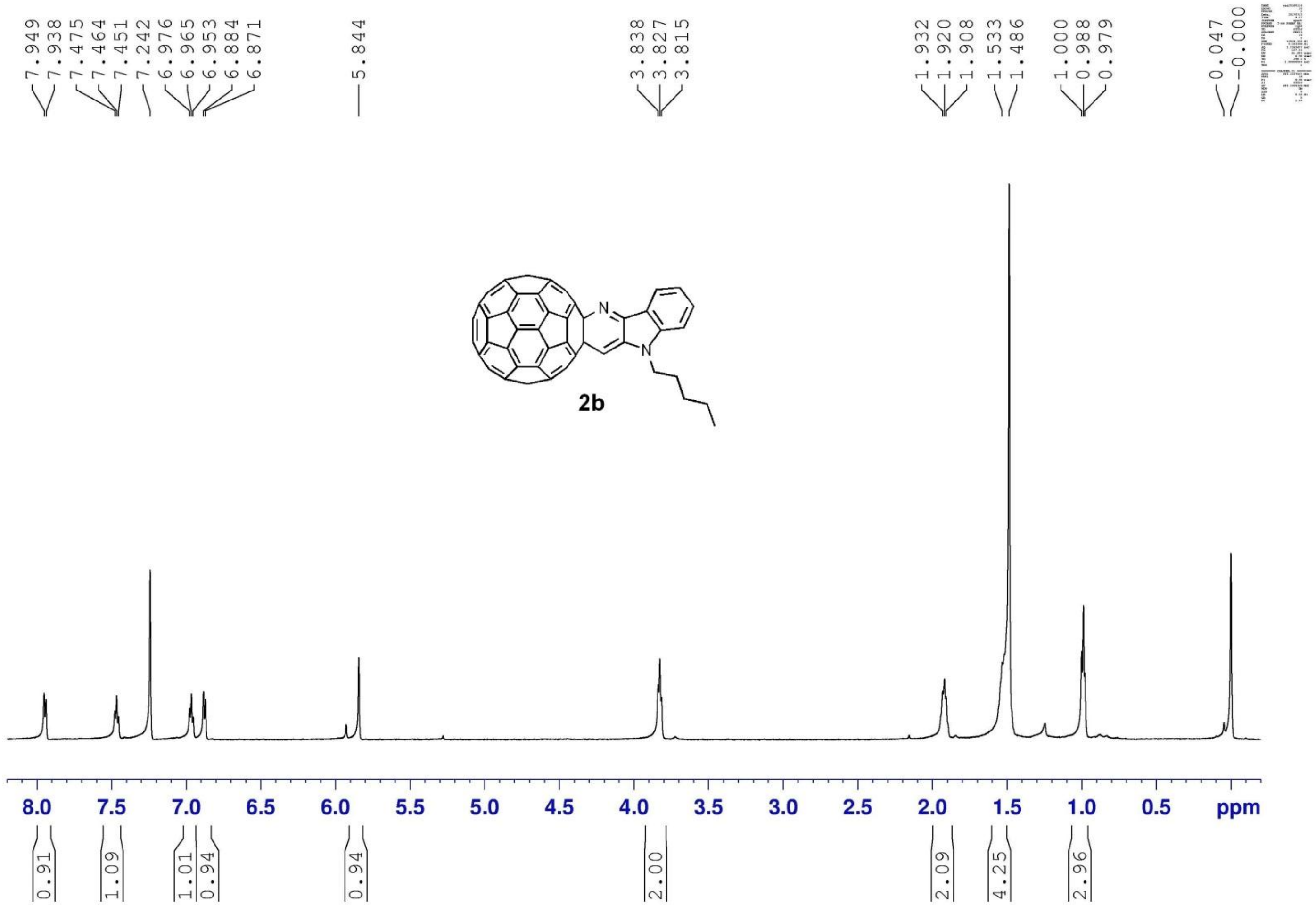
^{1}H NMR (400 MHz, CD_2Cl_2/CS_2) of compound 2a



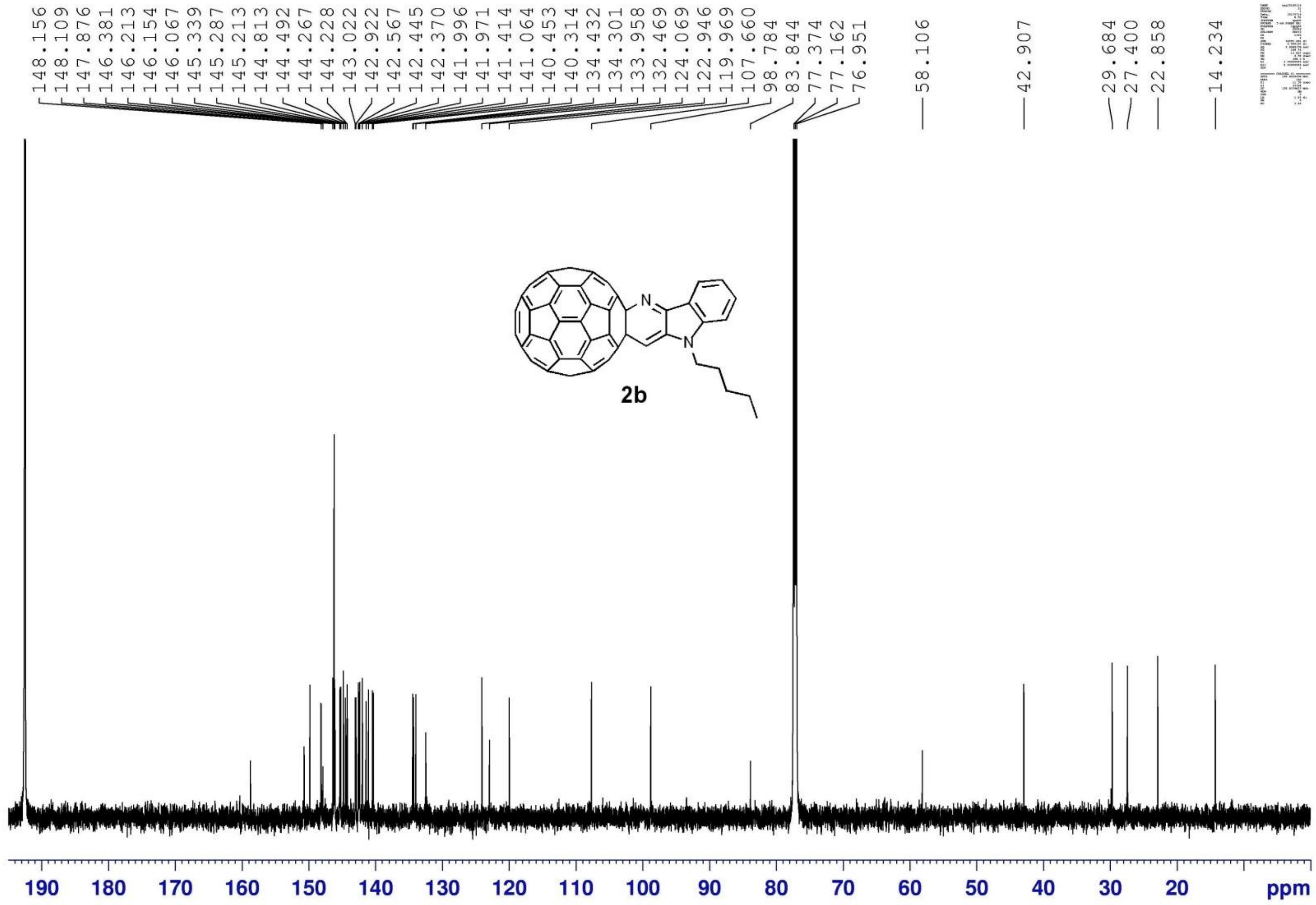
^{13}C NMR (150 MHz, DMSO-d_6/CS_2) of compound 2a



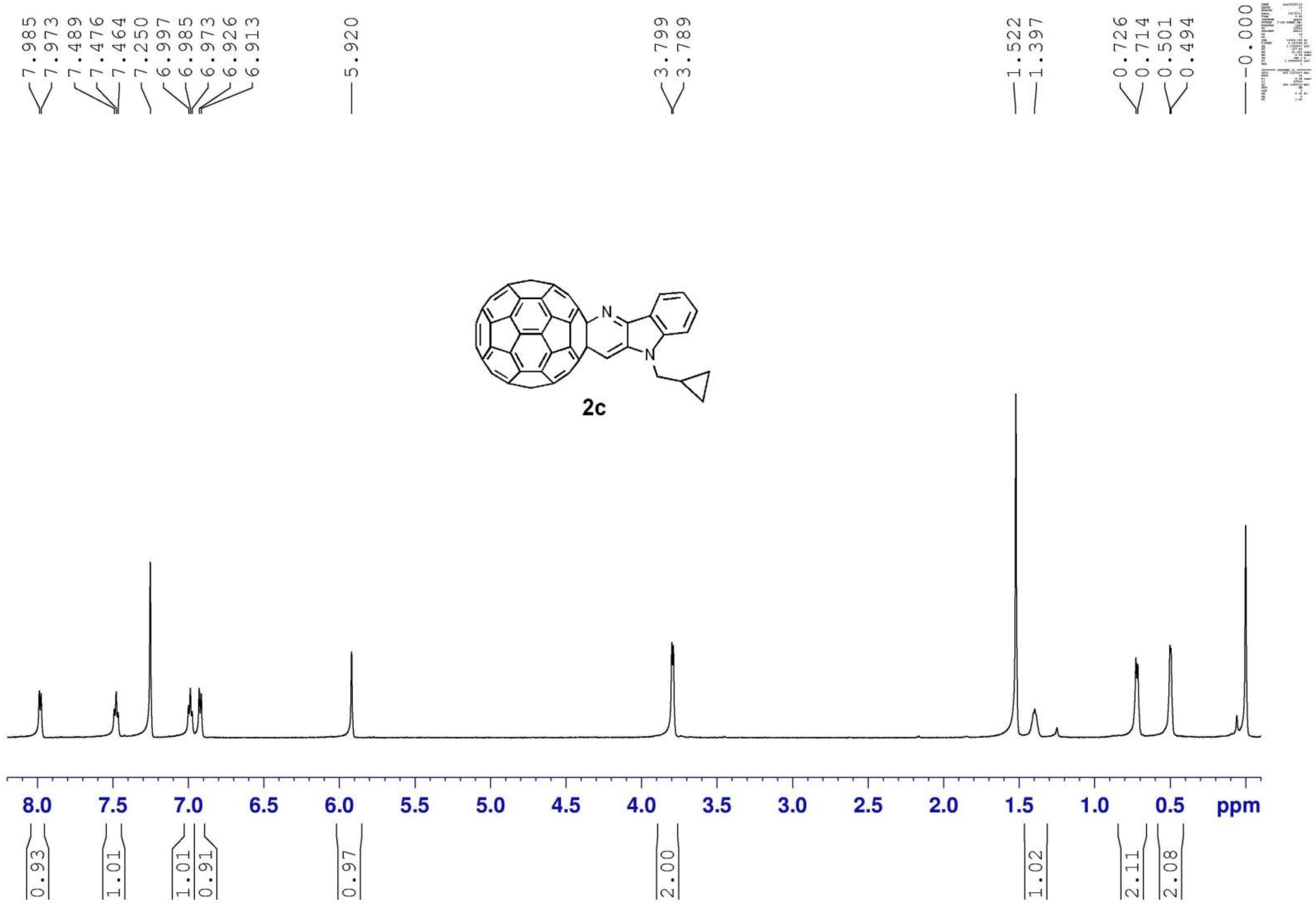
^1H NMR (600 MHz, $CDCl_3/CS_2$) of compound 2b



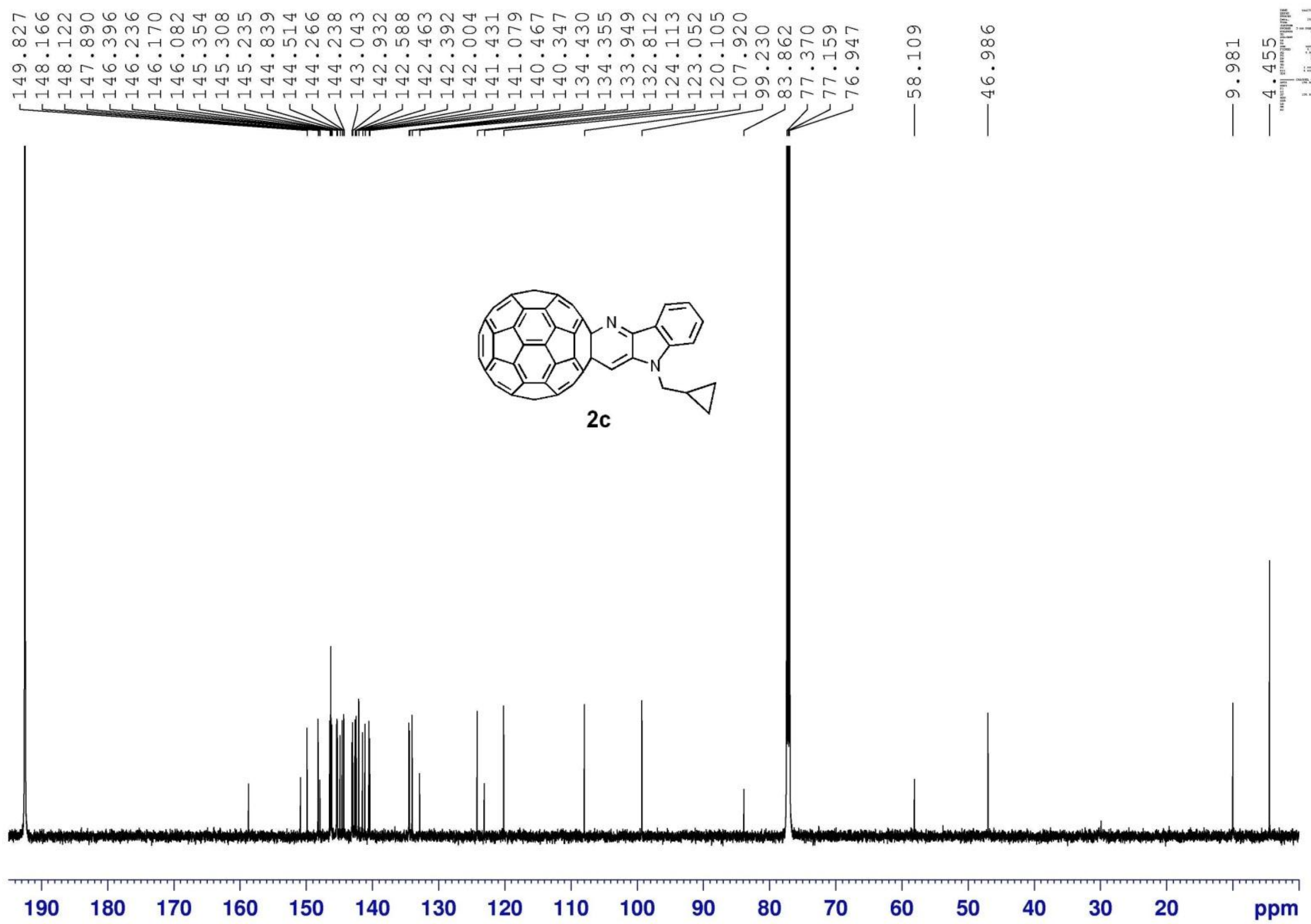
^{13}C NMR (150 MHz, $CDCl_3/CS_2$) of compound 2b



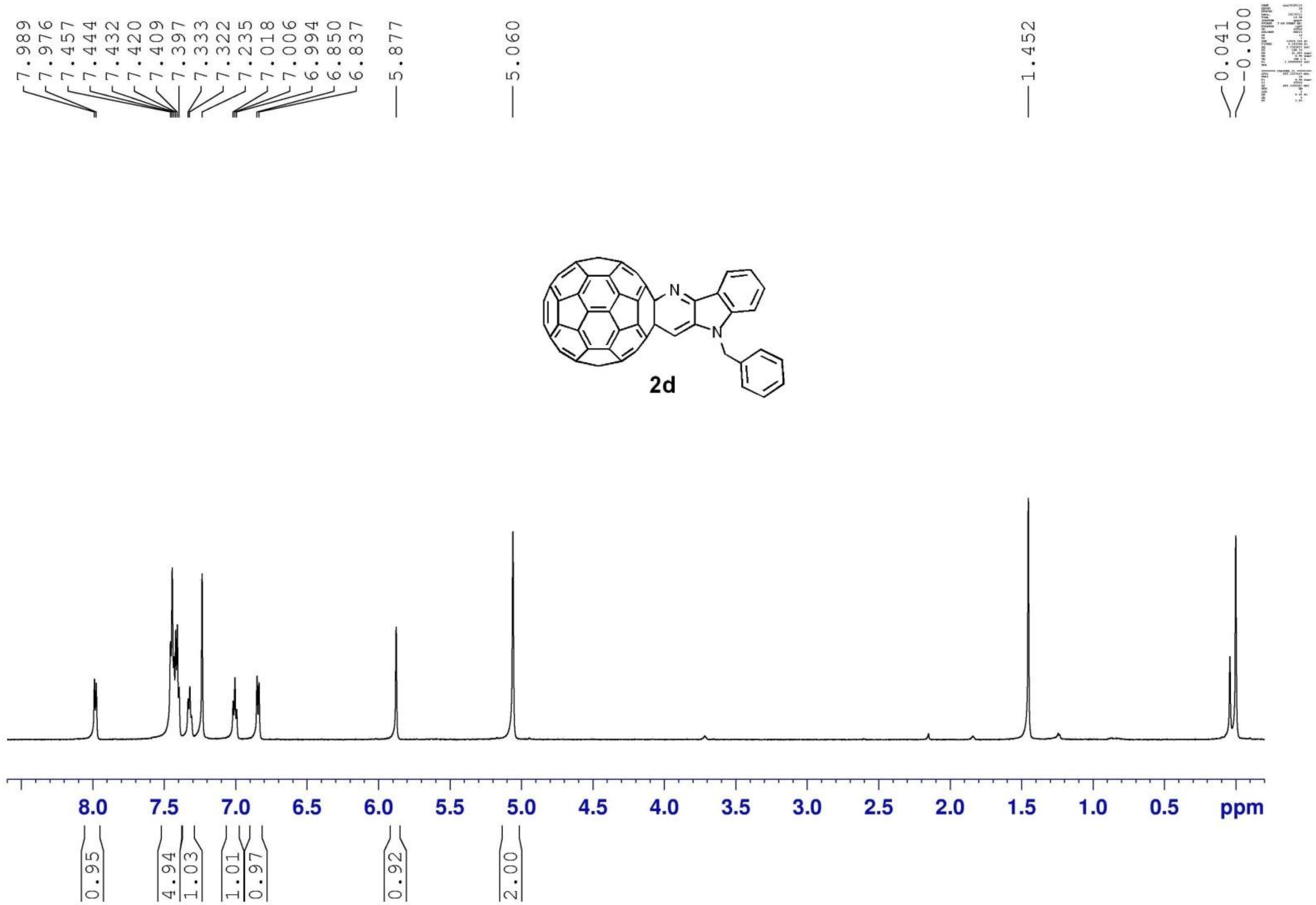
^1H NMR (600 MHz, $CDCl_3/CS_2$) of compound 2c



^{13}C NMR (150 MHz, $CDCl_3/CS_2$) of compound 2c

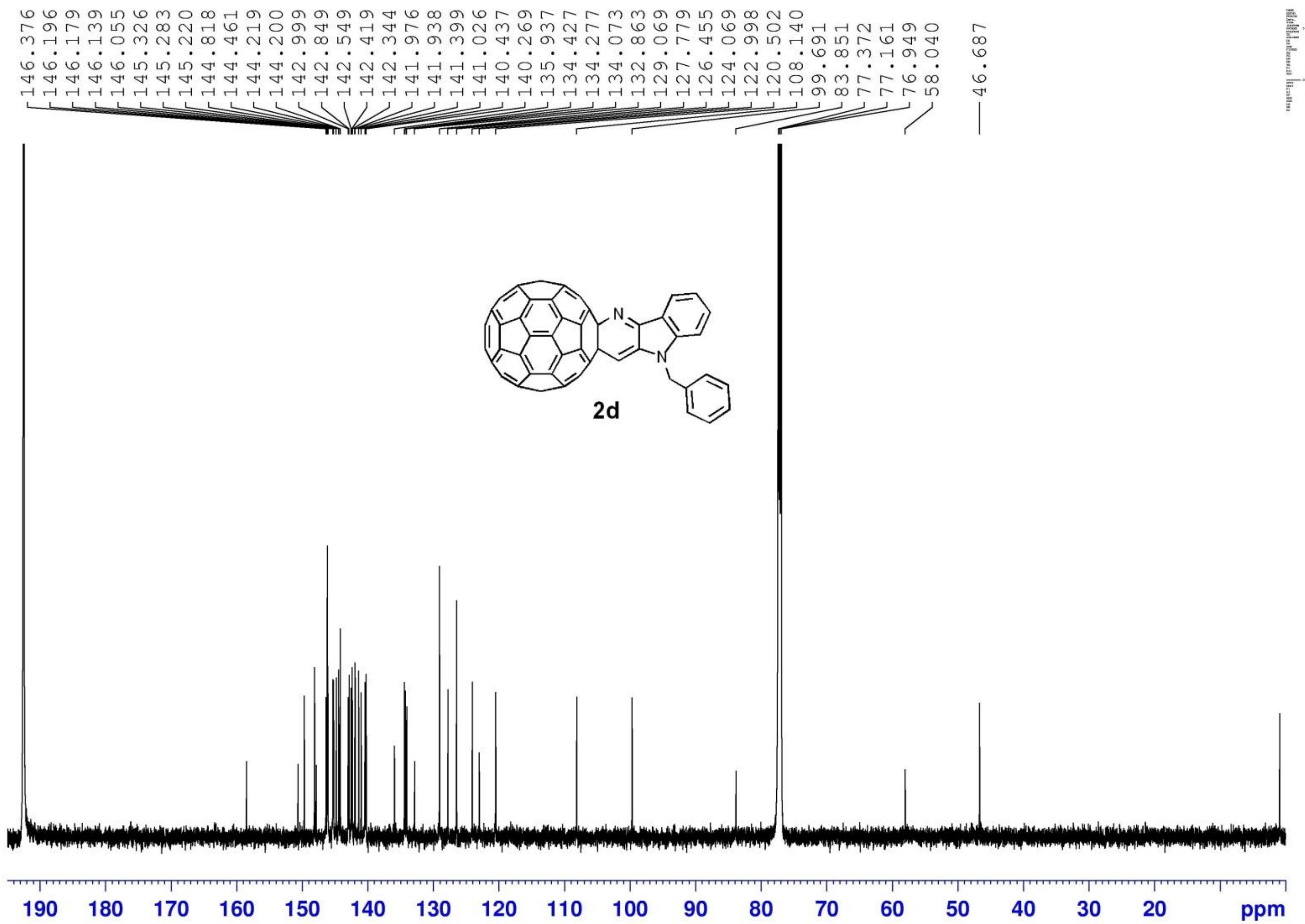


^{1}H NMR (600 MHz, $CDCl_3/CS_2$) of compound 2d

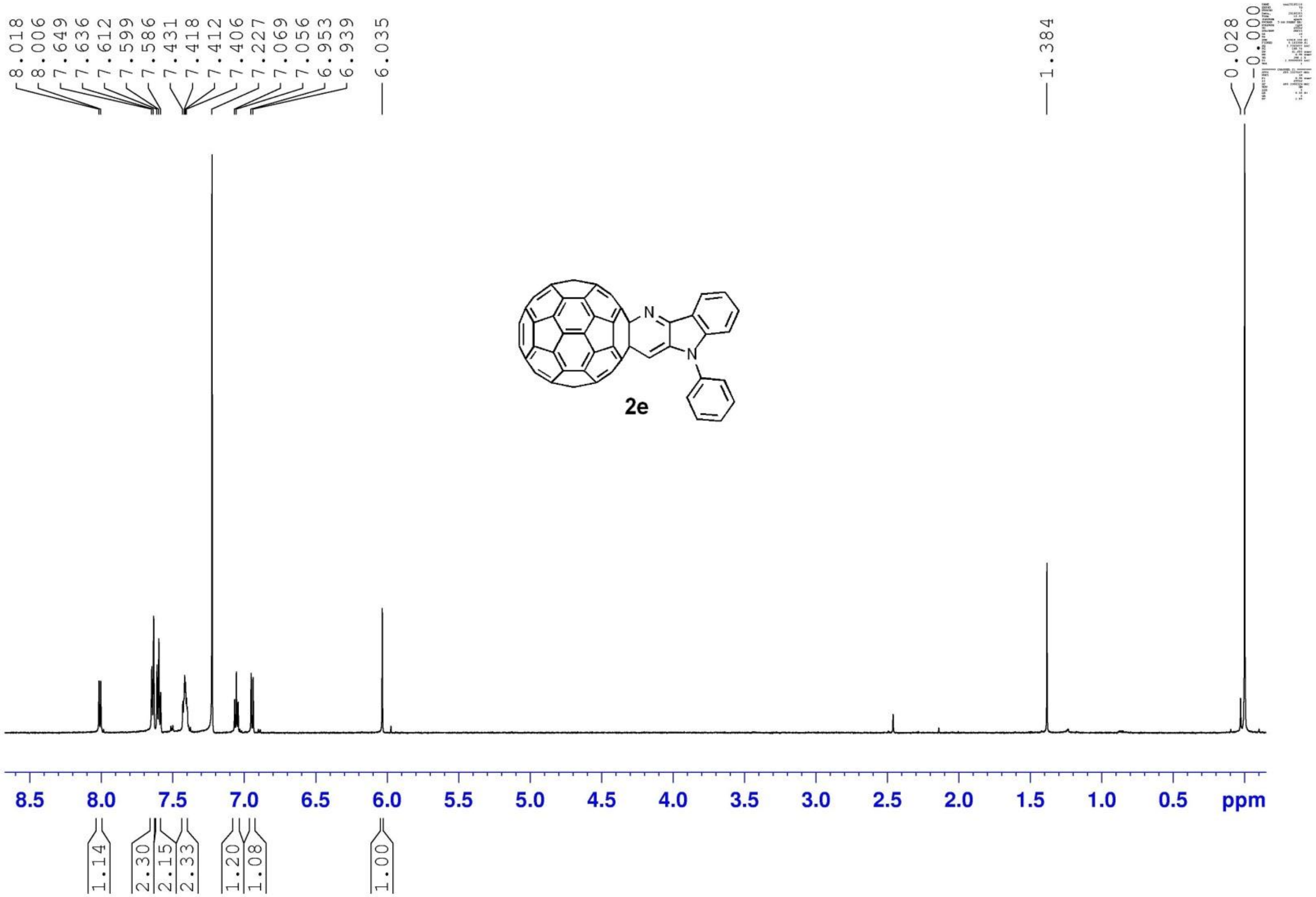


2d

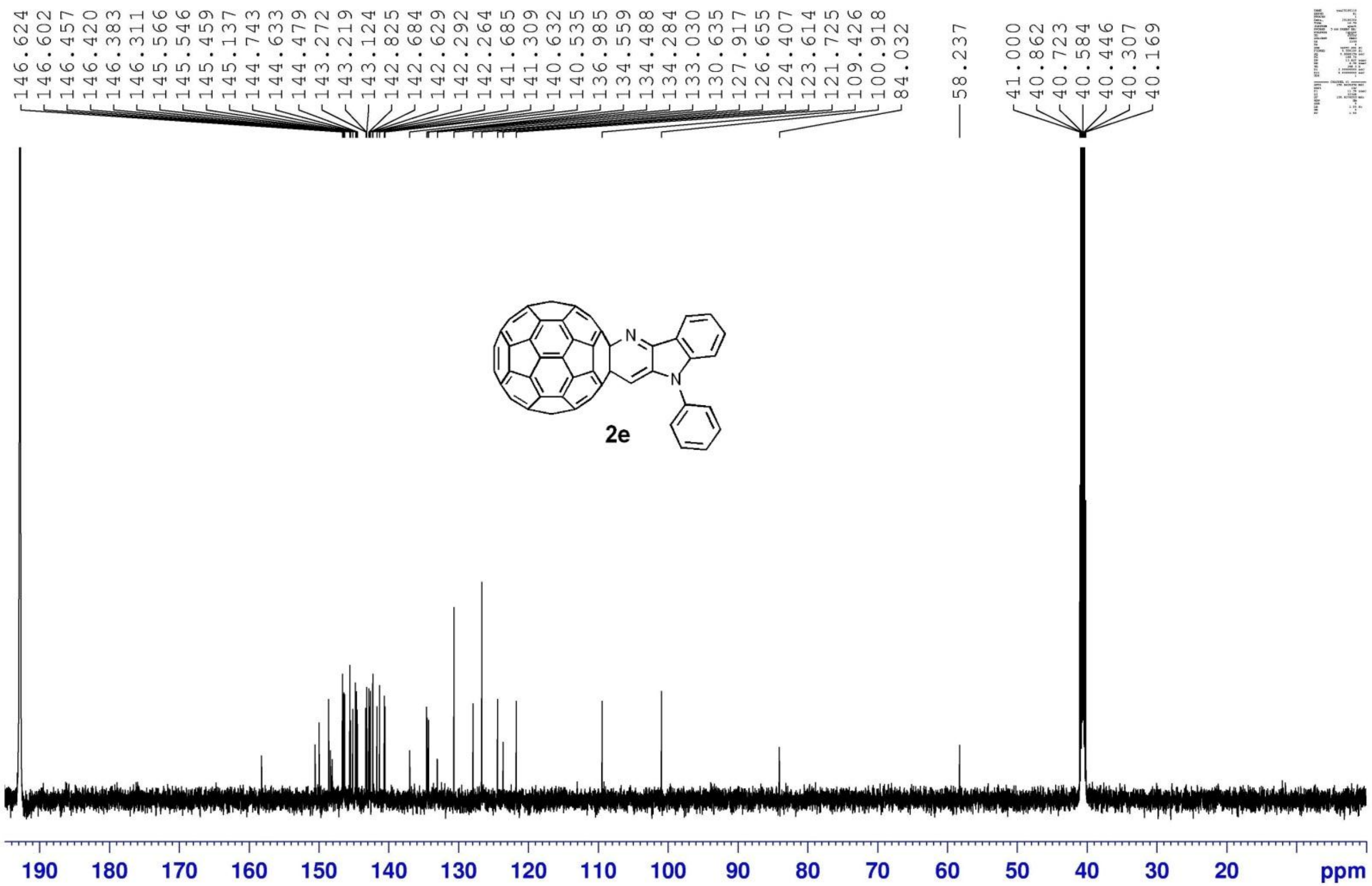
^{13}C NMR (150 MHz, $CDCl_3/CS_2$) of compound 2d



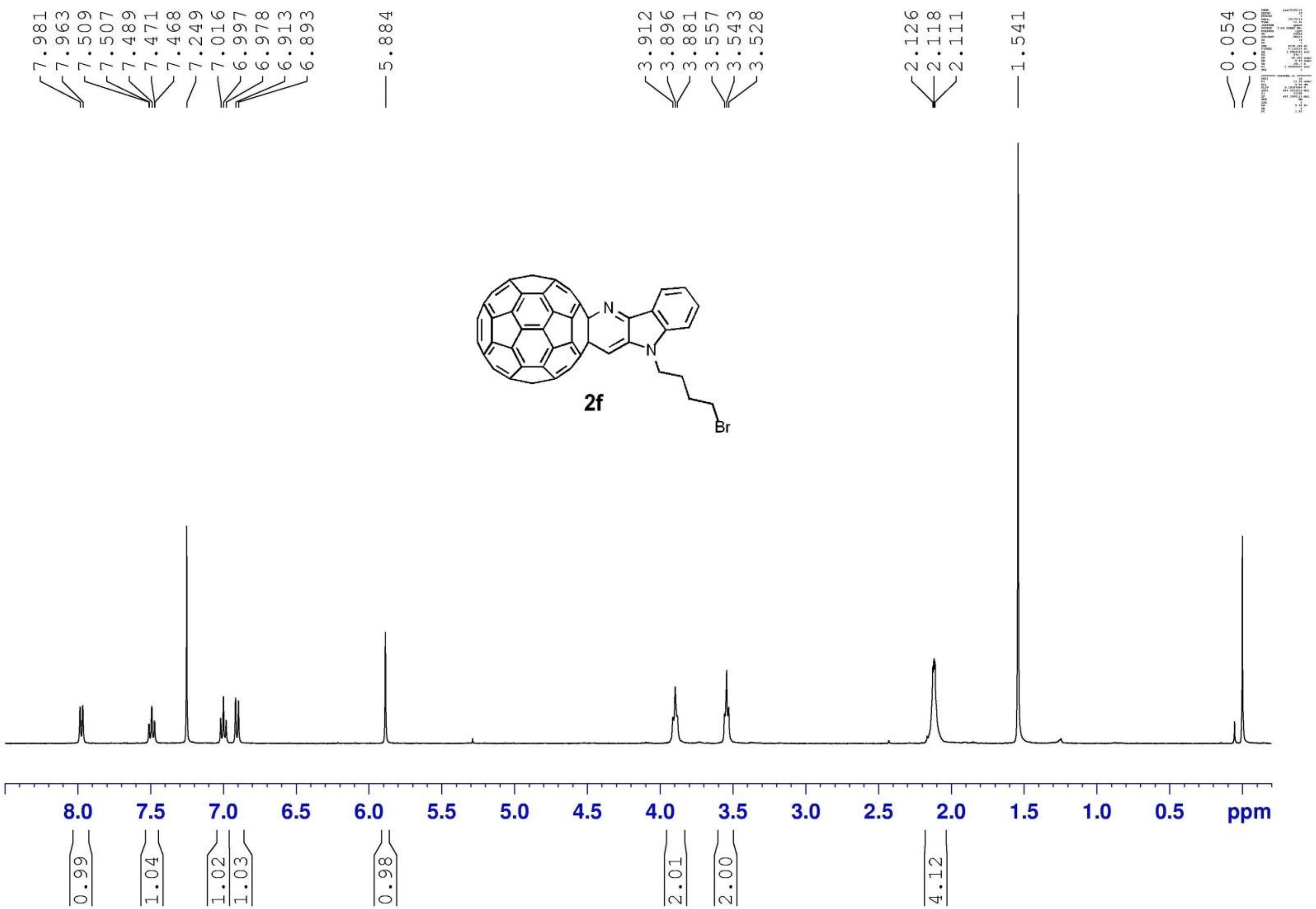
^1H NMR (600 MHz, $CDCl_3/CS_2$) of compound 2e



^{13}C NMR (150 MHz, DMSO-d_6/CS_2) of compound 2e

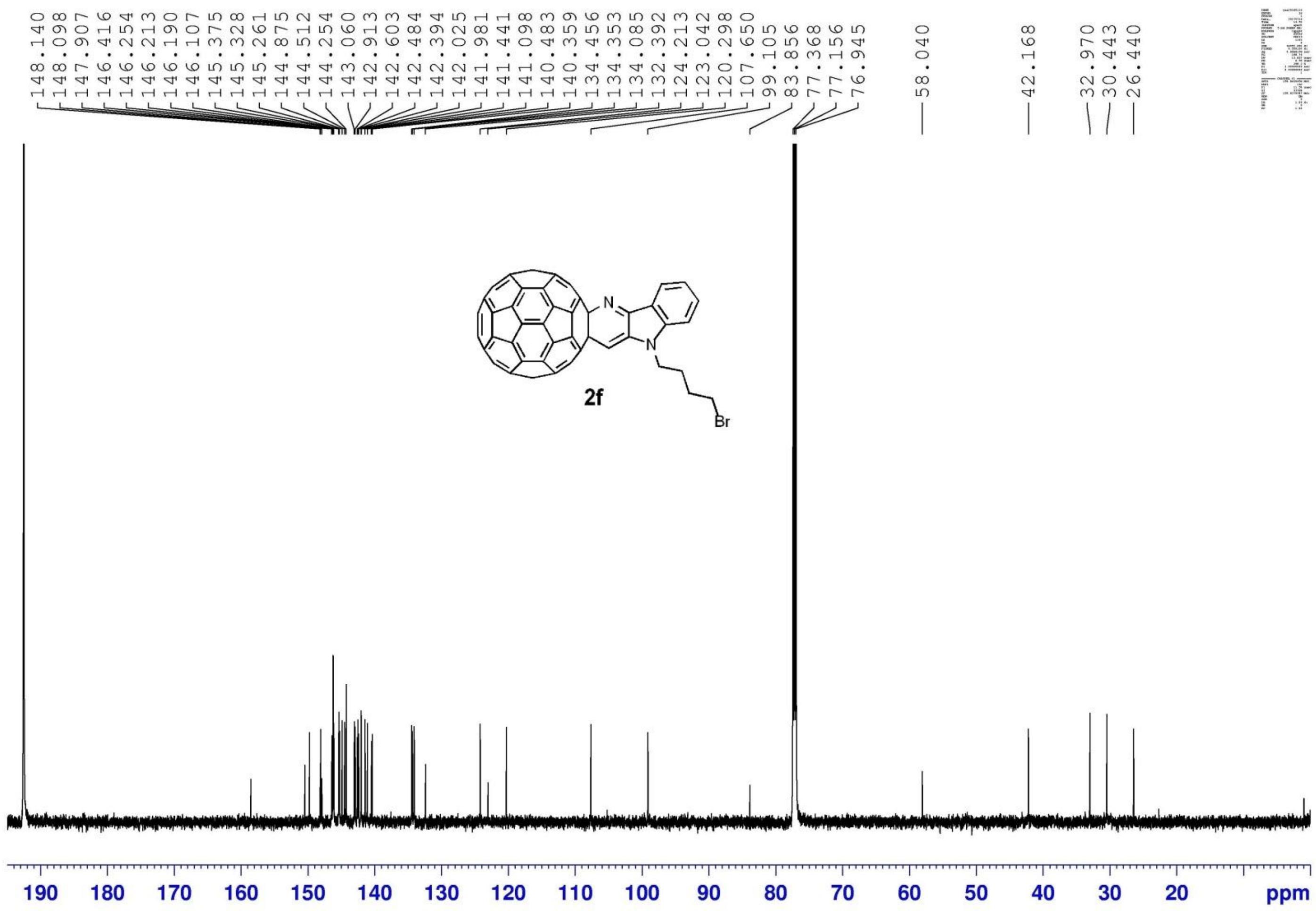


^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 2f

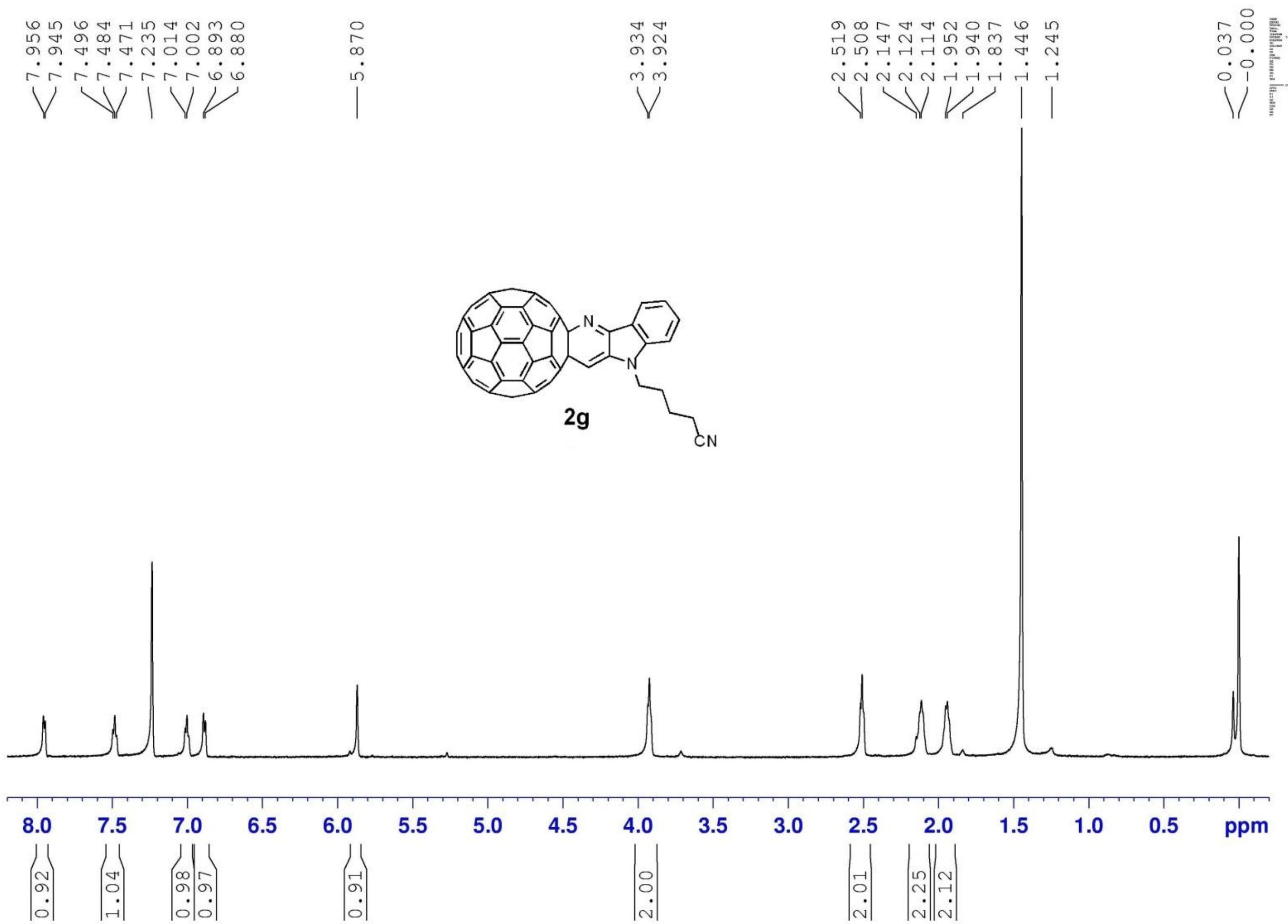


2f

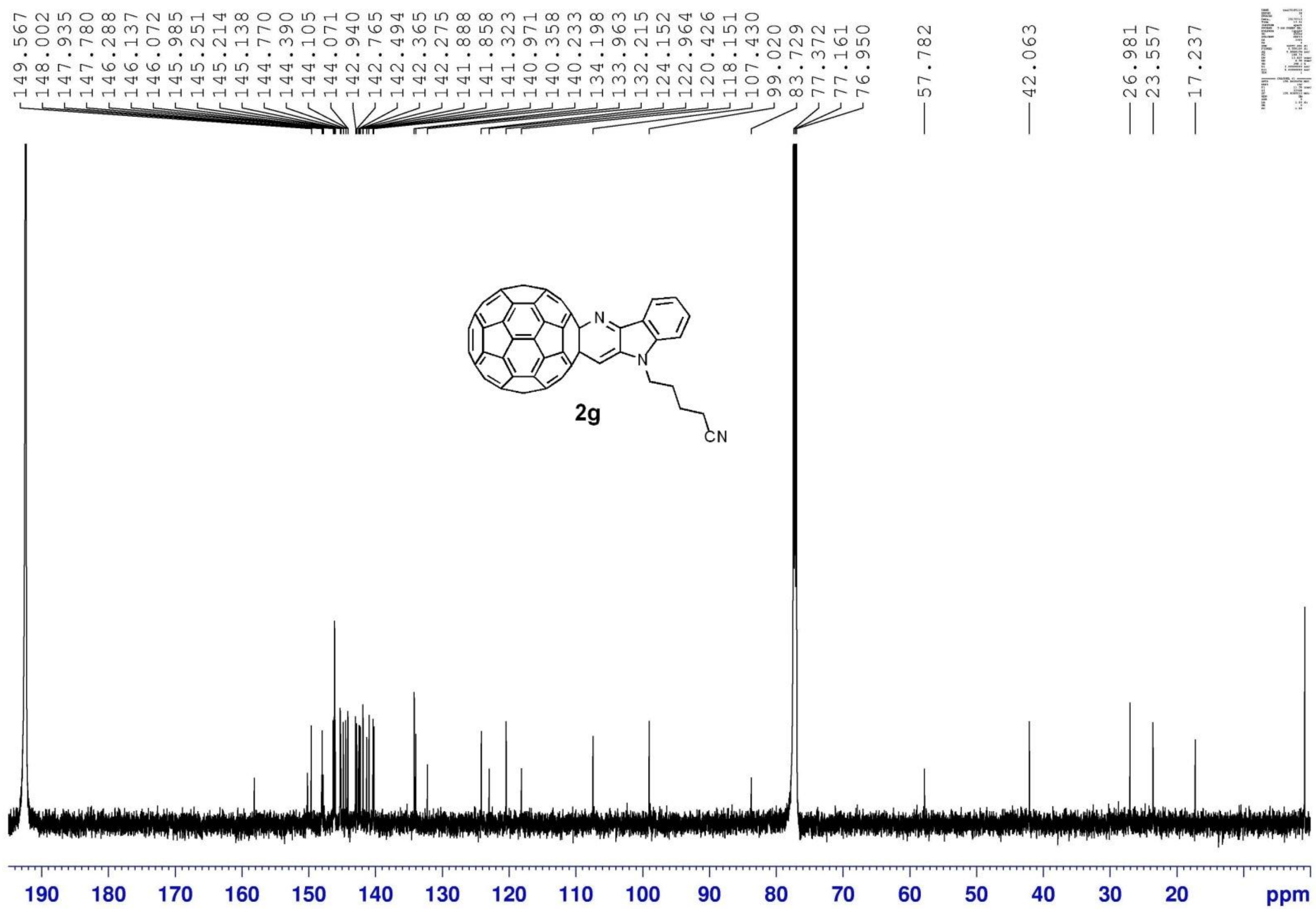
^{13}C NMR (150 MHz, $CDCl_3/CS_2$) of compound 2f



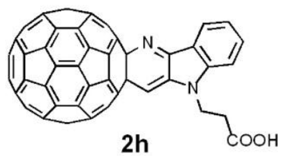
^1H NMR (600 MHz, $CDCl_3/CS_2$) of compound 2g



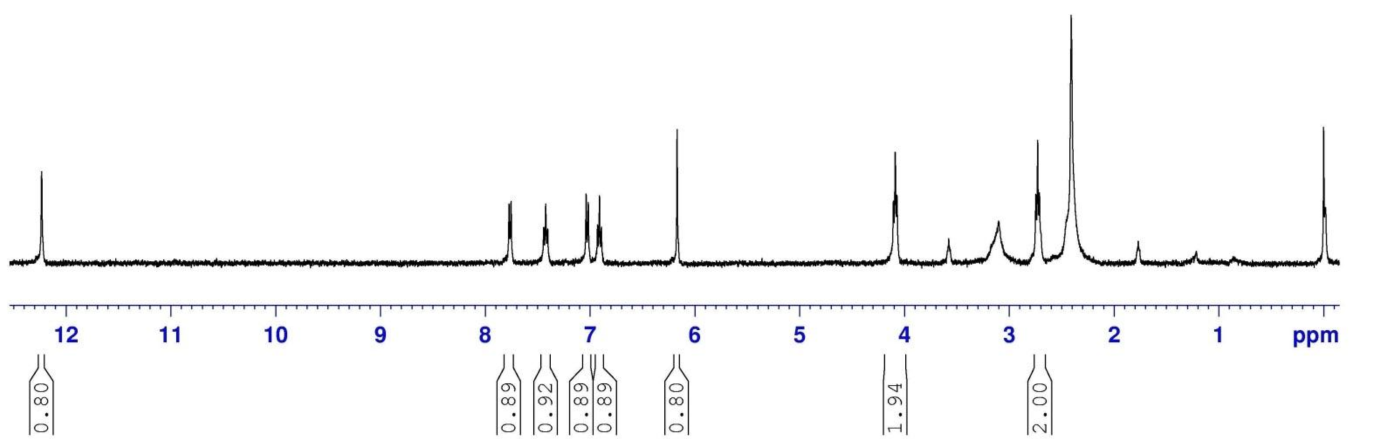
^{13}C NMR (150 MHz, $CDCl_3/CS_2$) of compound 2g



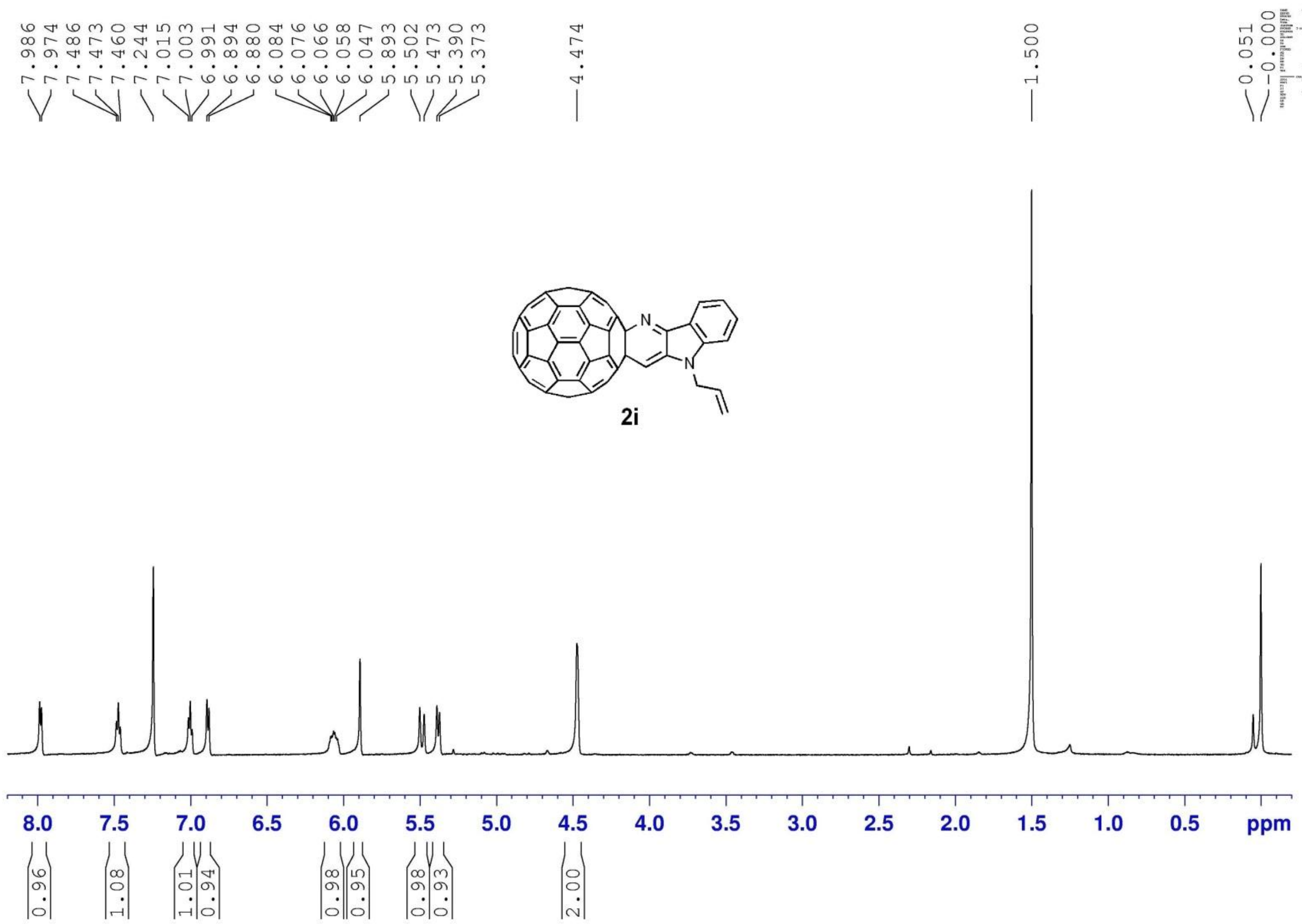
^{1}H NMR (400 MHz, DMSO-d_6/CS_2) of compound 2h



2h

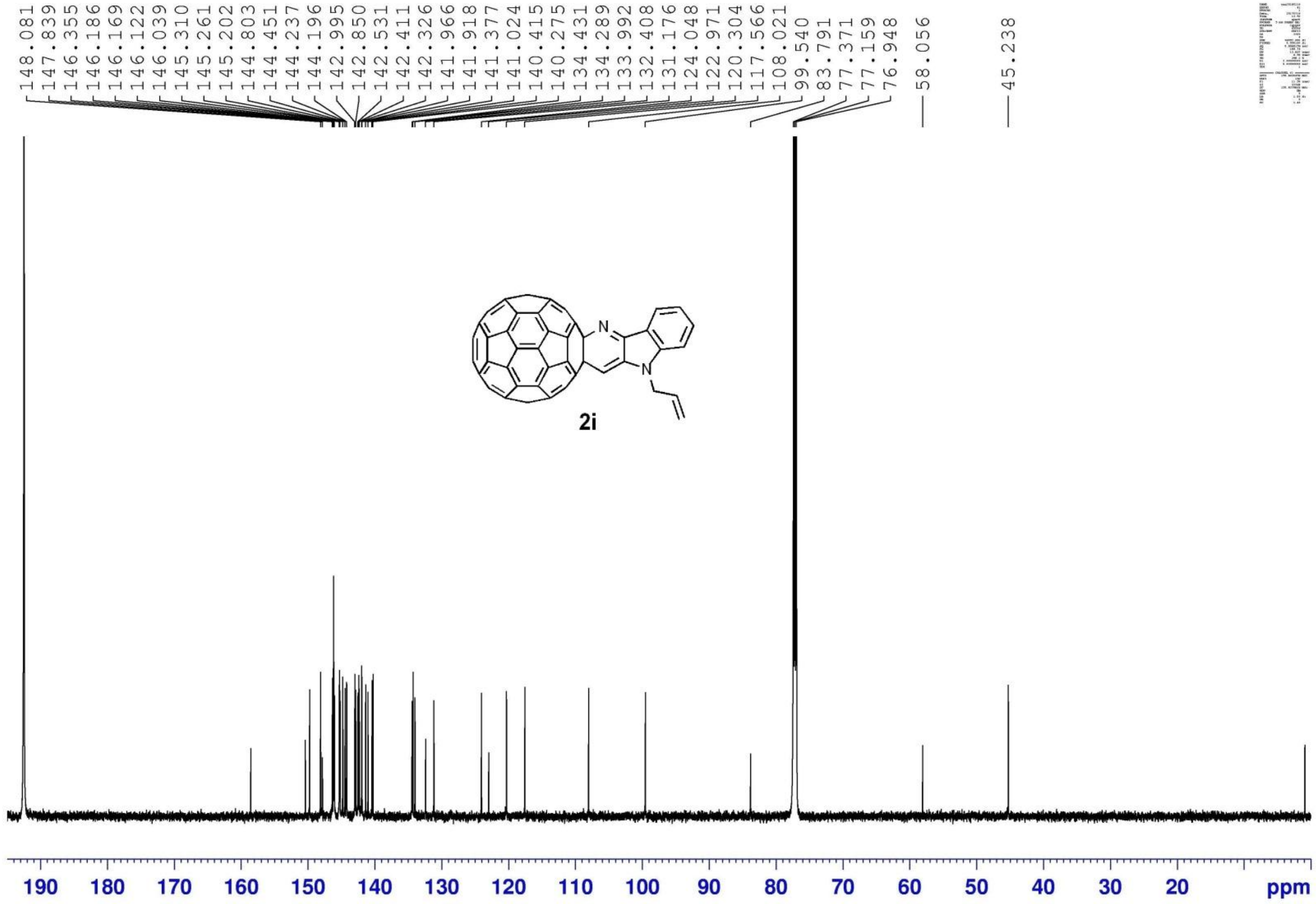


^{1}H NMR (600 MHz, $CDCl_3/CS_2$) of compound 2i

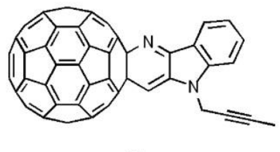


2i

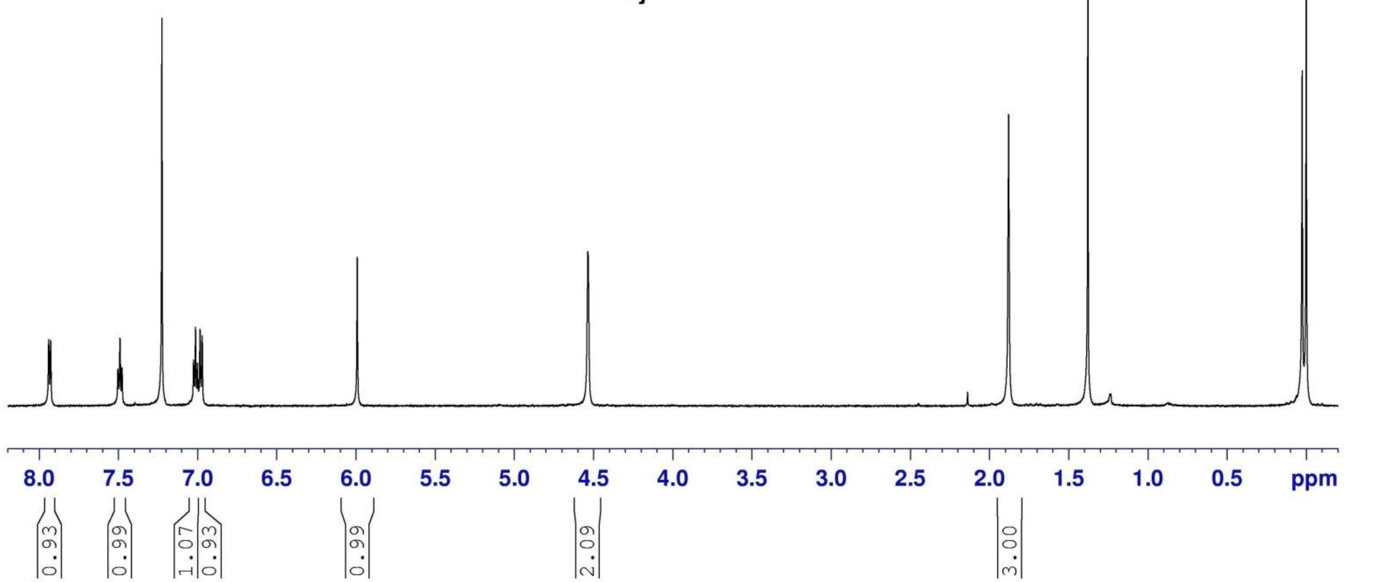
^{13}C NMR (150 MHz, $CDCl_3/CS_2$) of compound 2i



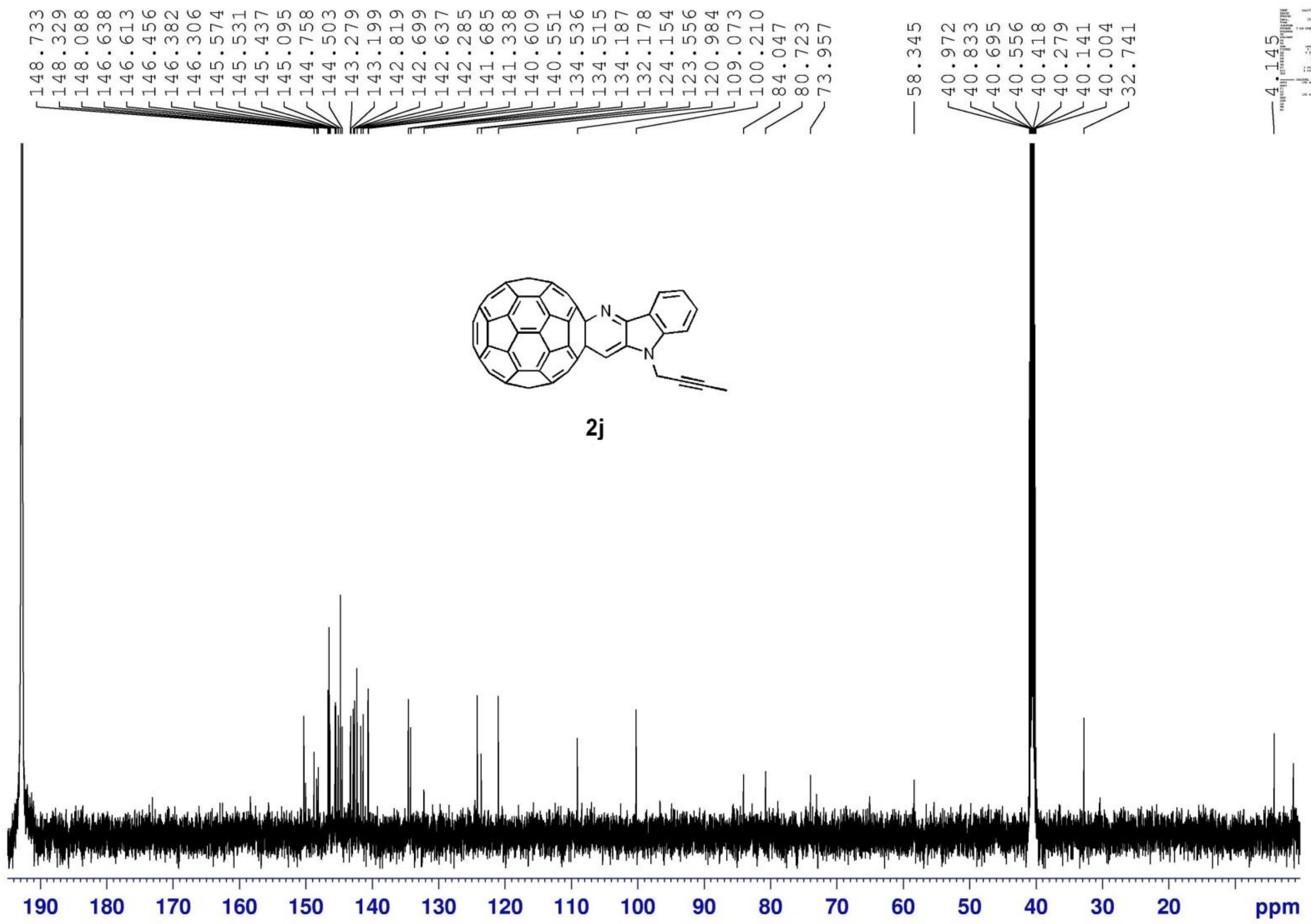
^{1}H NMR (600 MHz, $CDCl_3/CS_2$) of compound 2j



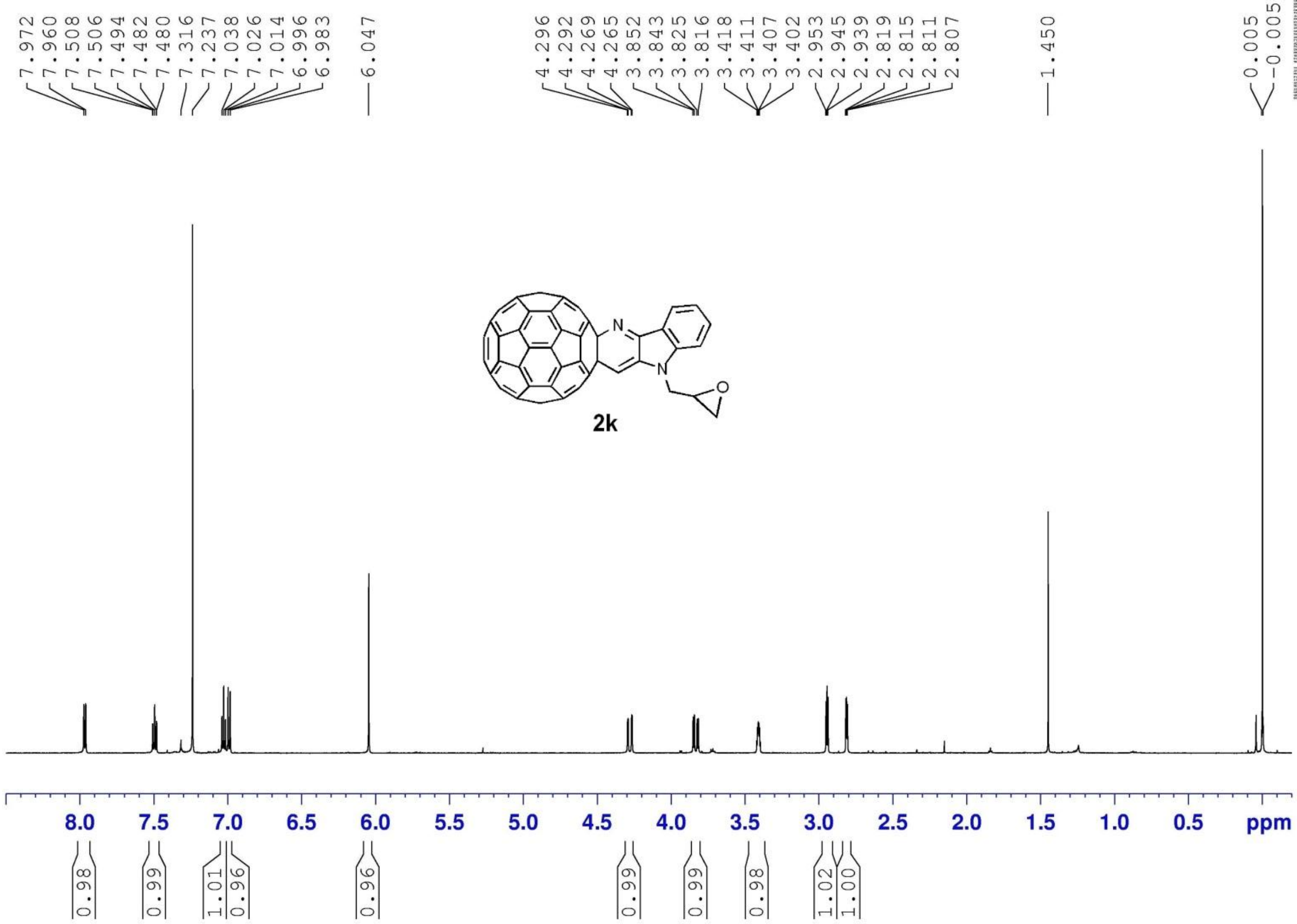
2j



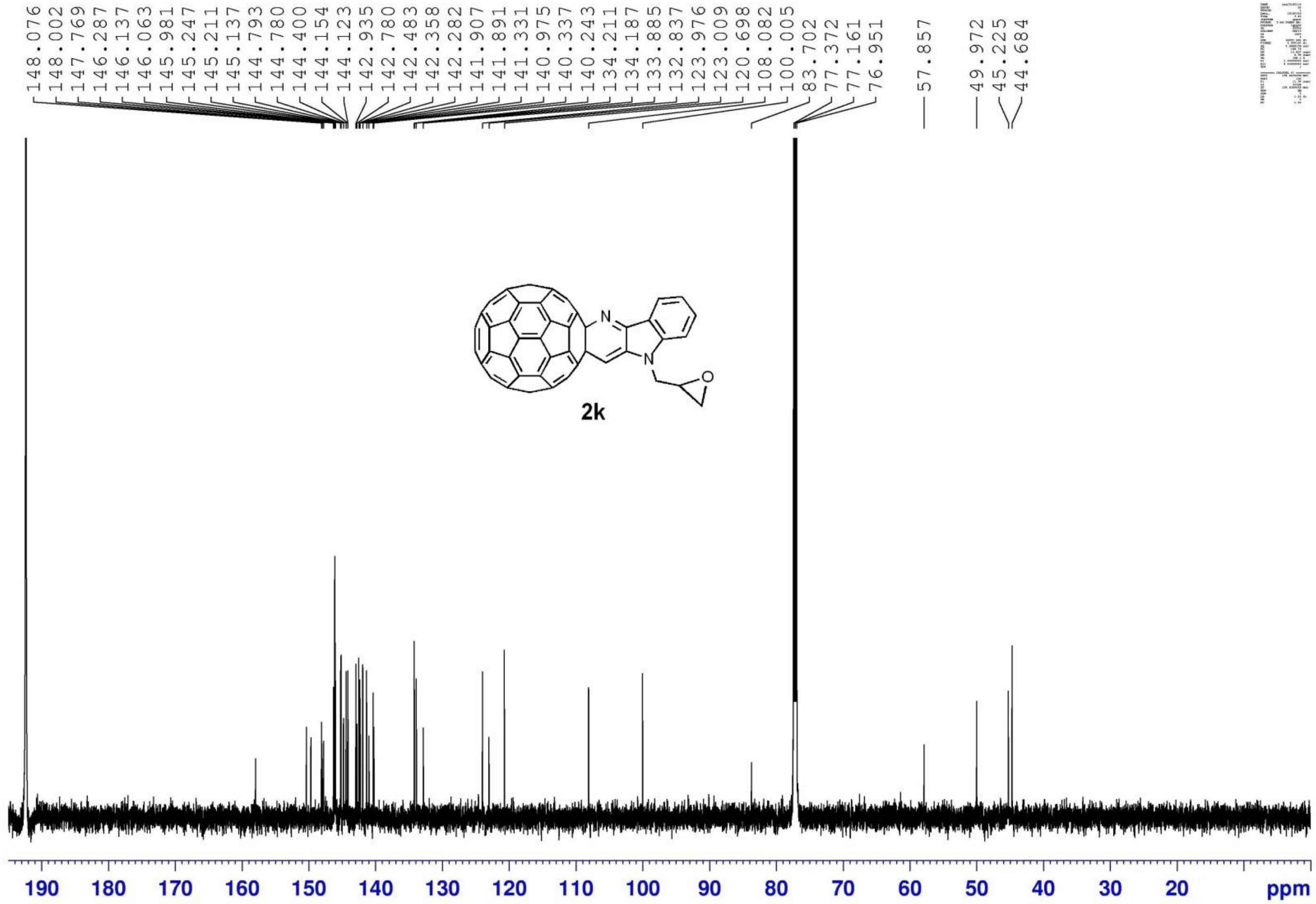
^{13}C NMR (150 MHz, DMSO-d_6/CS_2) of compound 2j



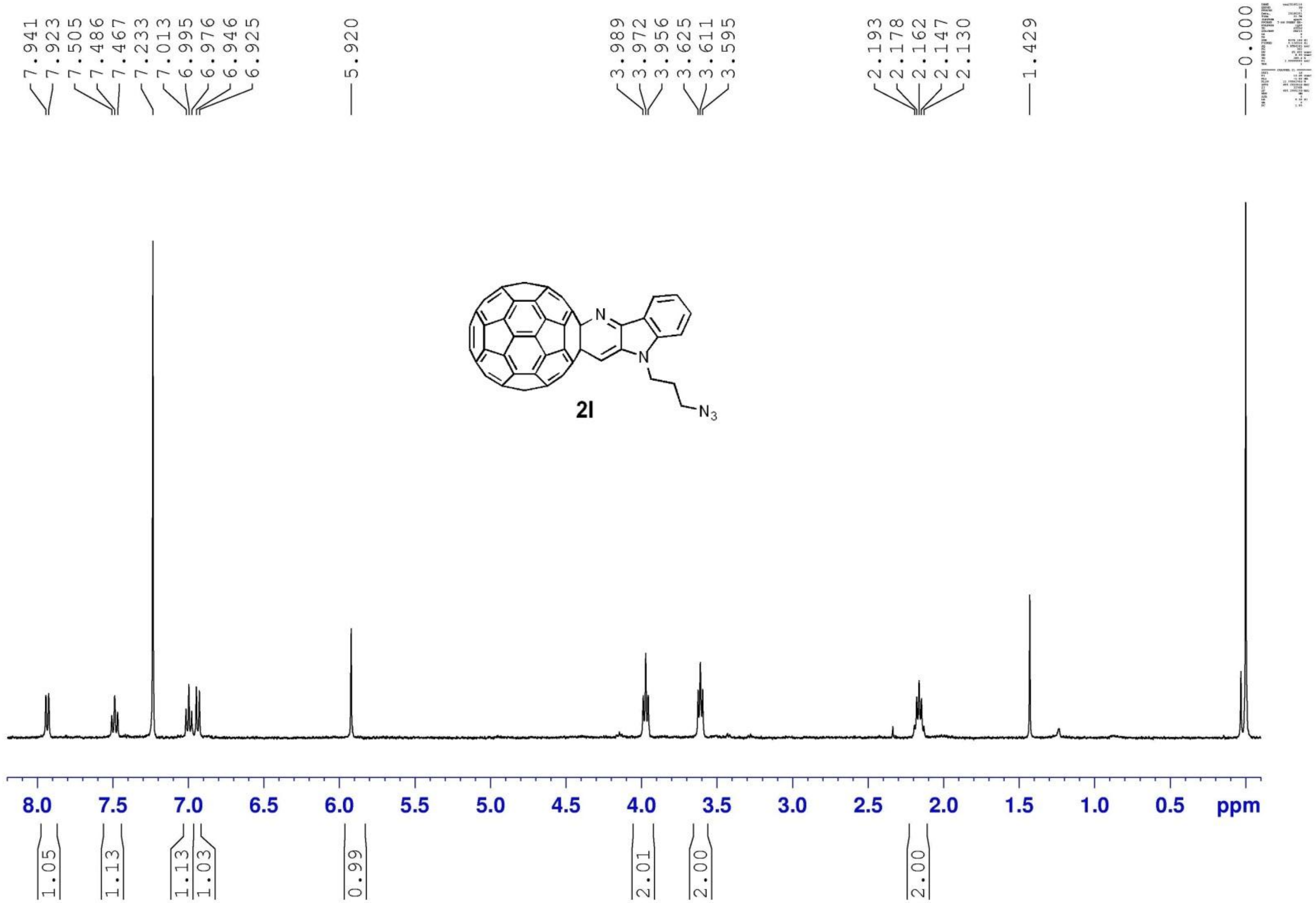
^1H NMR (600 MHz, $CDCl_3/CS_2$) of compound 2k



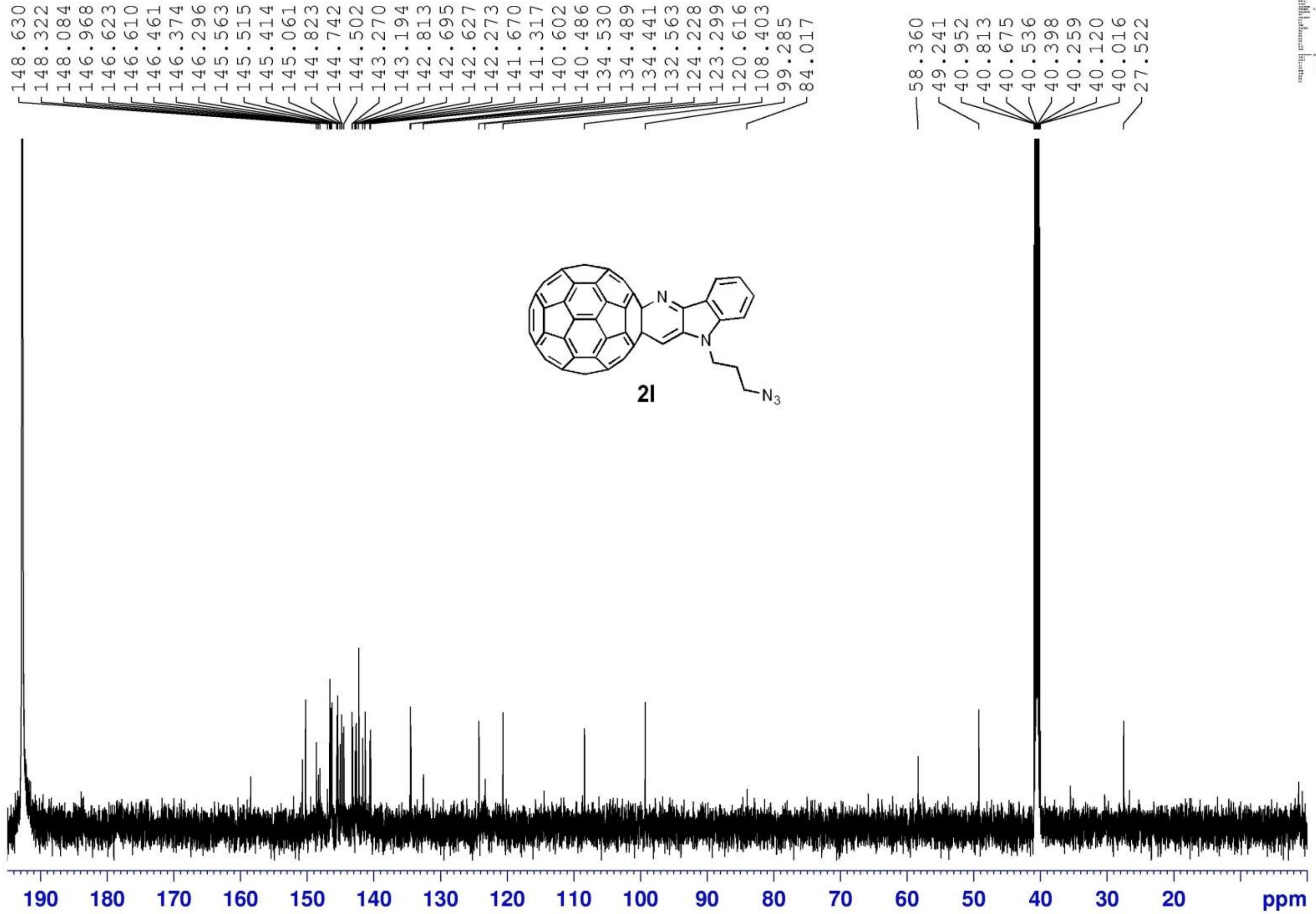
^{13}C NMR (150 MHz, $CDCl_3/CS_2$) of compound 2k



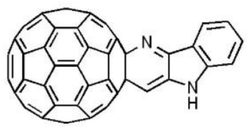
^1H NMR (400 MHz, $CDCl_3/CS_2$) of compound 2l



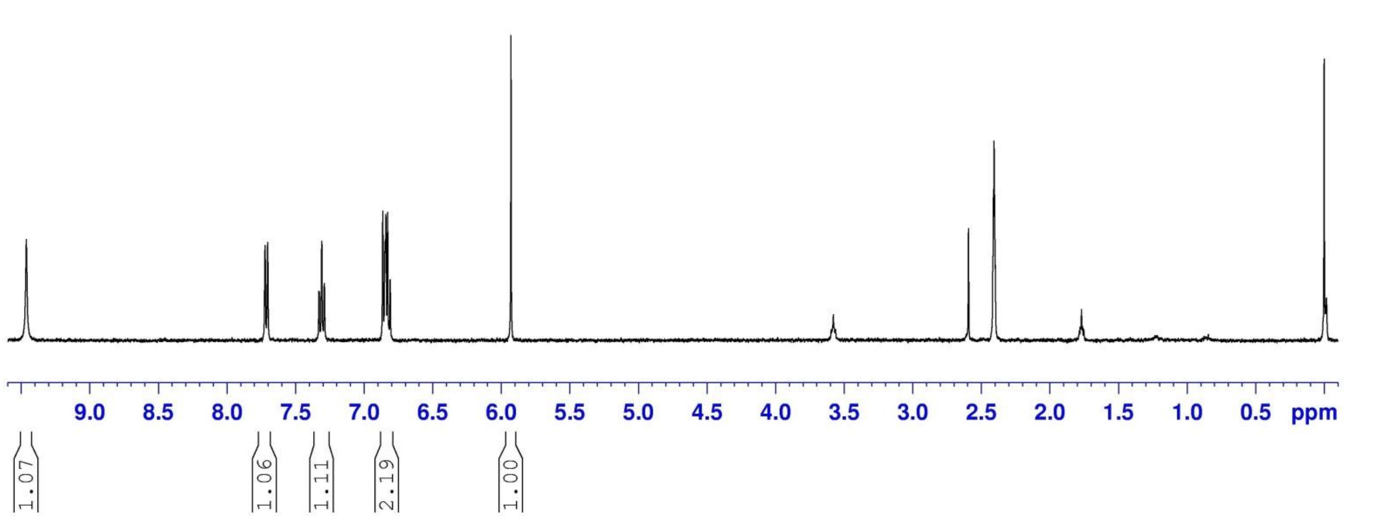
^{13}C NMR (150 MHz, DMSO-d_6/CS_2) of compound 2l



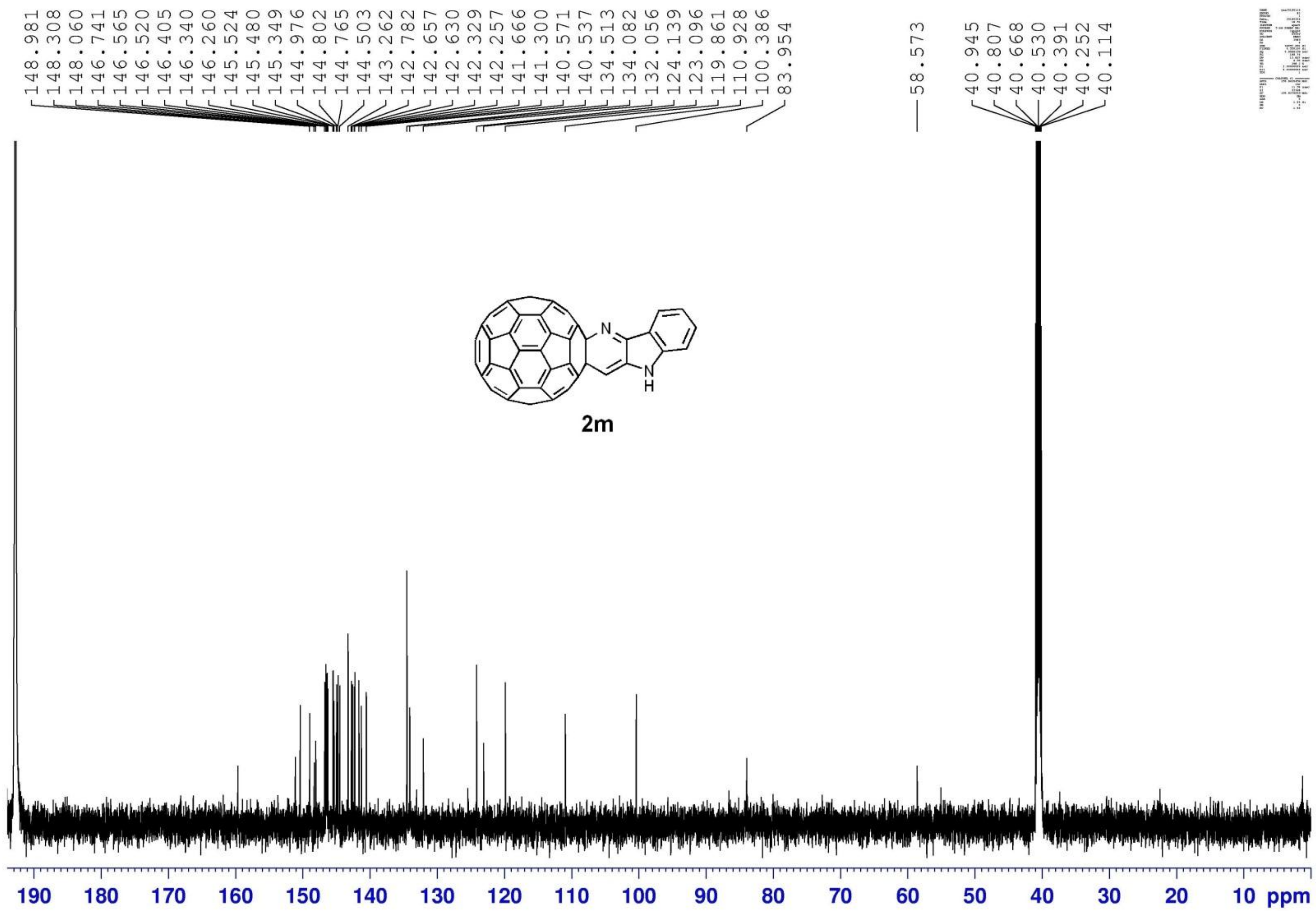
^{1}H NMR (400 MHz, DMSO-d_6/CS_2) of compound 2m



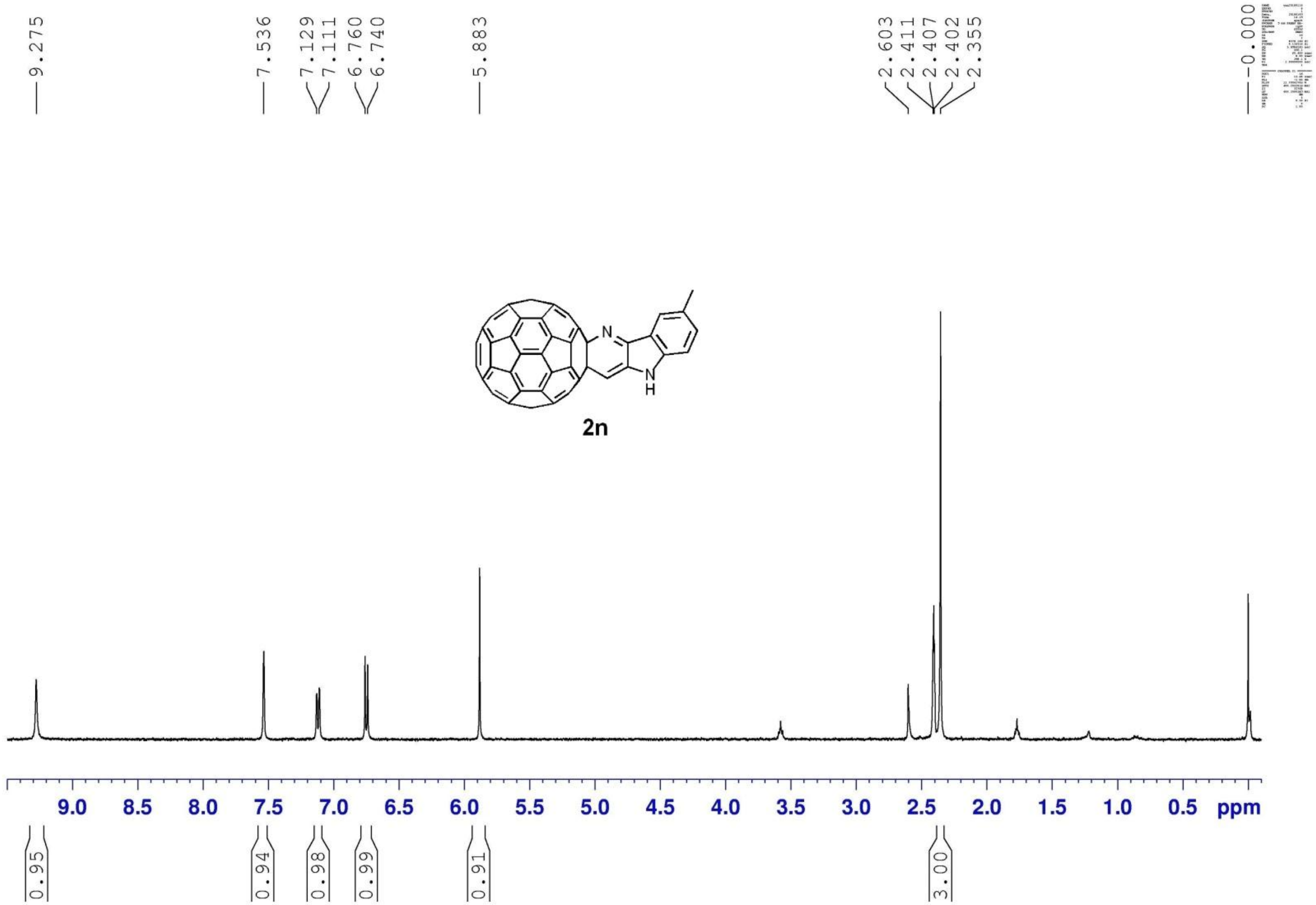
2m



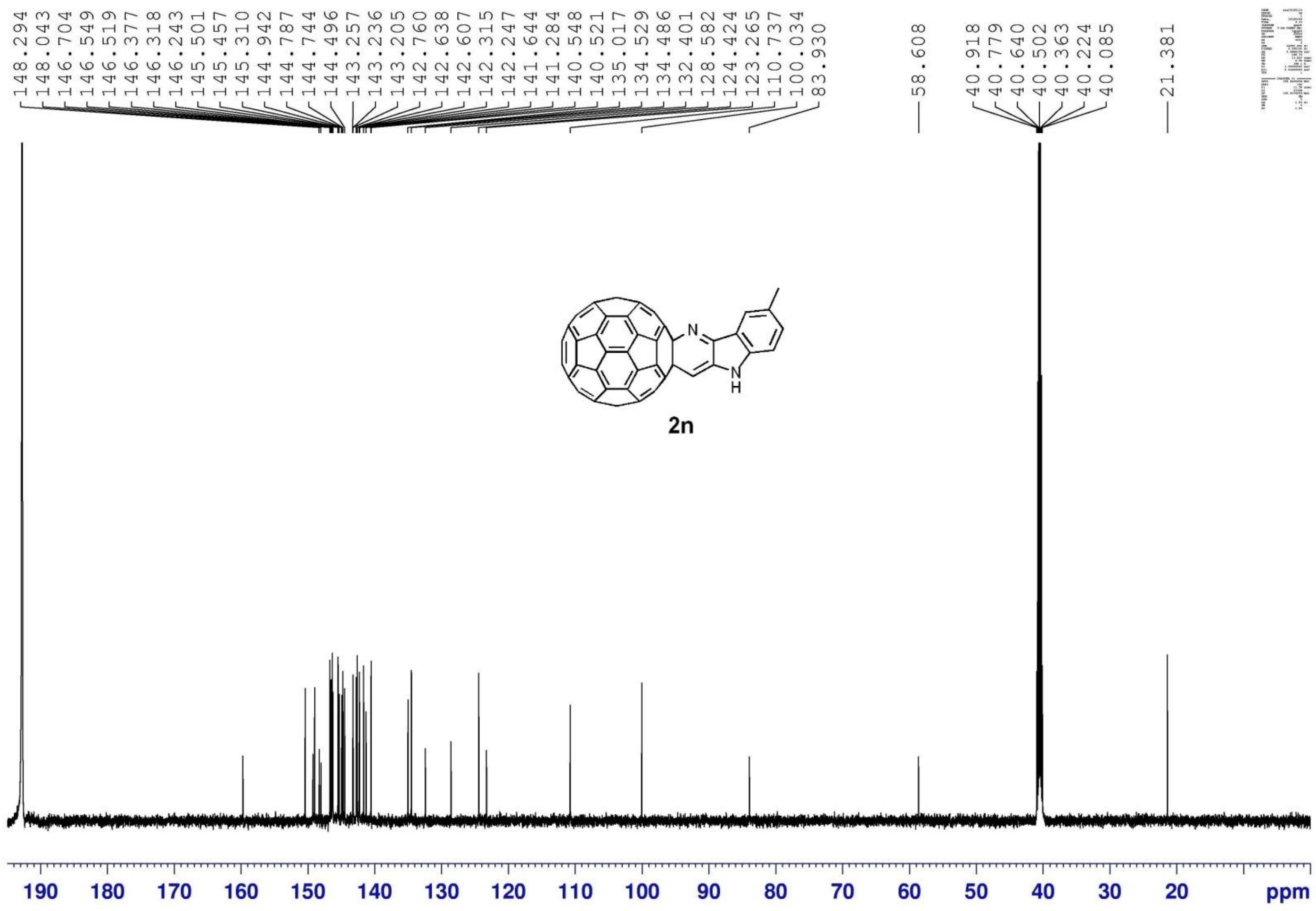
^{13}C NMR (150 MHz, DMSO-d_6/CS_2) of compound 2m



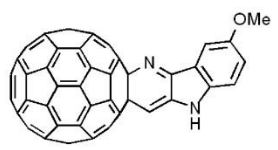
^{1}H NMR (400 MHz, DMSO-d_6/CS_2) of compound 2n



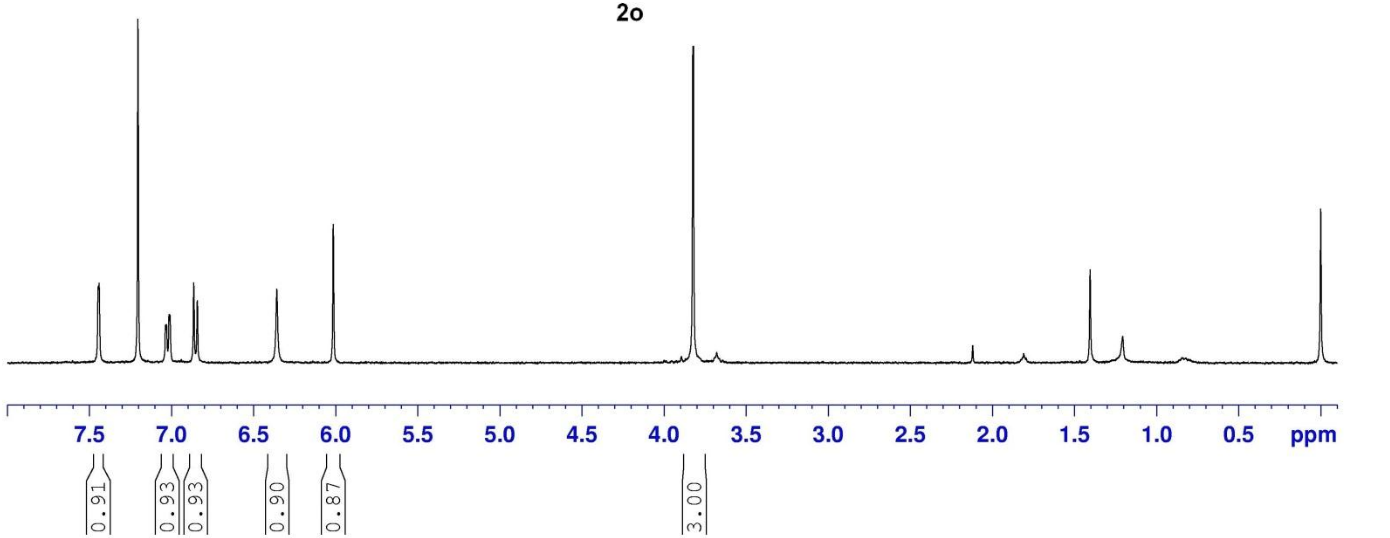
^{13}C NMR (150 MHz, DMSO-d_6/CS_2) of compound 2n



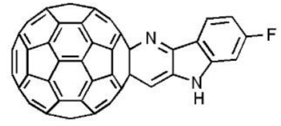
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 2o



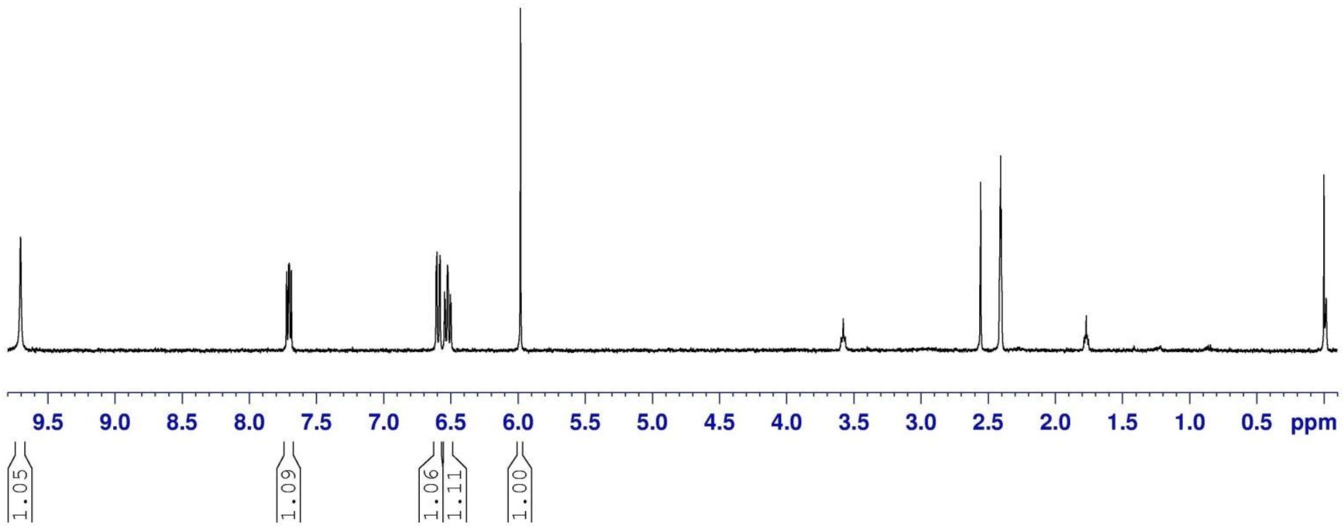
2o



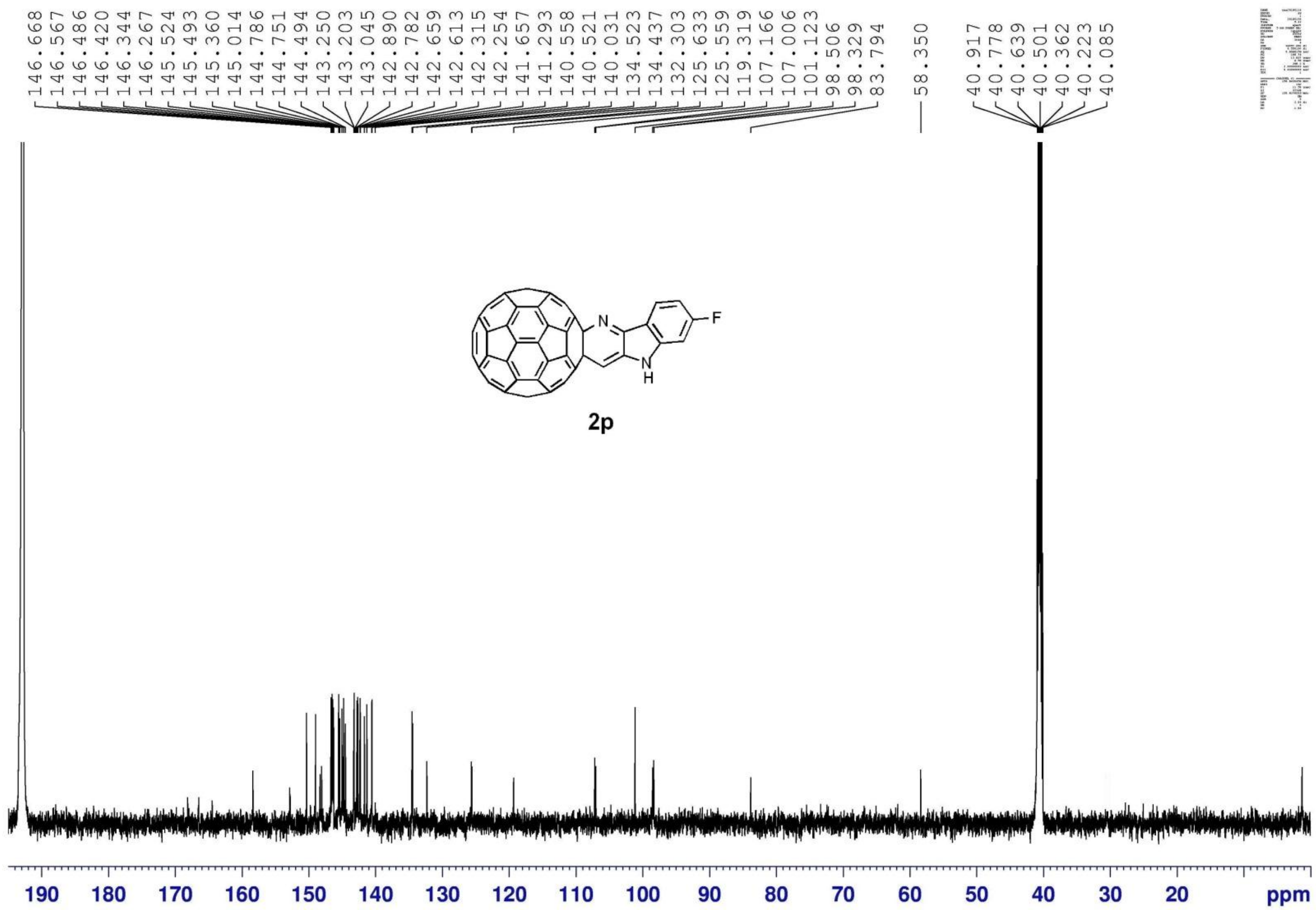
^{1}H NMR (400 MHz, DMSO-d_6/CS_2) of compound 2p



2p

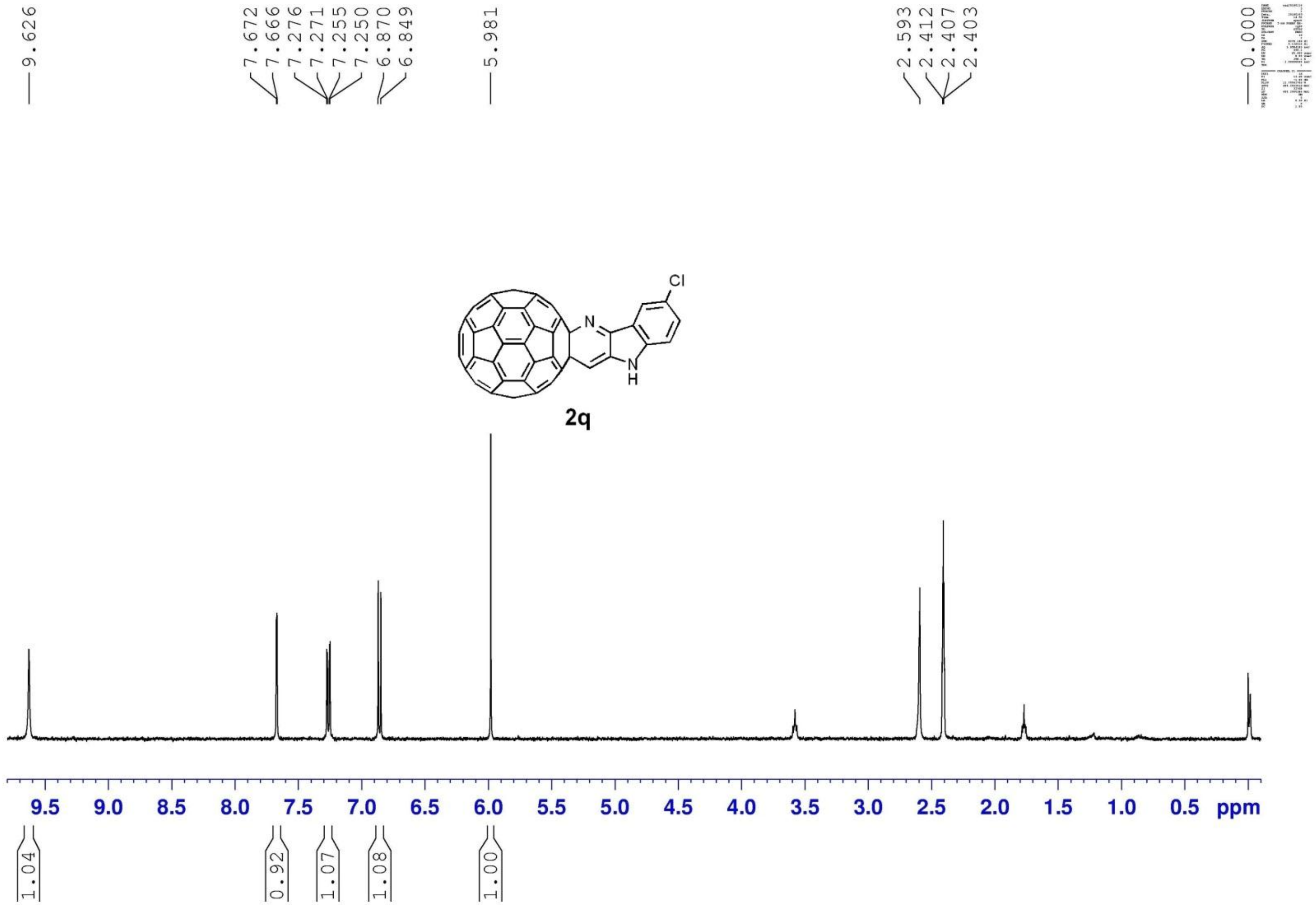


^{13}C NMR (150 MHz, DMSO-d_6/CS_2) of compound 2p

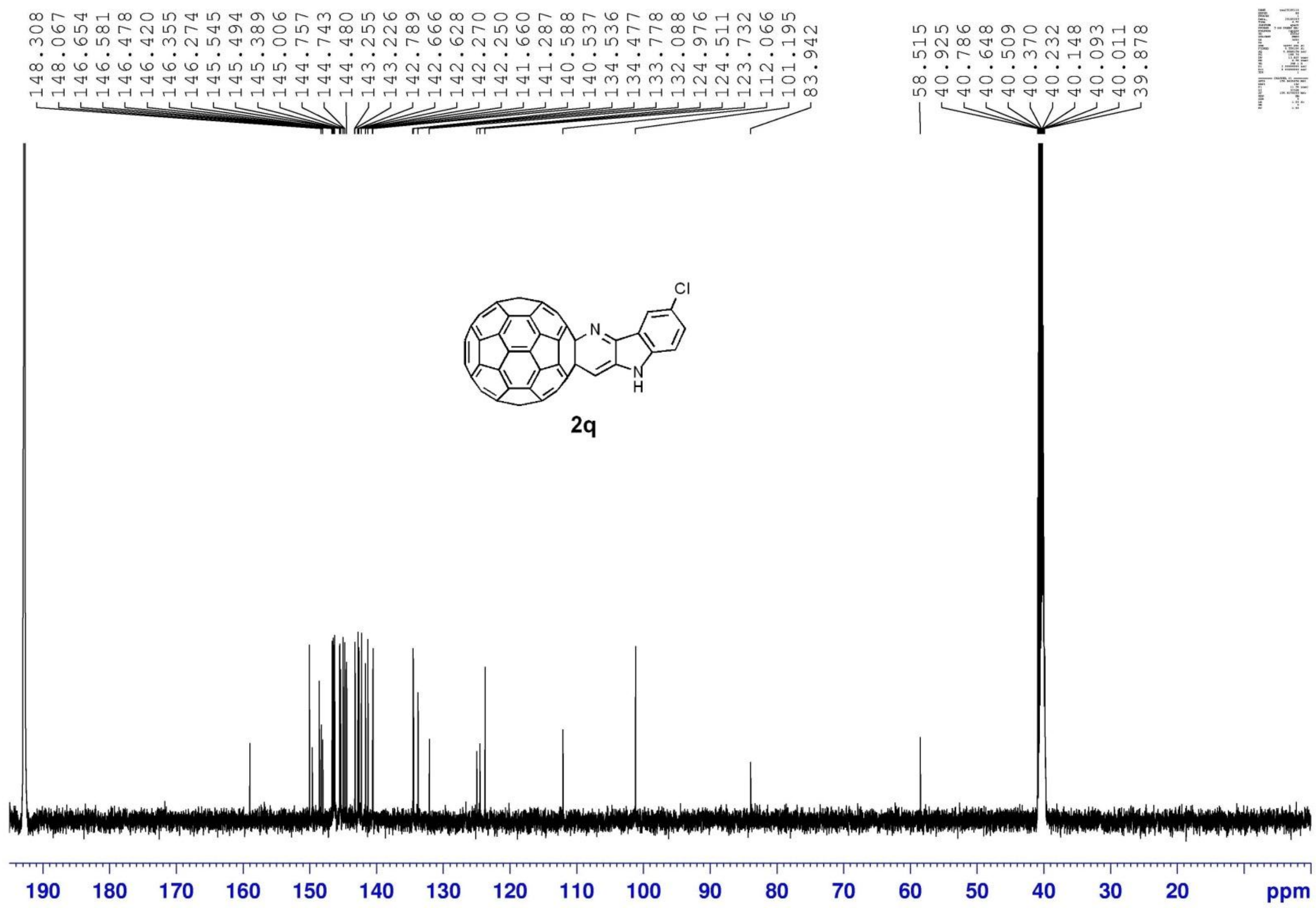


2p

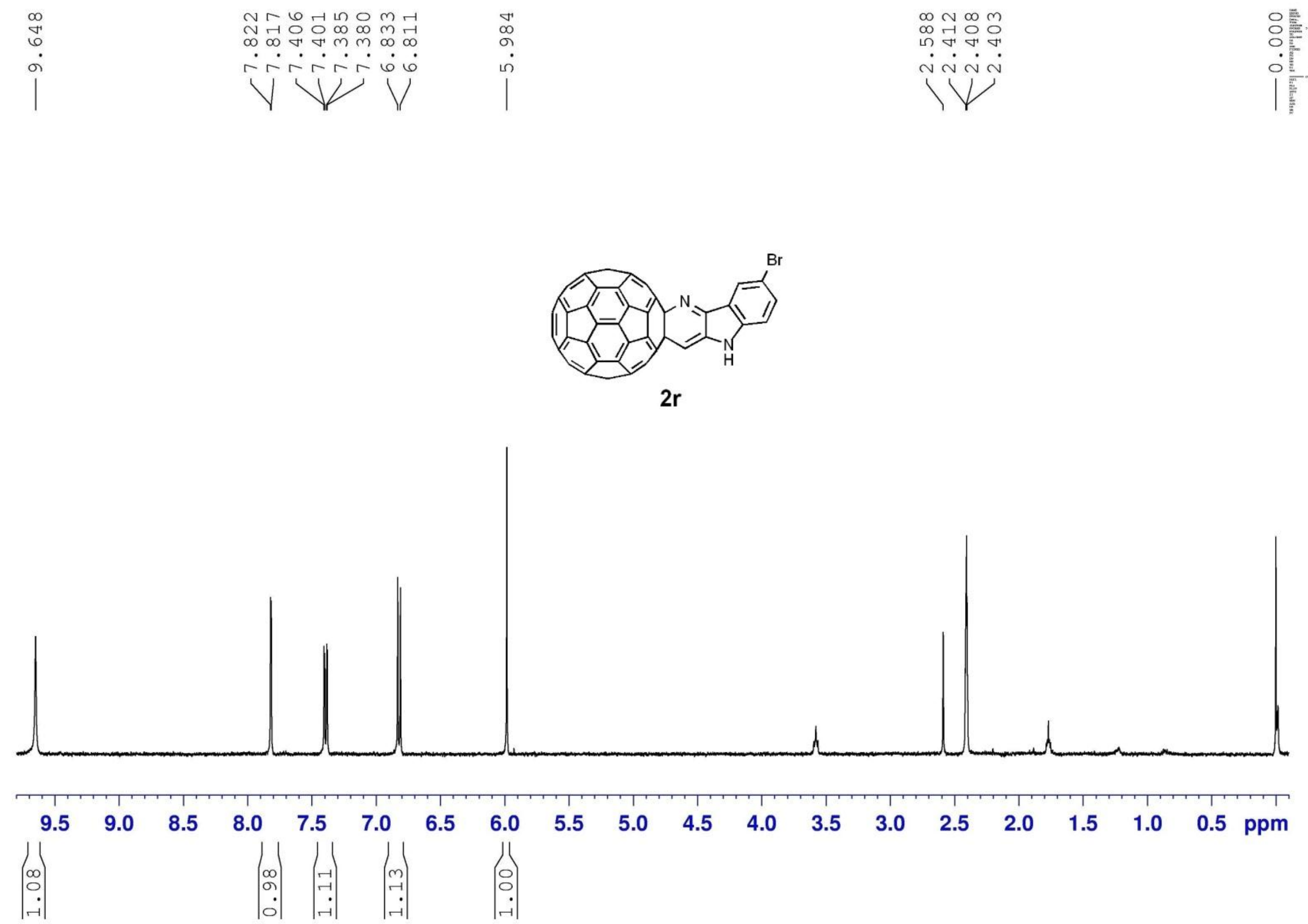
^{1}H NMR (400 MHz, DMSO-d_6/CS_2) of compound 2q



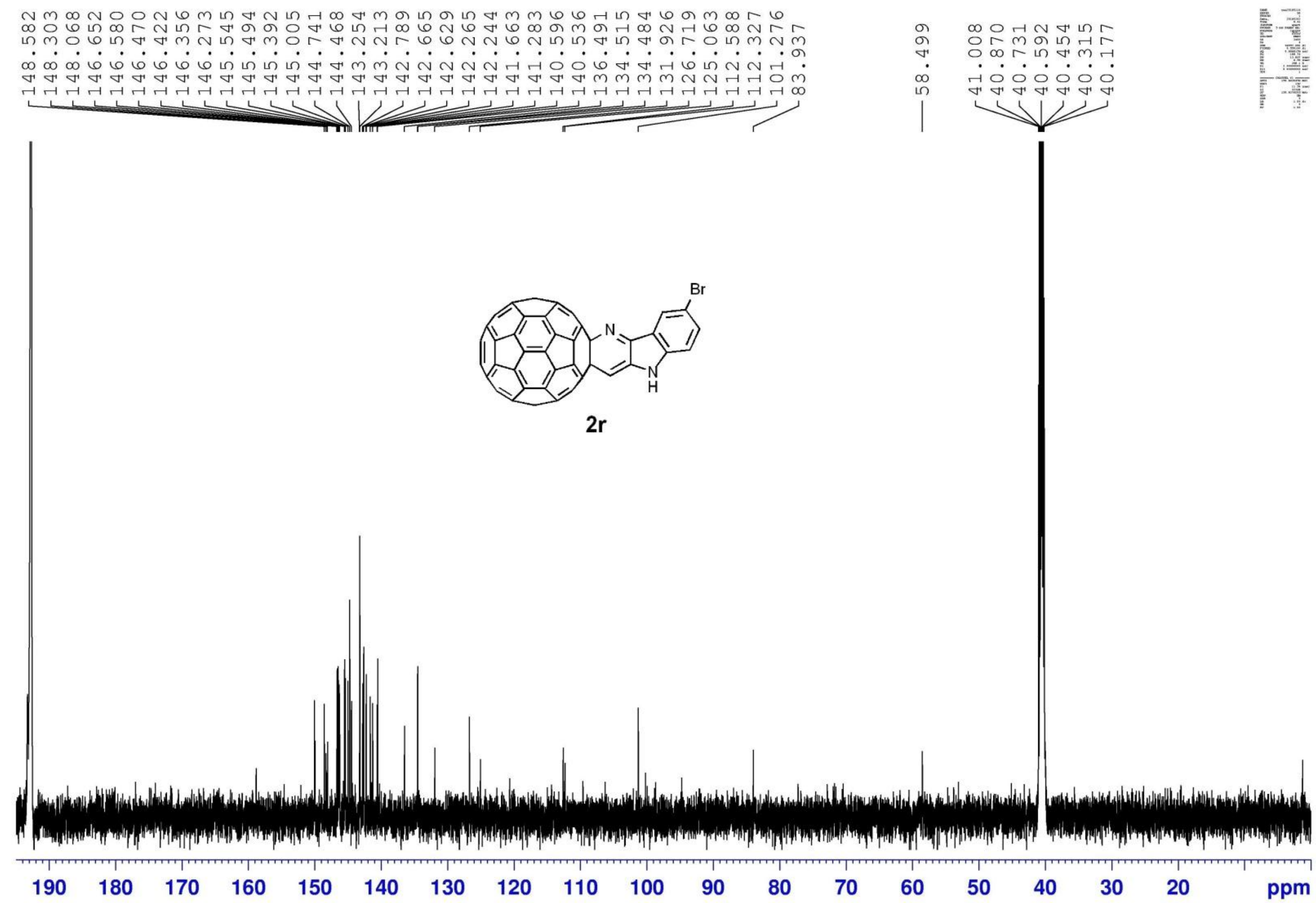
^{13}C NMR (150 MHz, DMSO-d_6/CS_2) of compound 2q



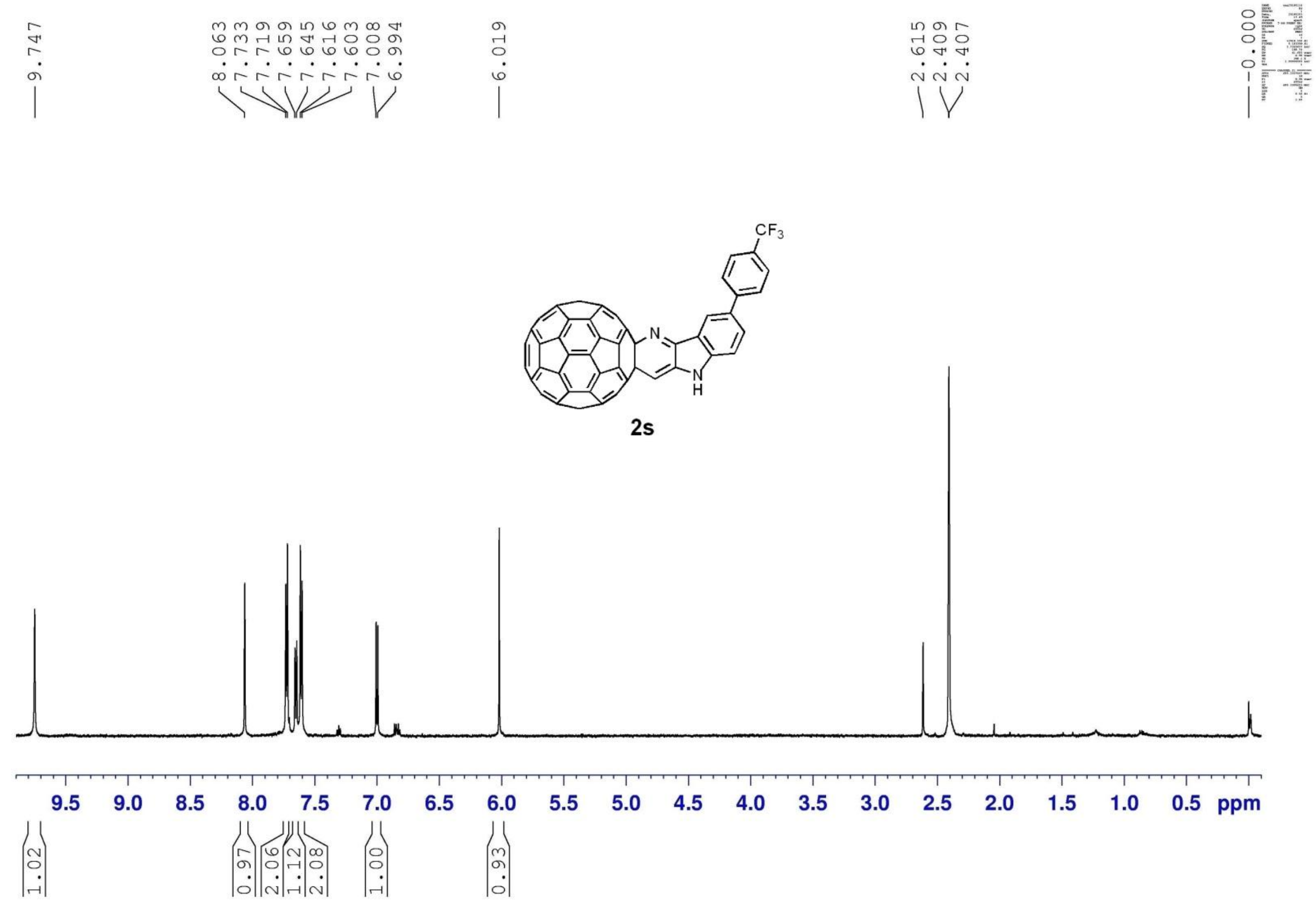
^{1}H NMR (400 MHz, DMSO-d_6/CS_2) of compound 2r



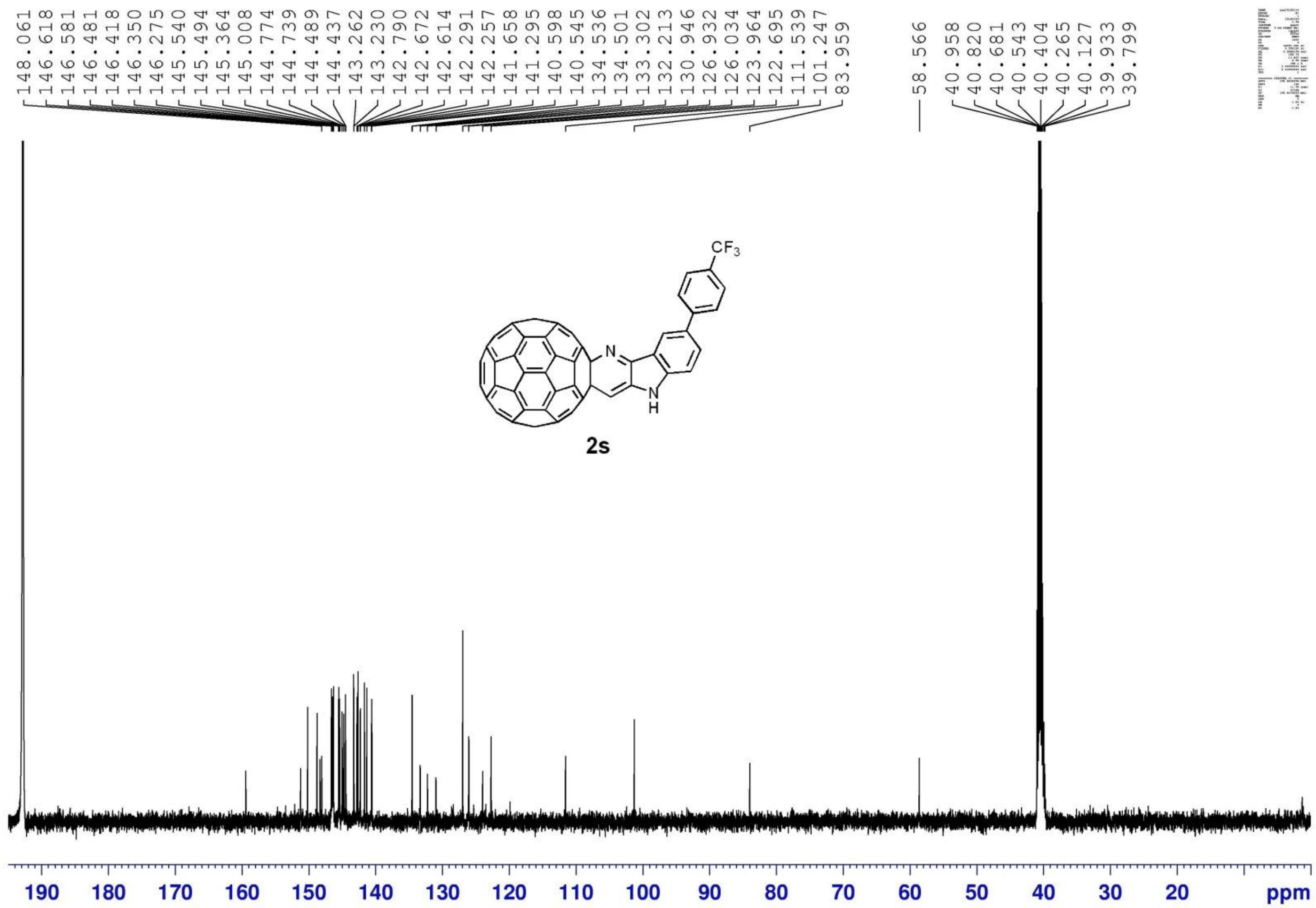
^{13}C NMR (150 MHz, DMSO-d_6/CS_2) of compound 2r



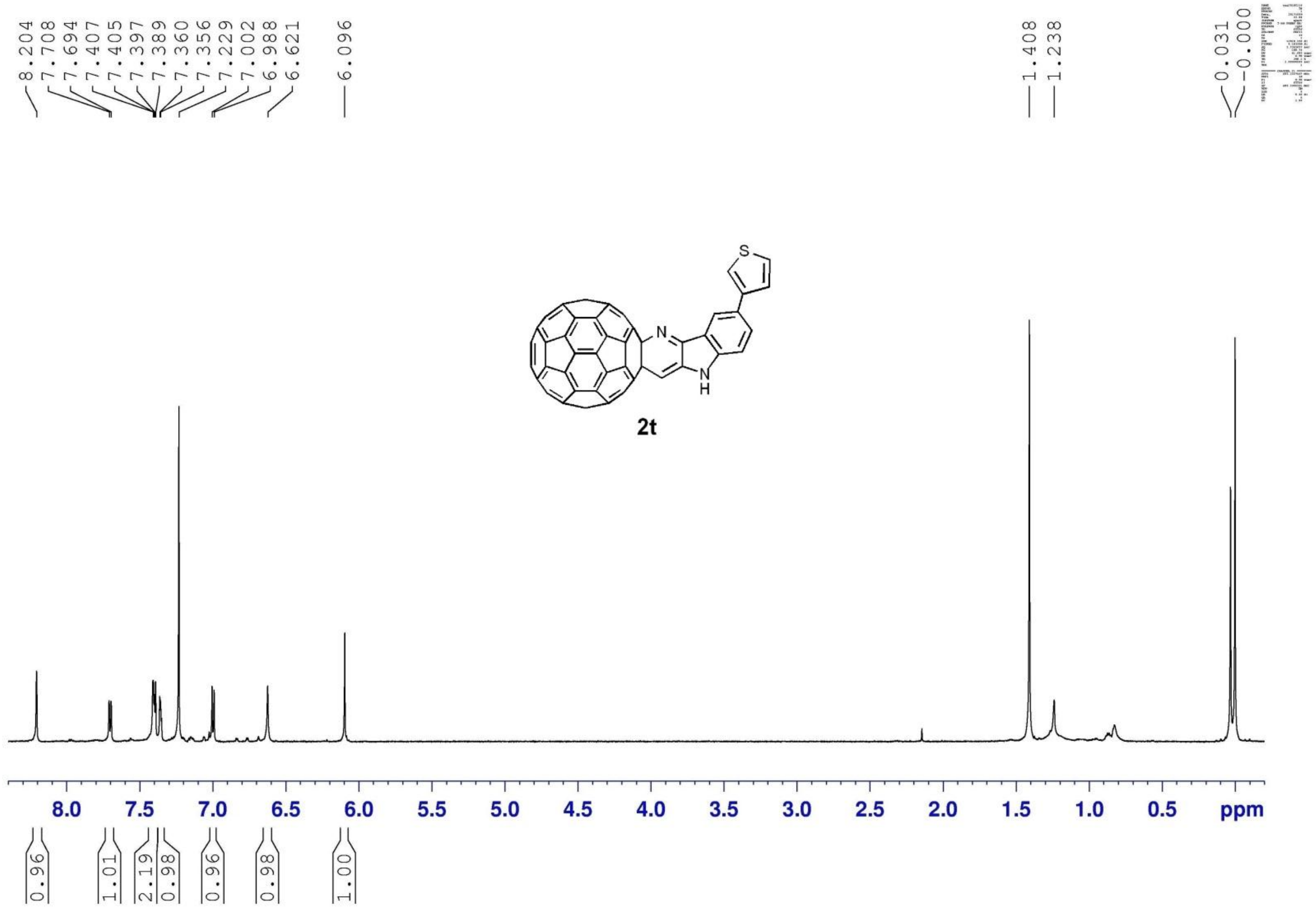
^1H NMR (600 MHz, DMSO-d_6/CS_2) of compound 2s



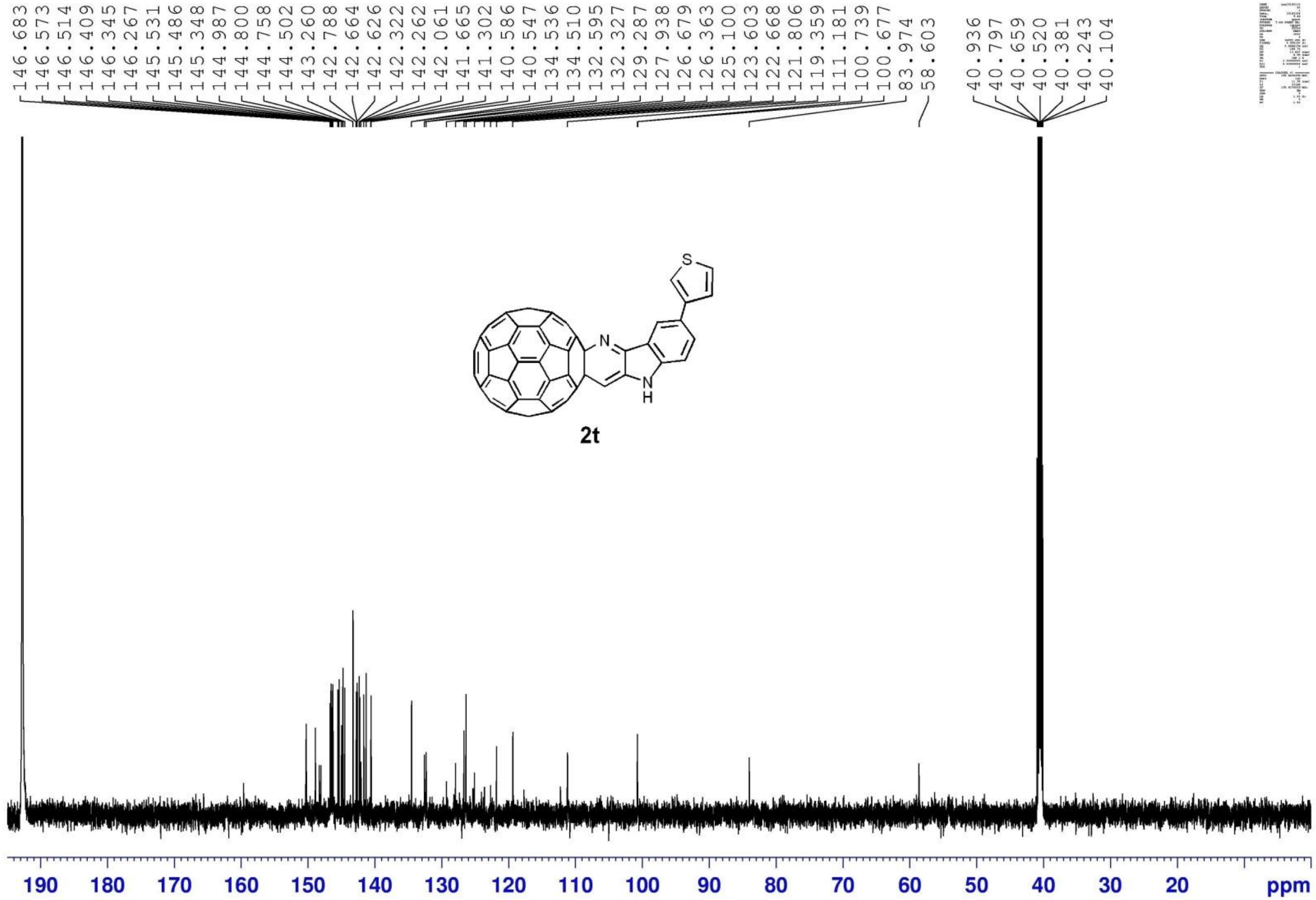
^{13}C NMR (150 MHz, DMSO-d_6/CS_2) of compound 2s



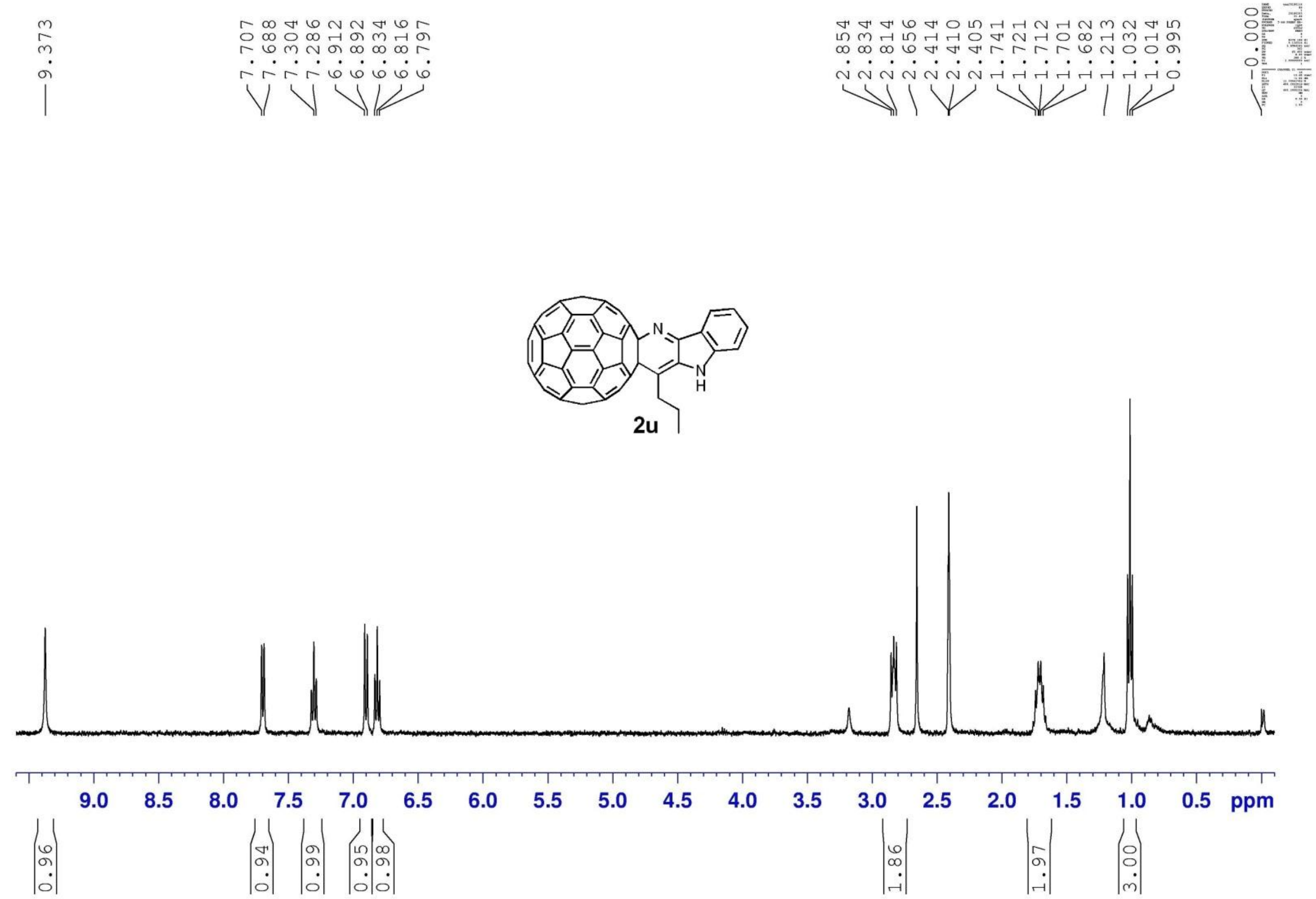
^1H NMR (600 MHz, $CDCl_3/CS_2$) of compound 2t



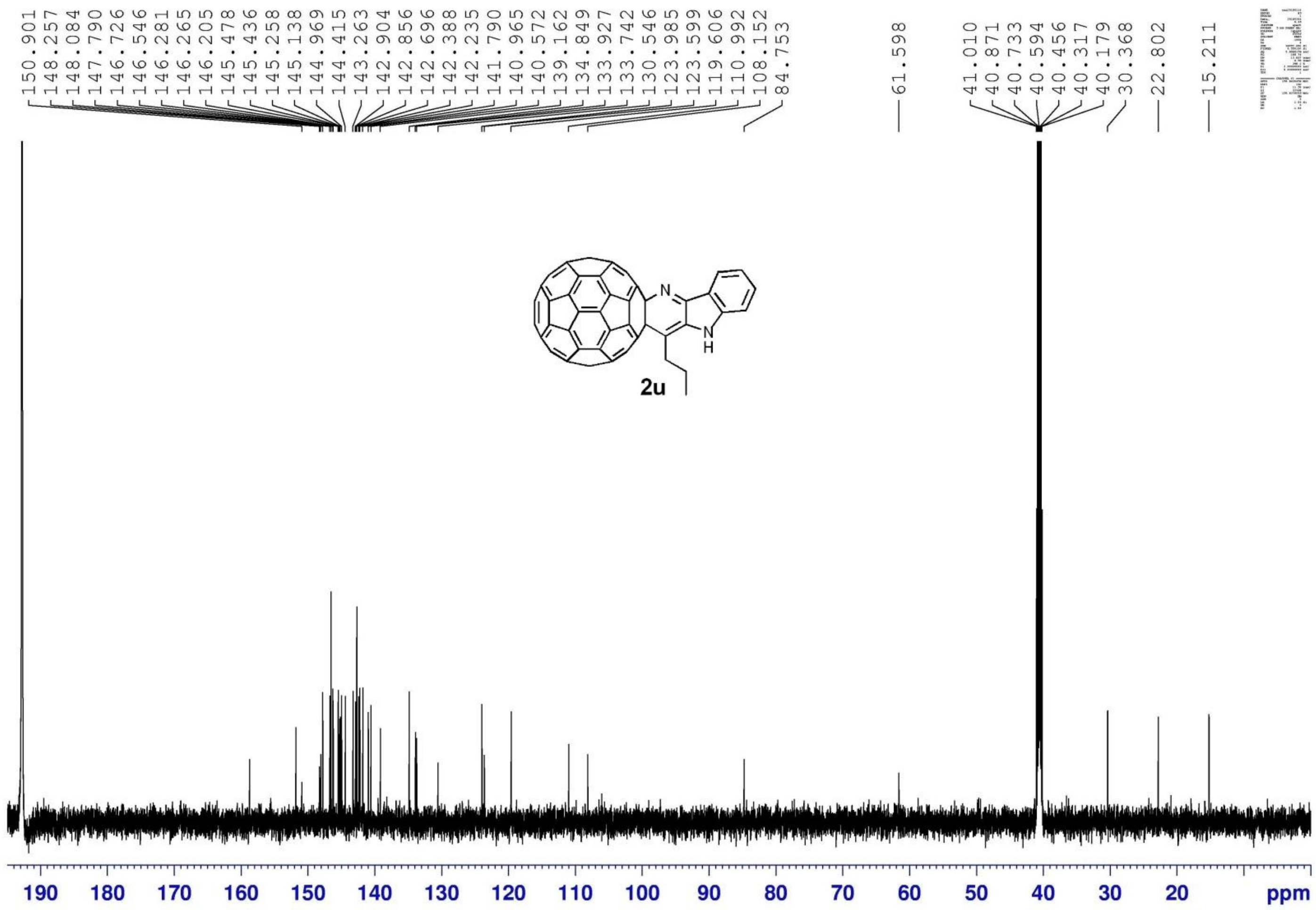
^{13}C NMR (150 MHz, DMSO-d_6/CS_2) of compound 2t



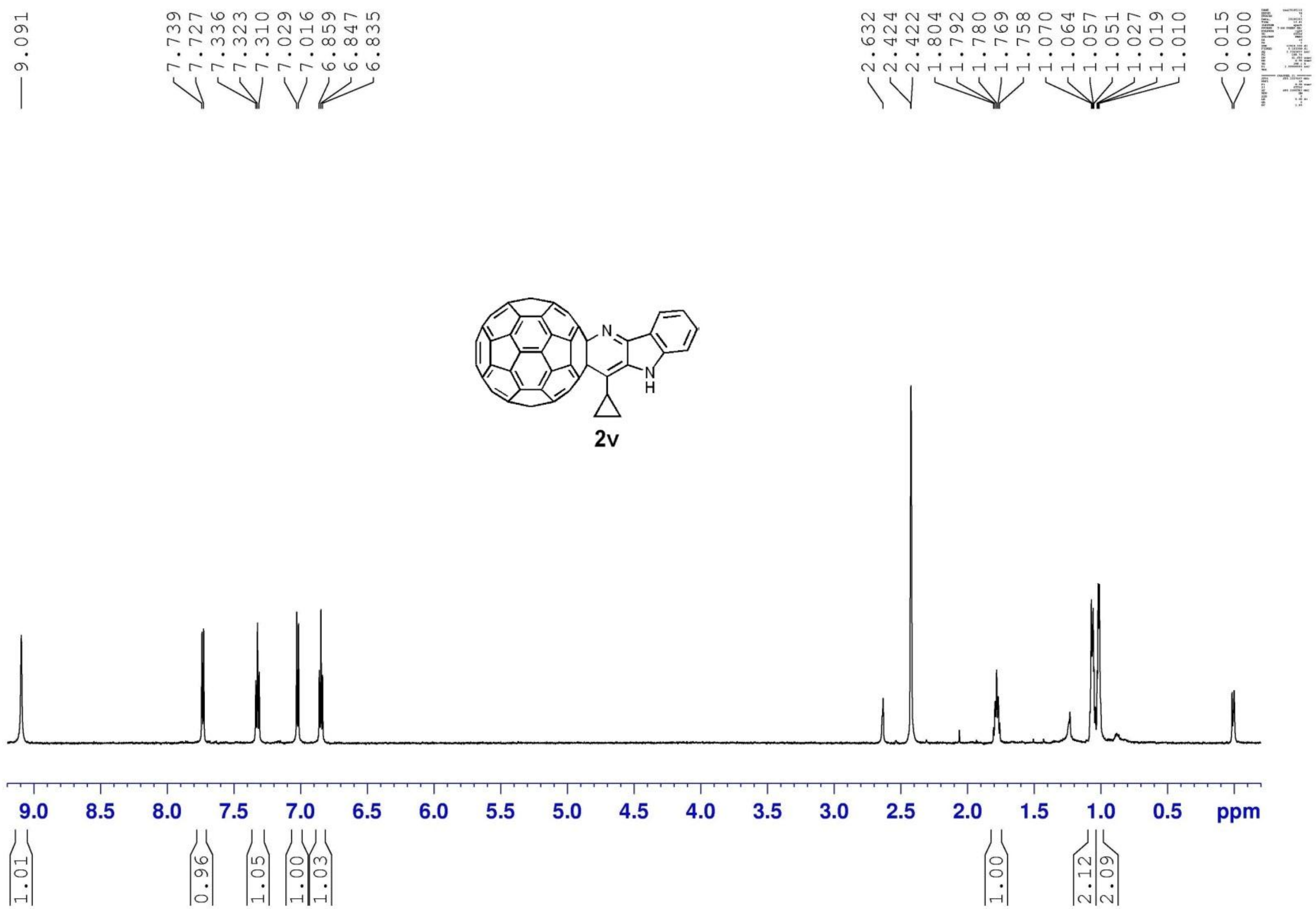
^{1}H NMR (400 MHz, DMSO-d_6/CS_2) of compound 2u



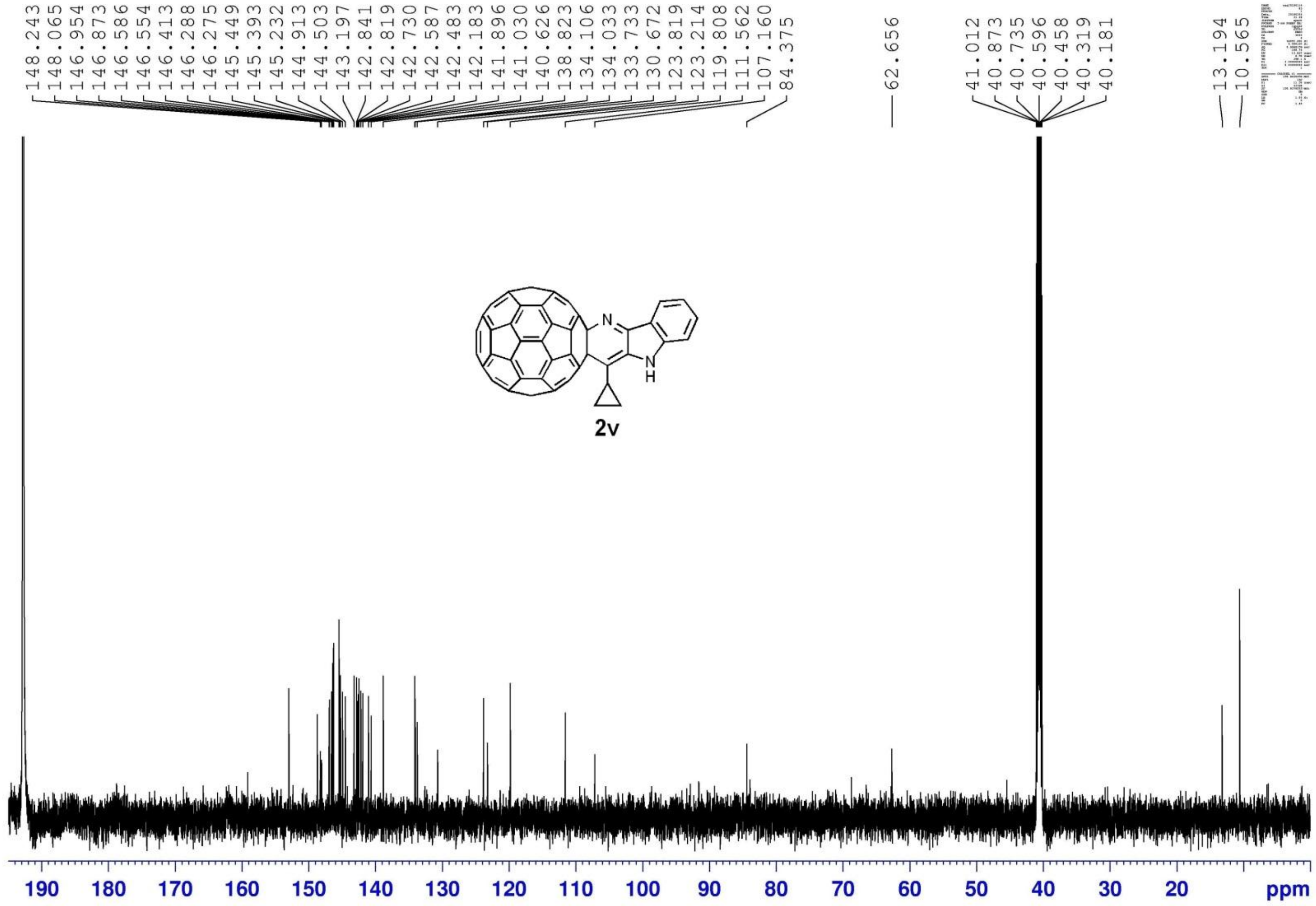
^{13}C NMR (150 MHz, DMSO-d_6/CS_2) of compound 2u



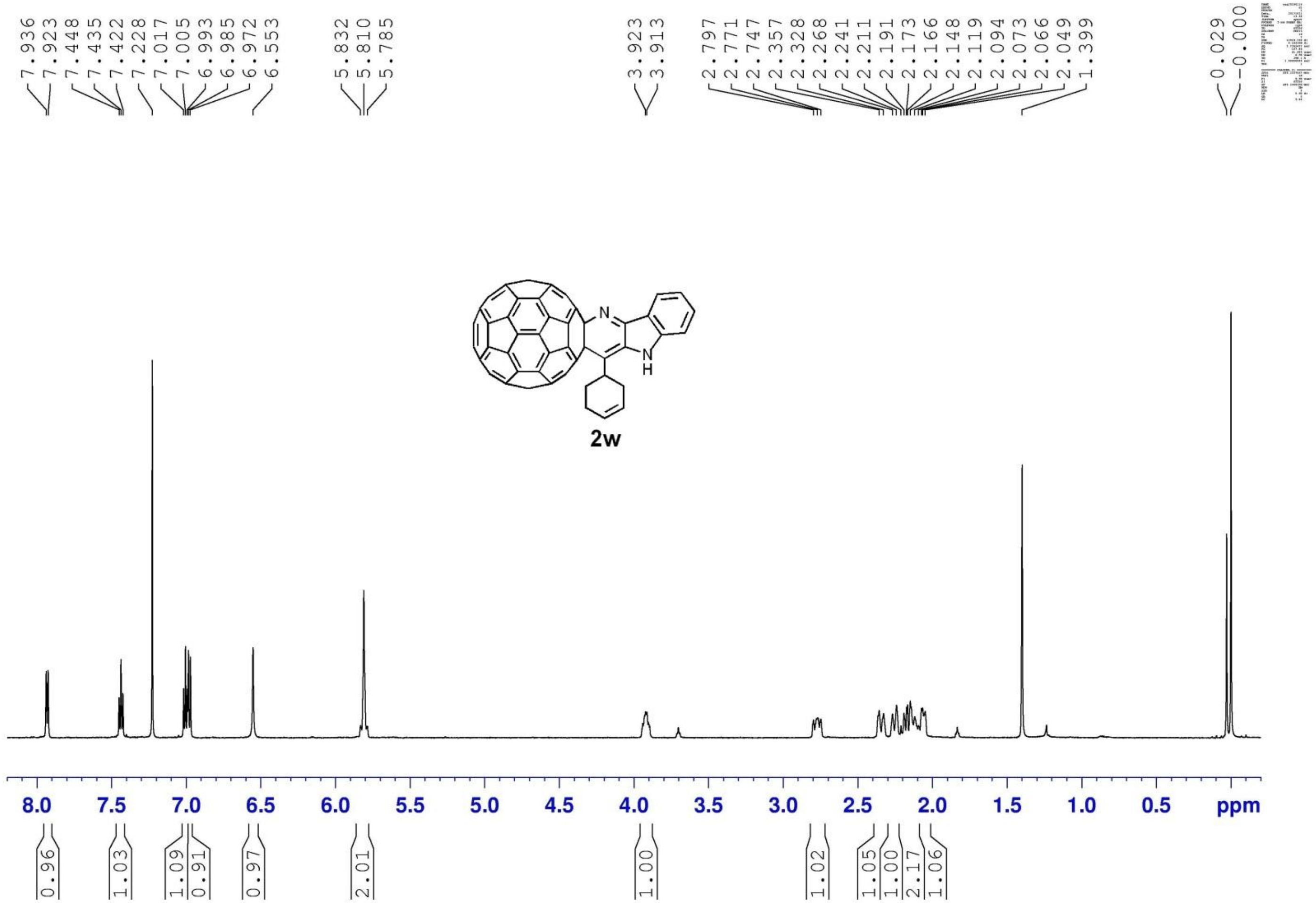
^{1}H NMR (600 MHz, DMSO-d_6/CS_2) of compound 2v



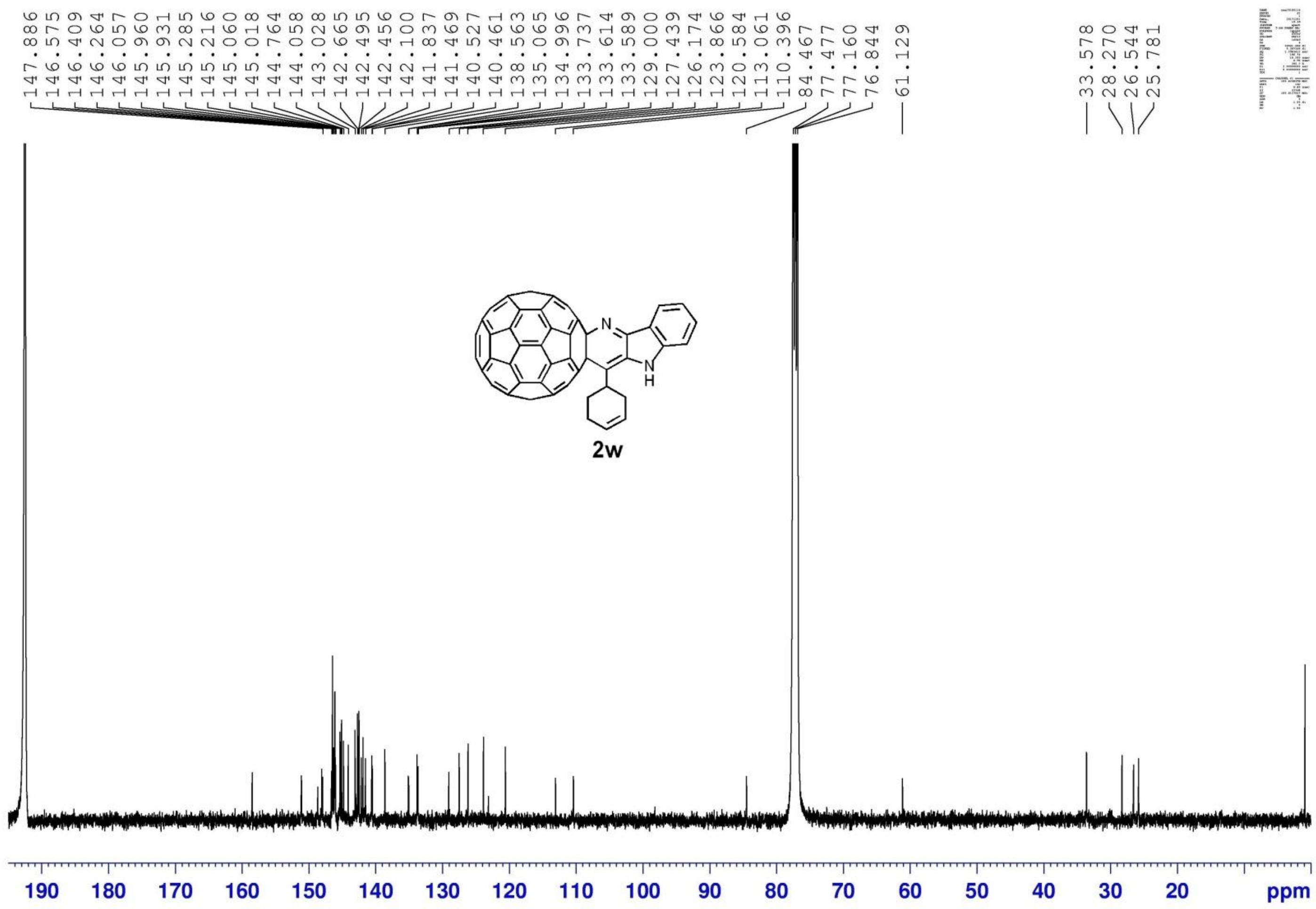
^{13}C NMR (150 MHz, DMSO-d_6/CS_2) of compound 2v



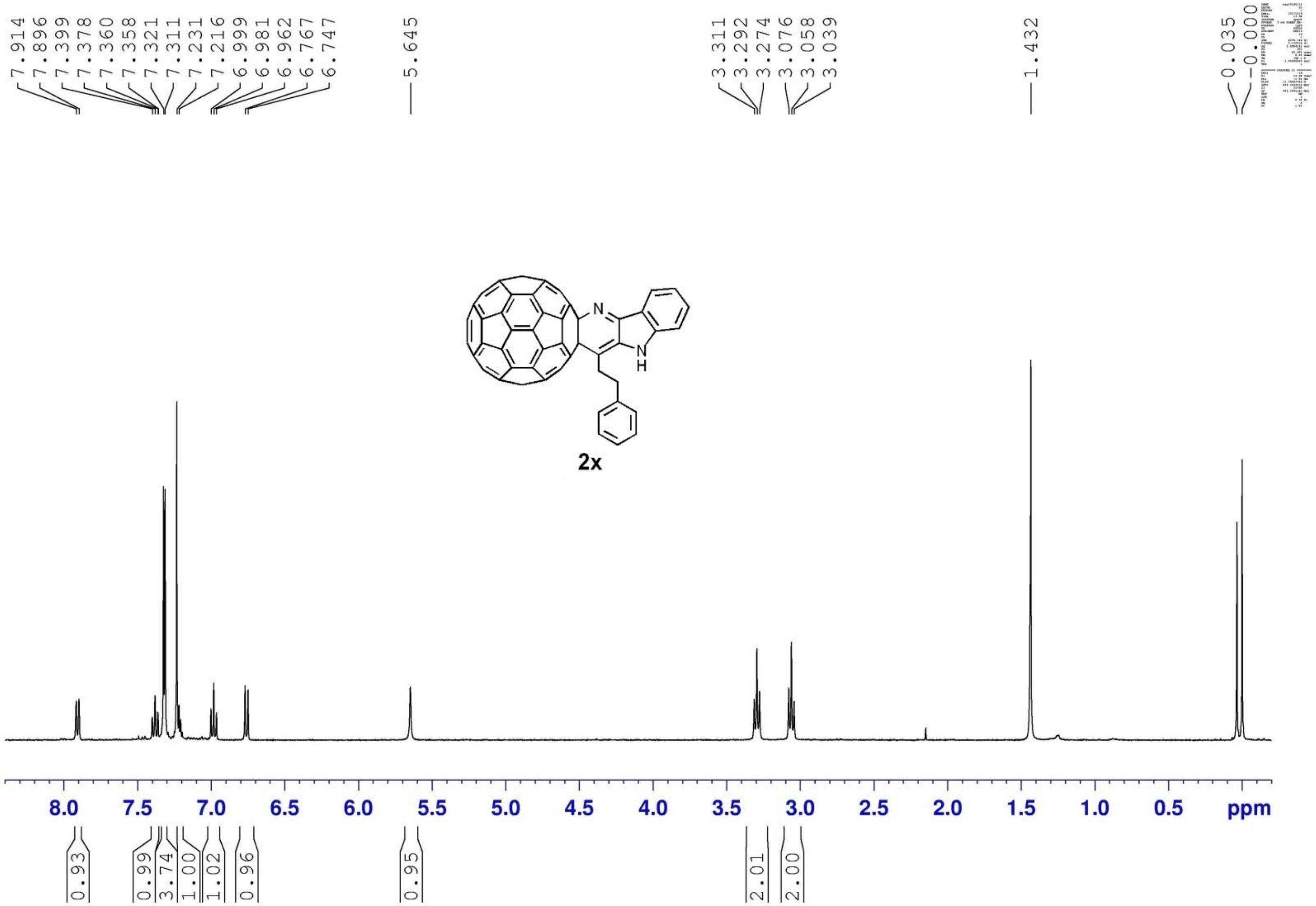
^{1}H NMR (600 MHz, $CDCl_3/CS_2$) of compound 2w



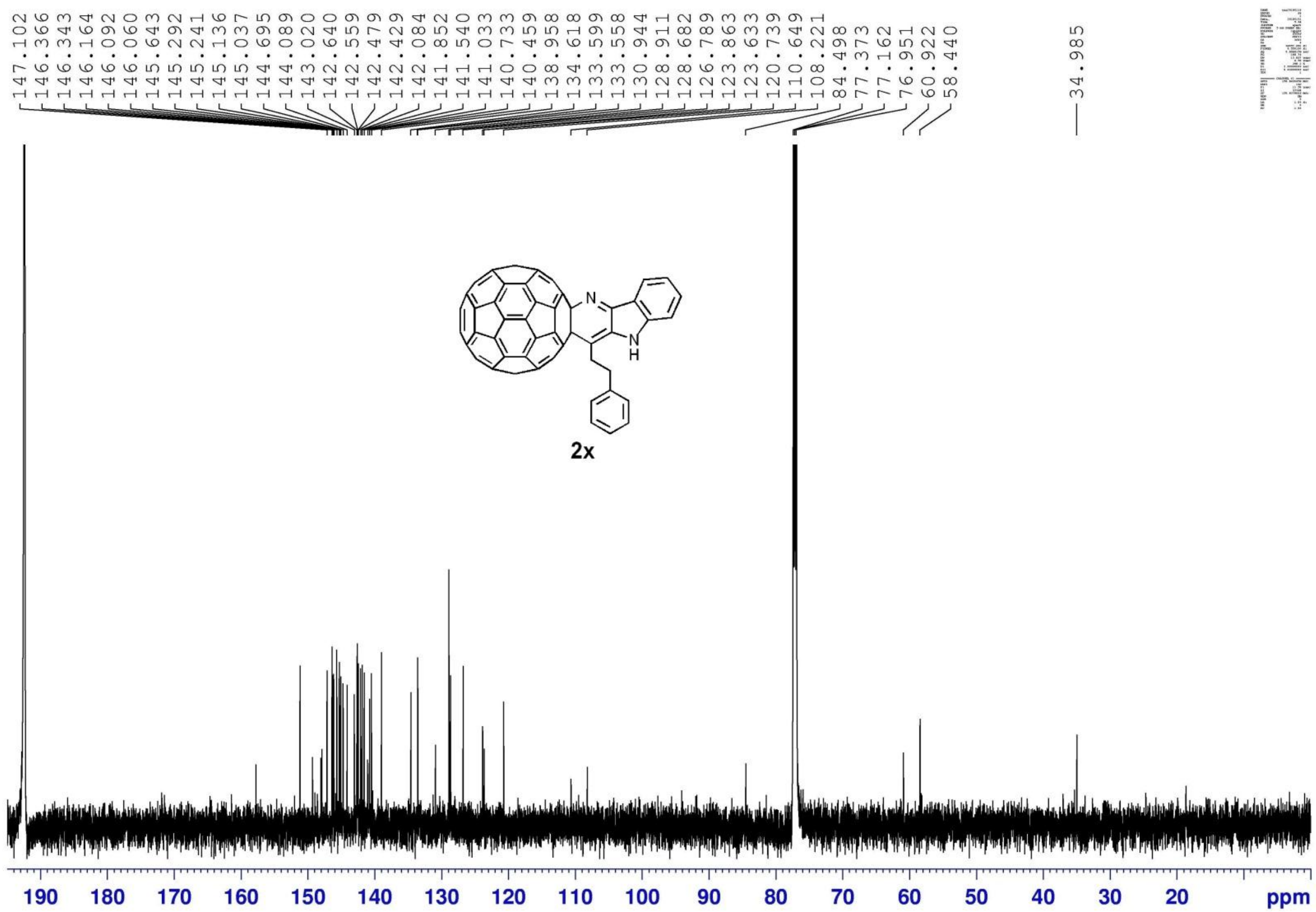
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 2w



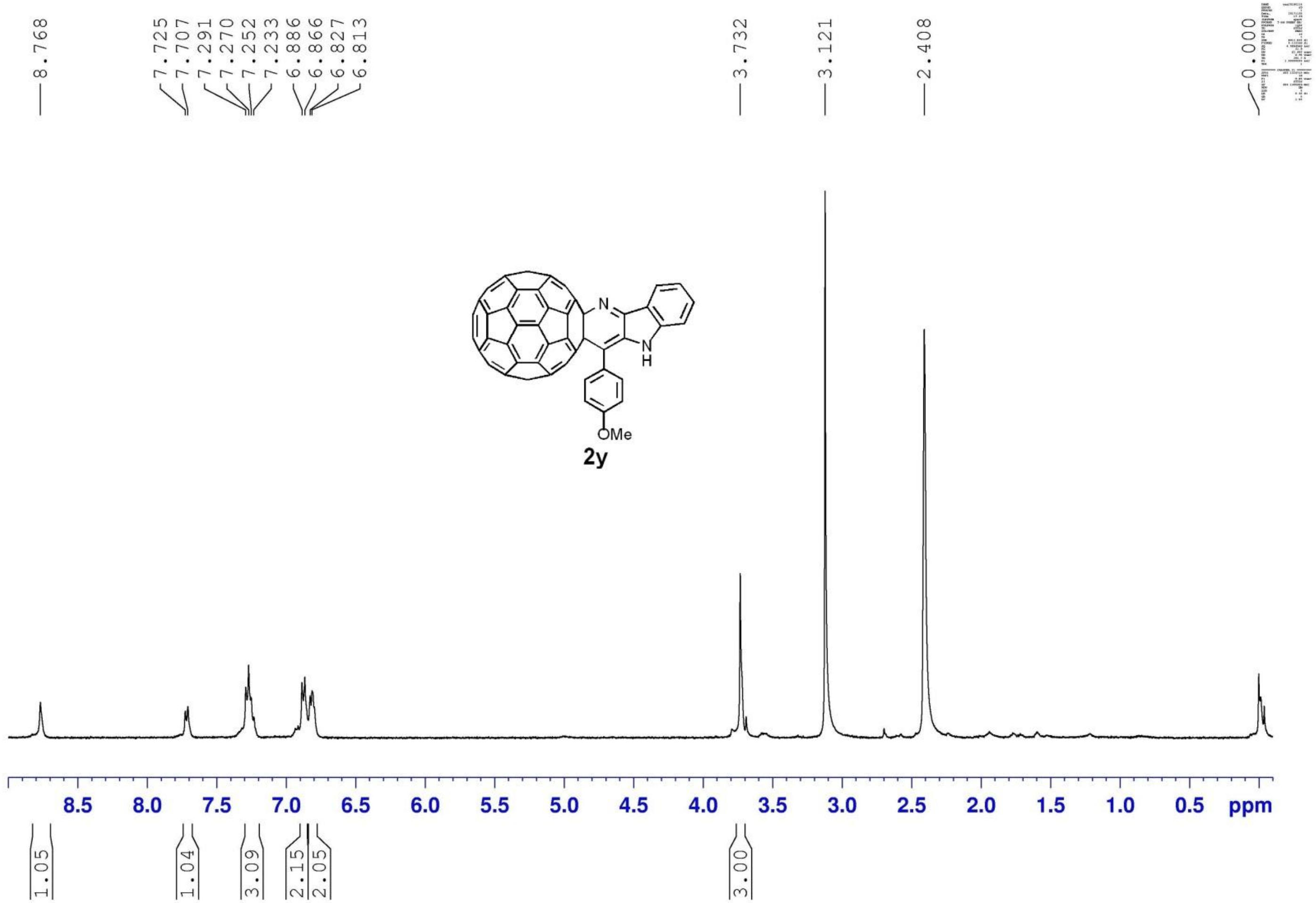
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 2x



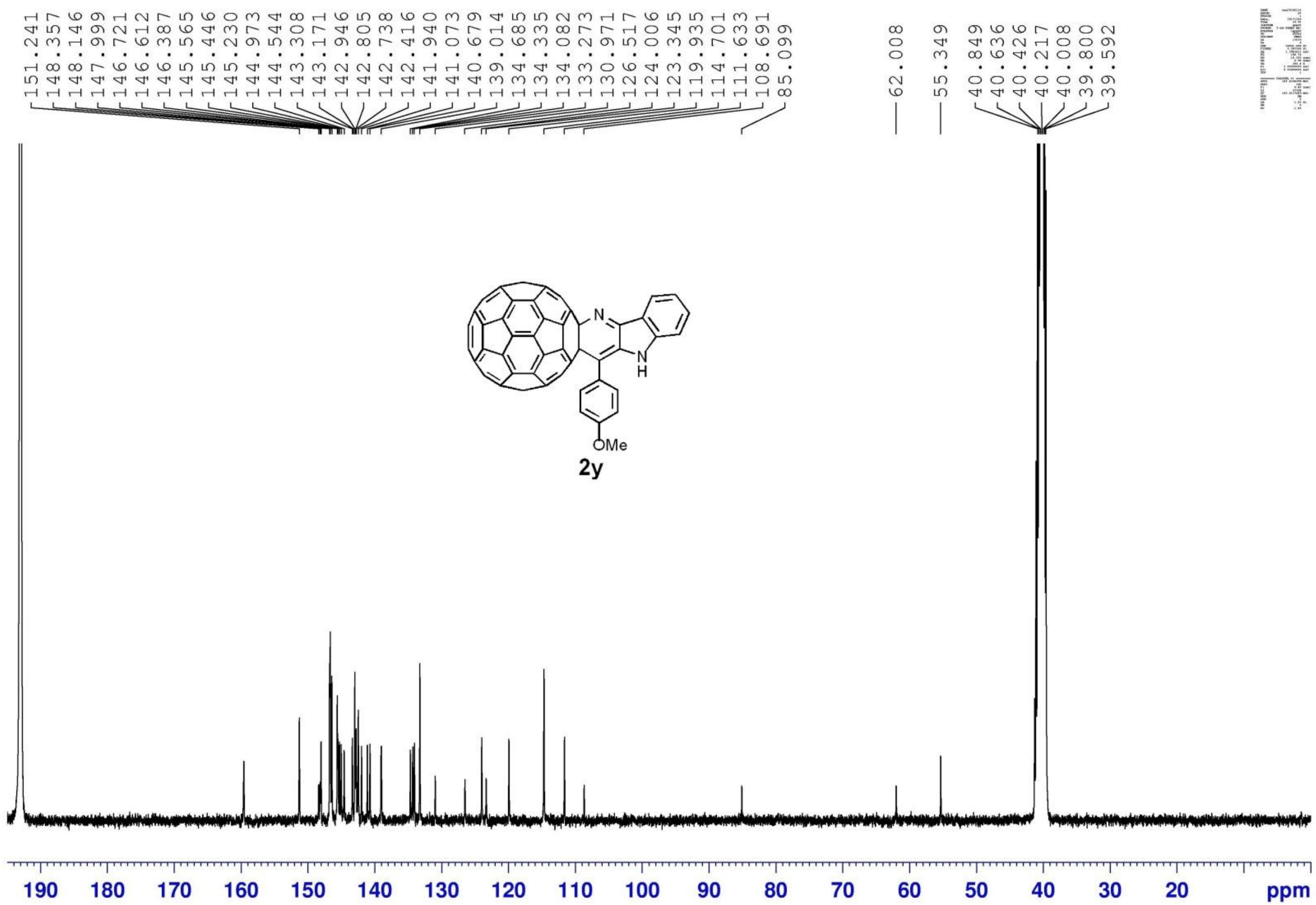
^{13}C NMR (150 MHz, $CDCl_3/CS_2$) of compound 2x



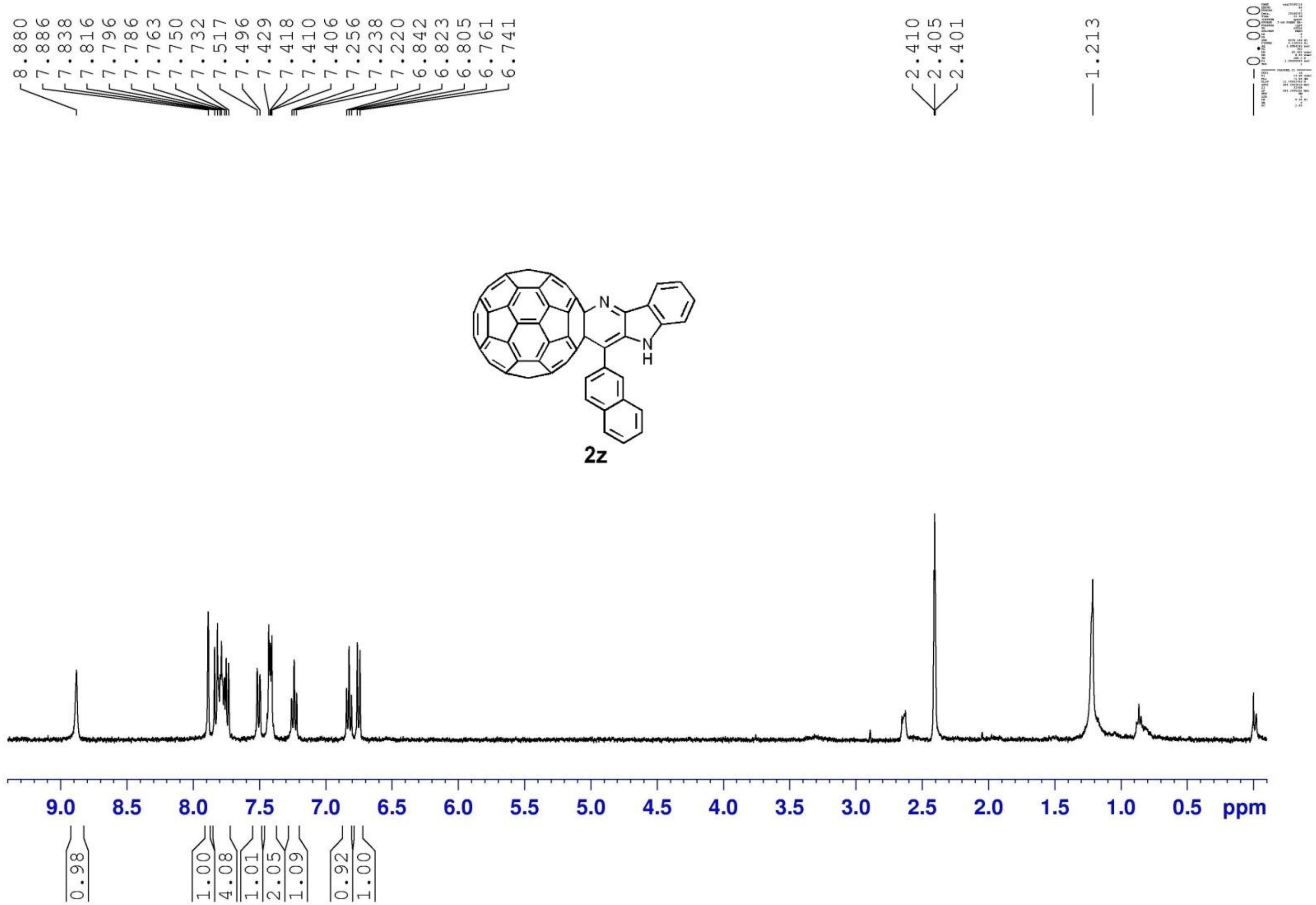
^{1}H NMR (400 MHz, DMSO-d_6/CS_2) of compound 2y



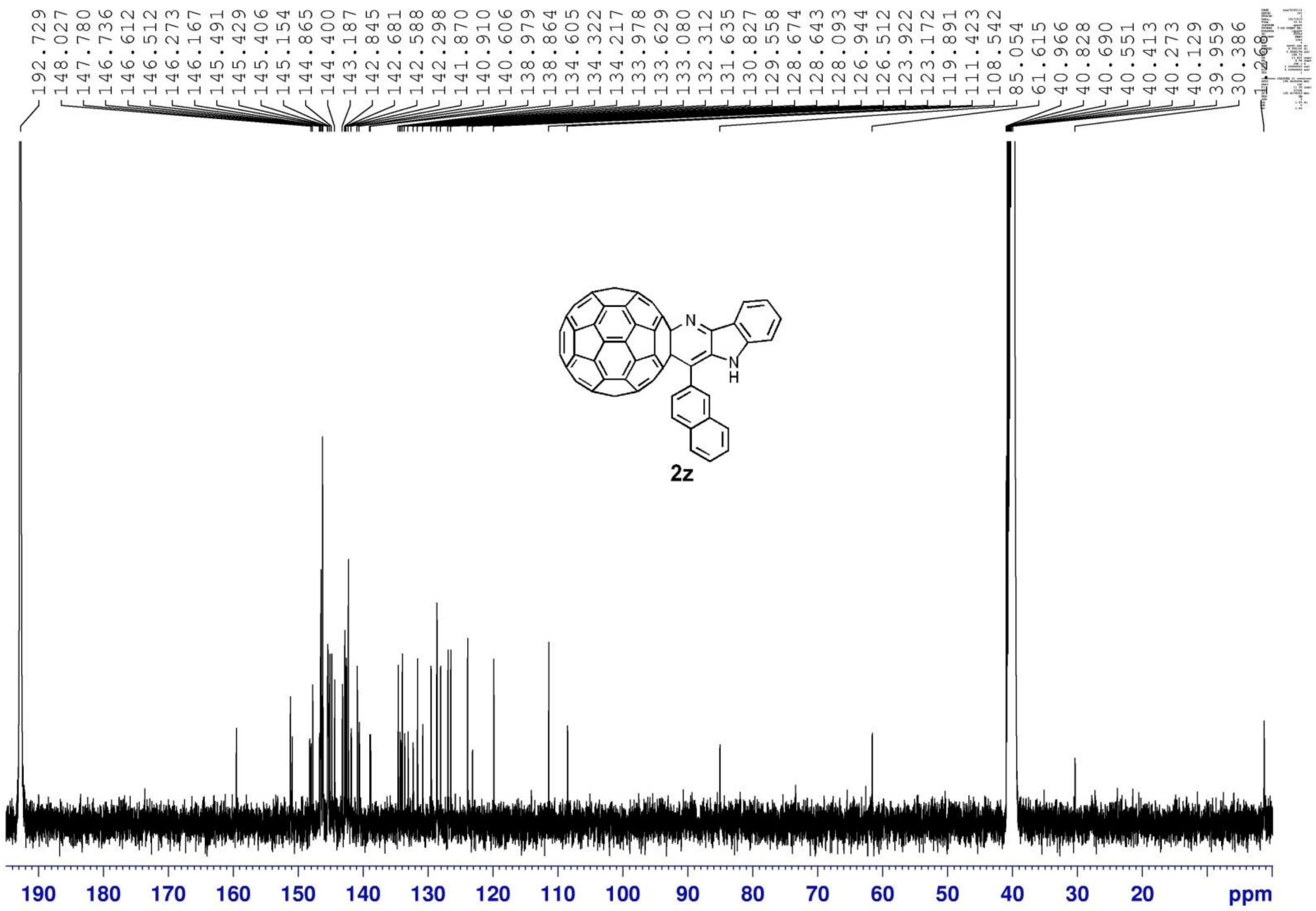
^{13}C NMR (100 MHz, DMSO-d_6/CS_2) of compound 2y



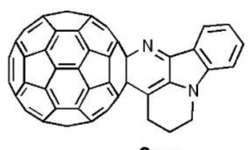
^{1}H NMR (400 MHz, DMSO-d_6/CS_2) of compound 2z



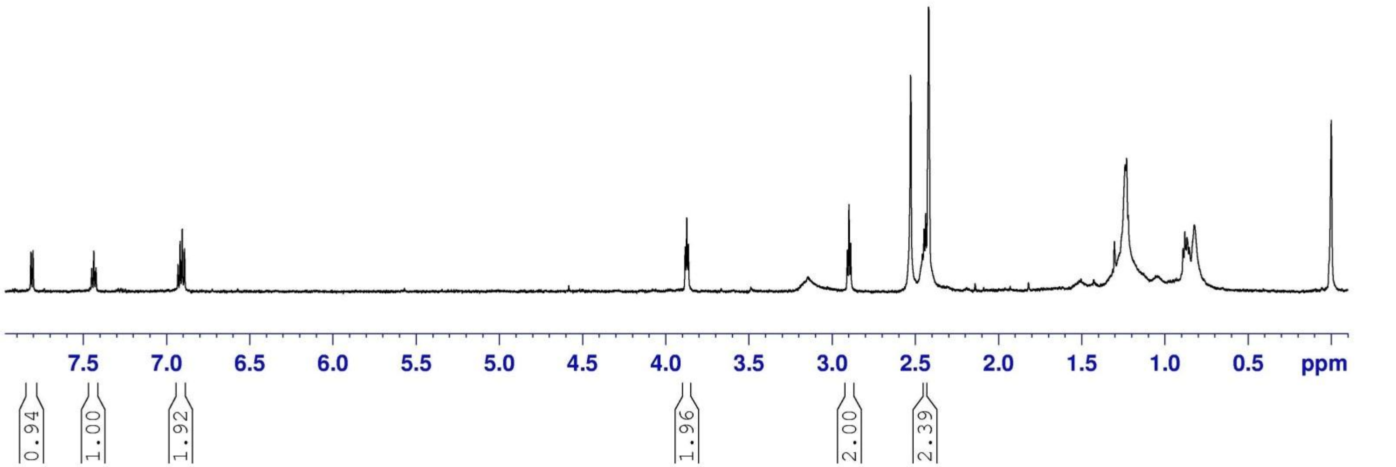
^{13}C NMR (150 MHz, d_6-DMSO/CS_2) of compound 2z



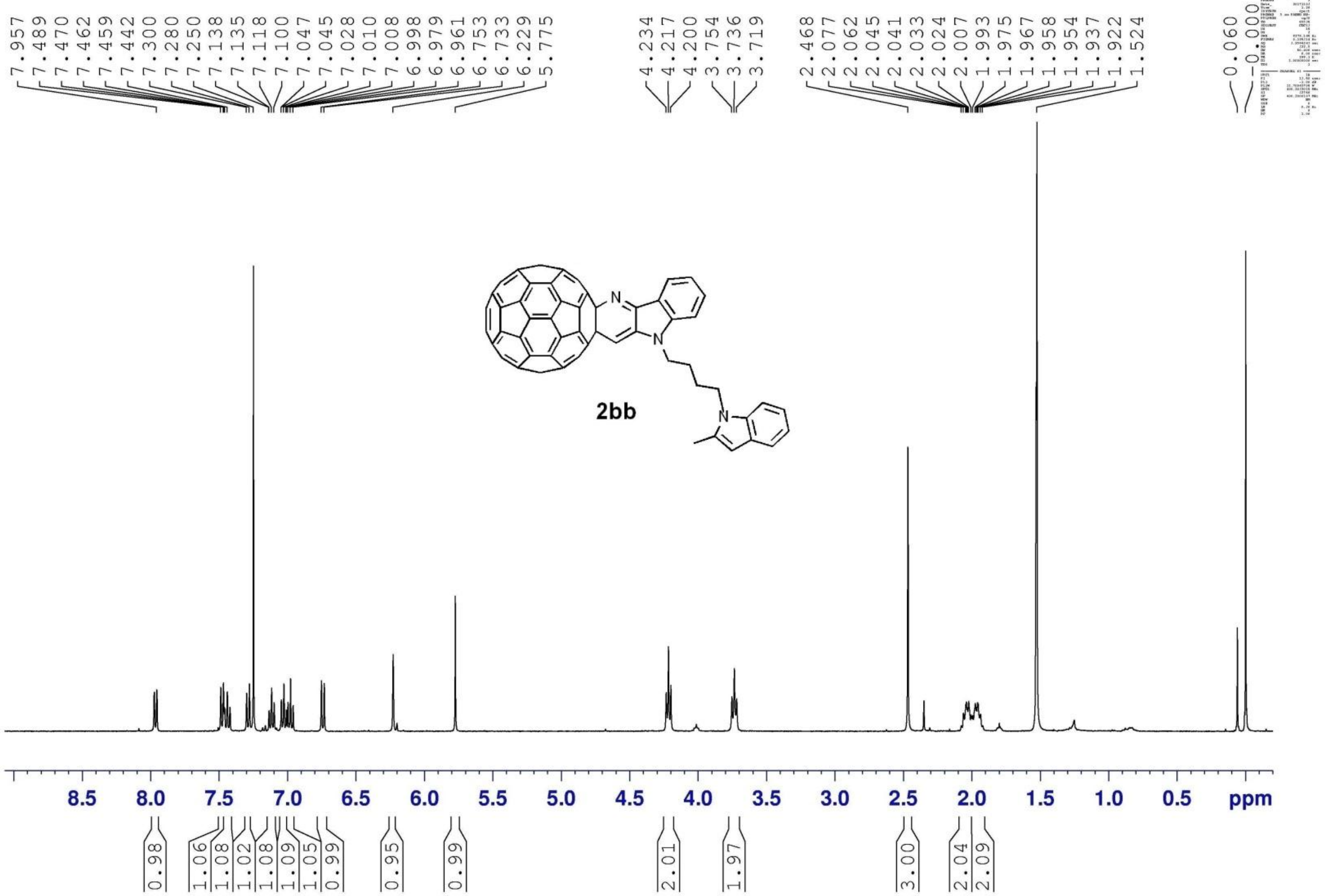
^{1}H NMR (600 MHz, DMSO-d_6/CS_2) of compound 2aa



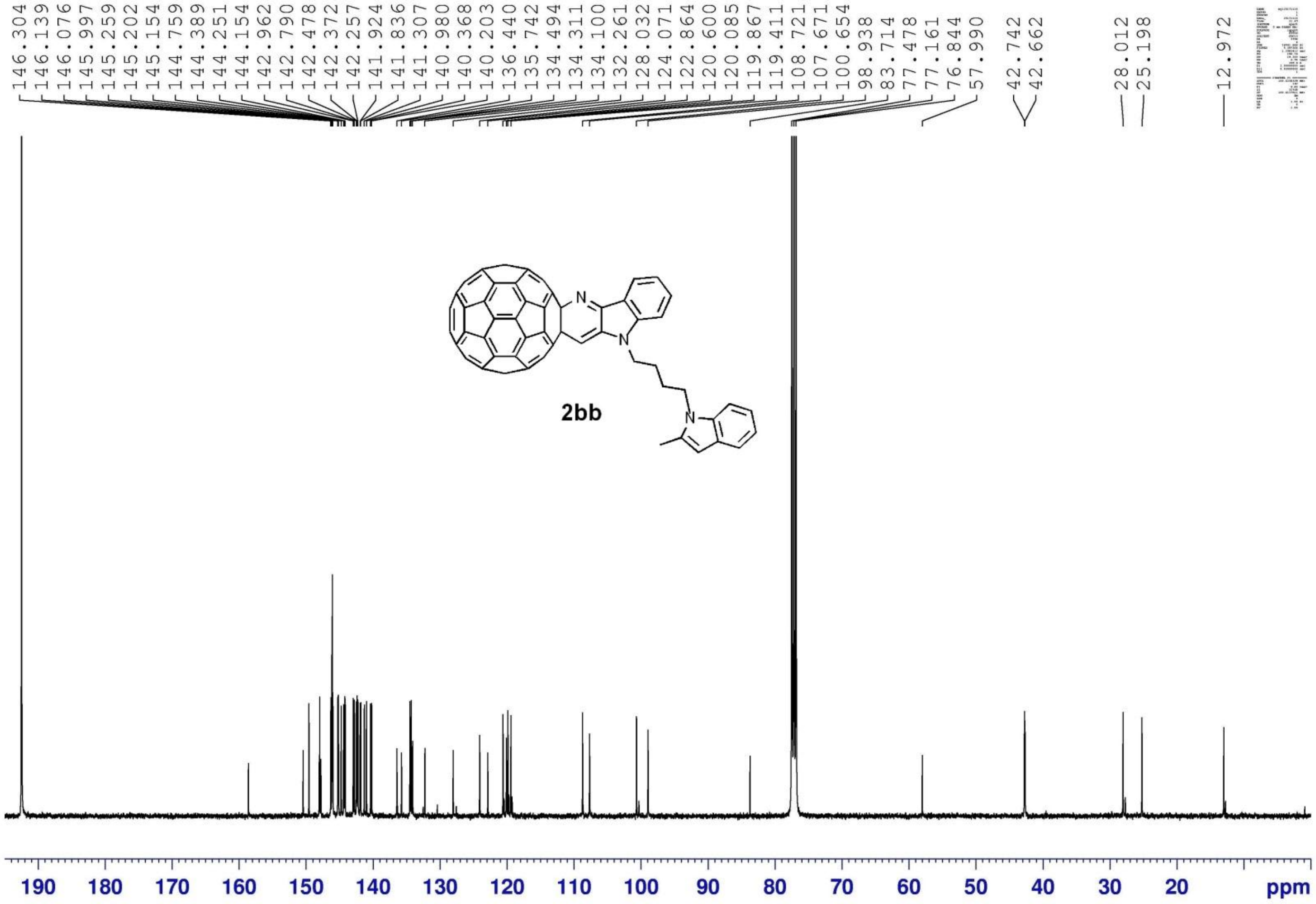
2aa



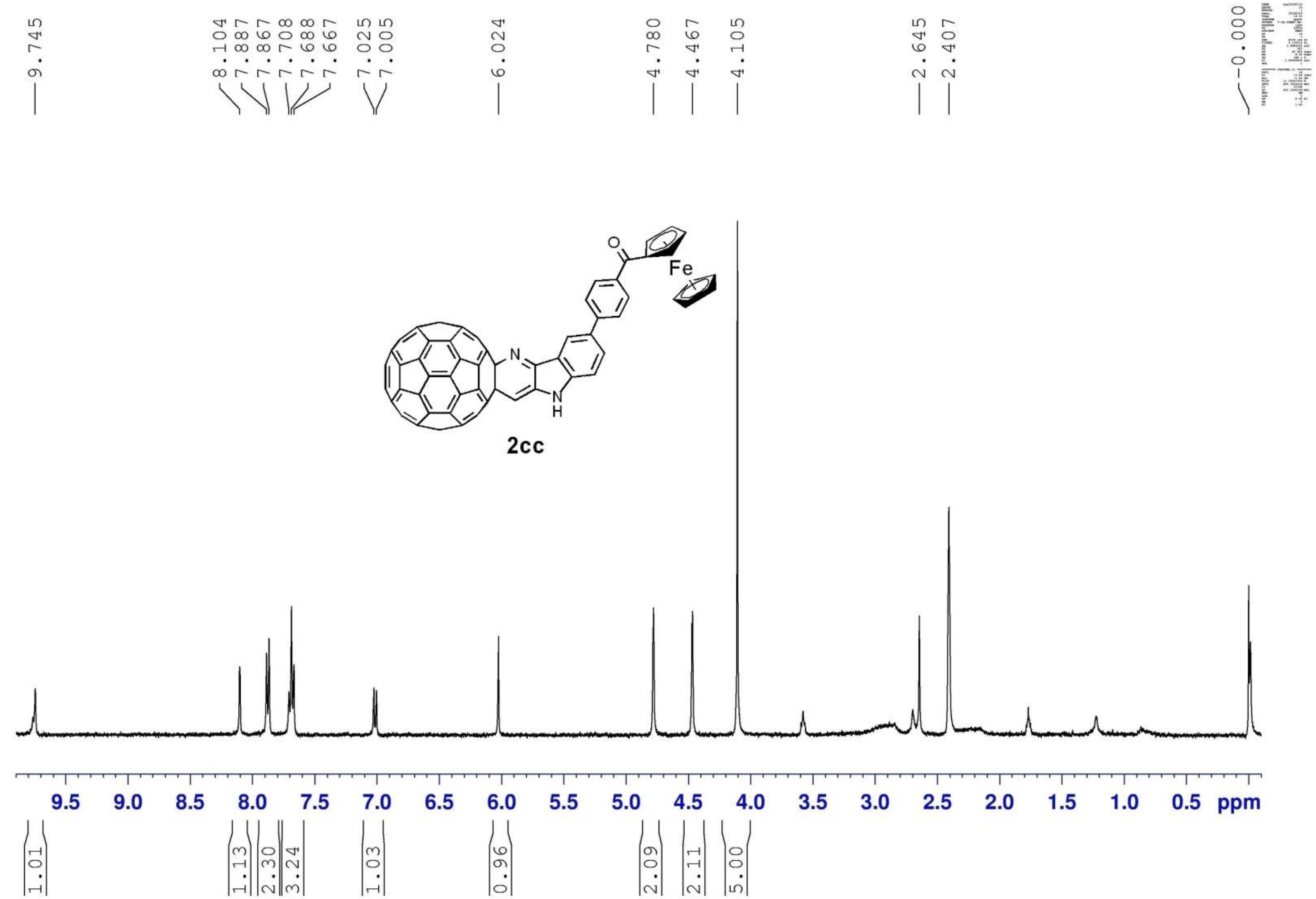
[1]H NMR (400 MHz, $CDCl_3/CS_2$) of compound 2bb



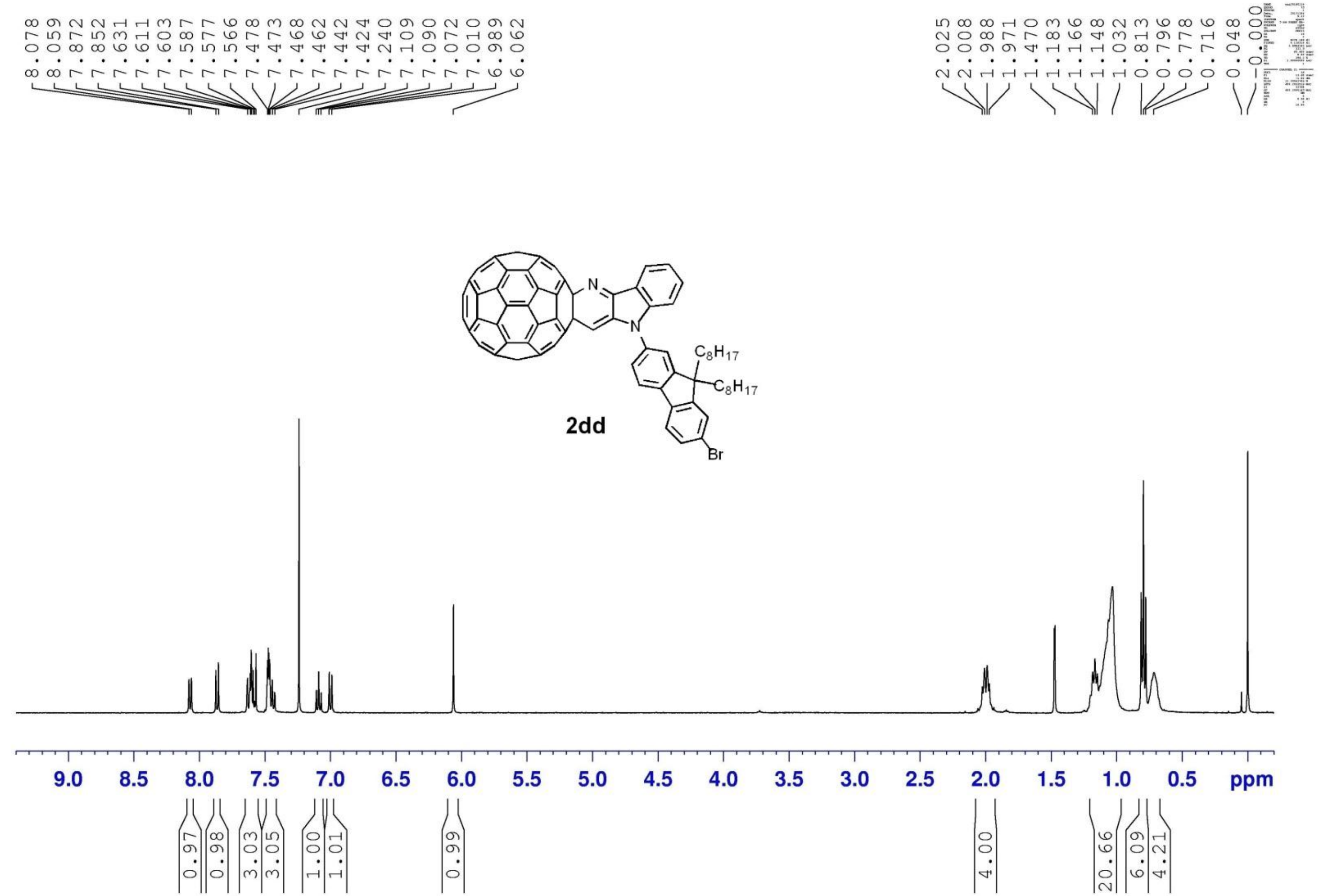
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 2bb



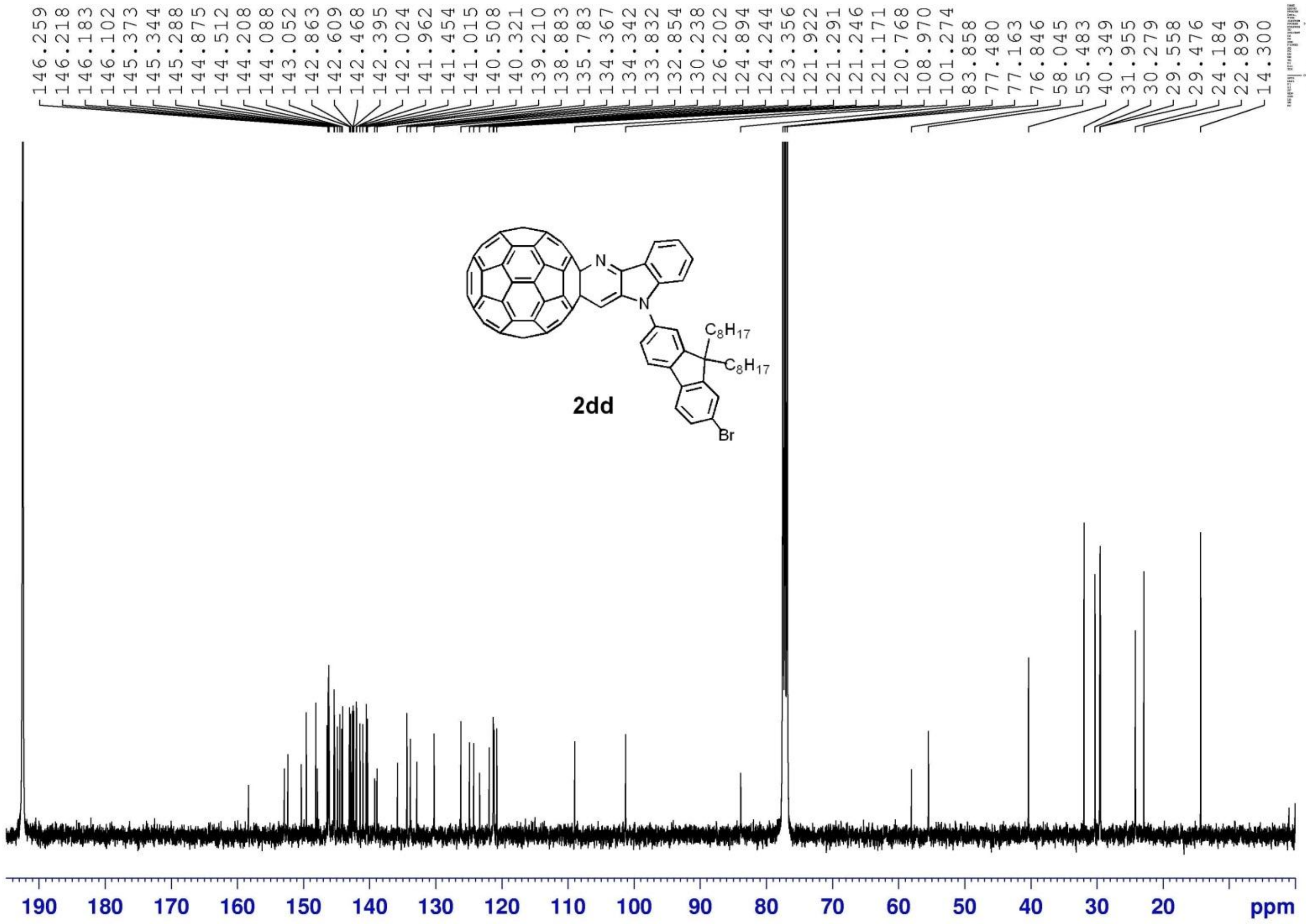
^{1}H NMR (400 MHz, DMSO-d_6/CS_2) of compound 2cc



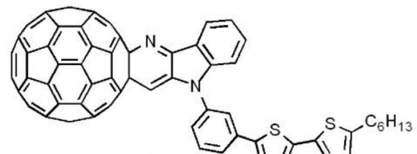
^{1}H NMR (400 MHz, $CDCl_3/CS_2$) of compound 2dd



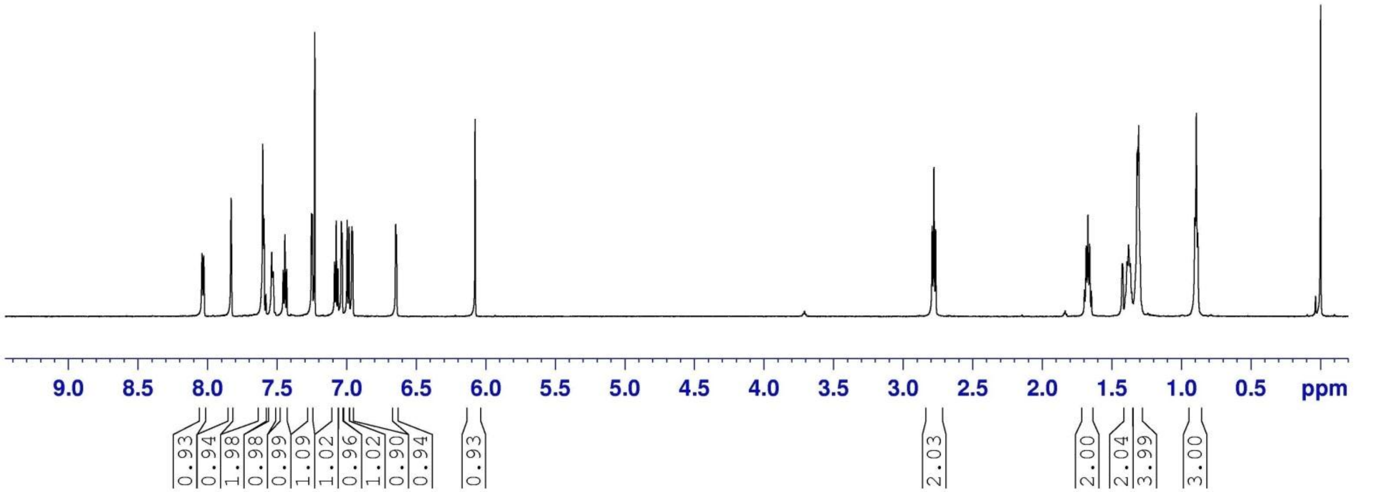
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 2dd



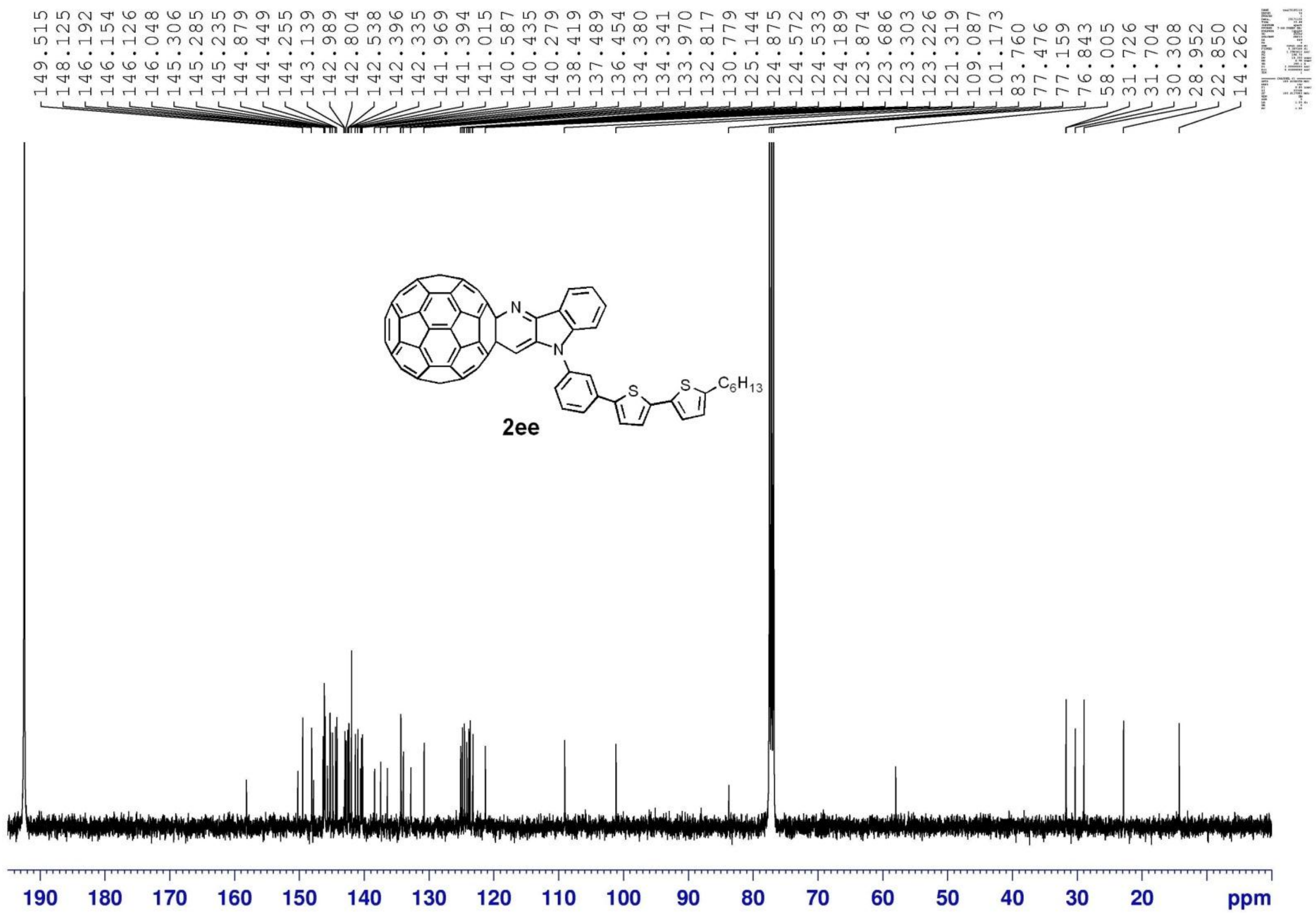
^{1}H NMR (600 MHz, $CDCl_3/CS_2$) of compound 2ee



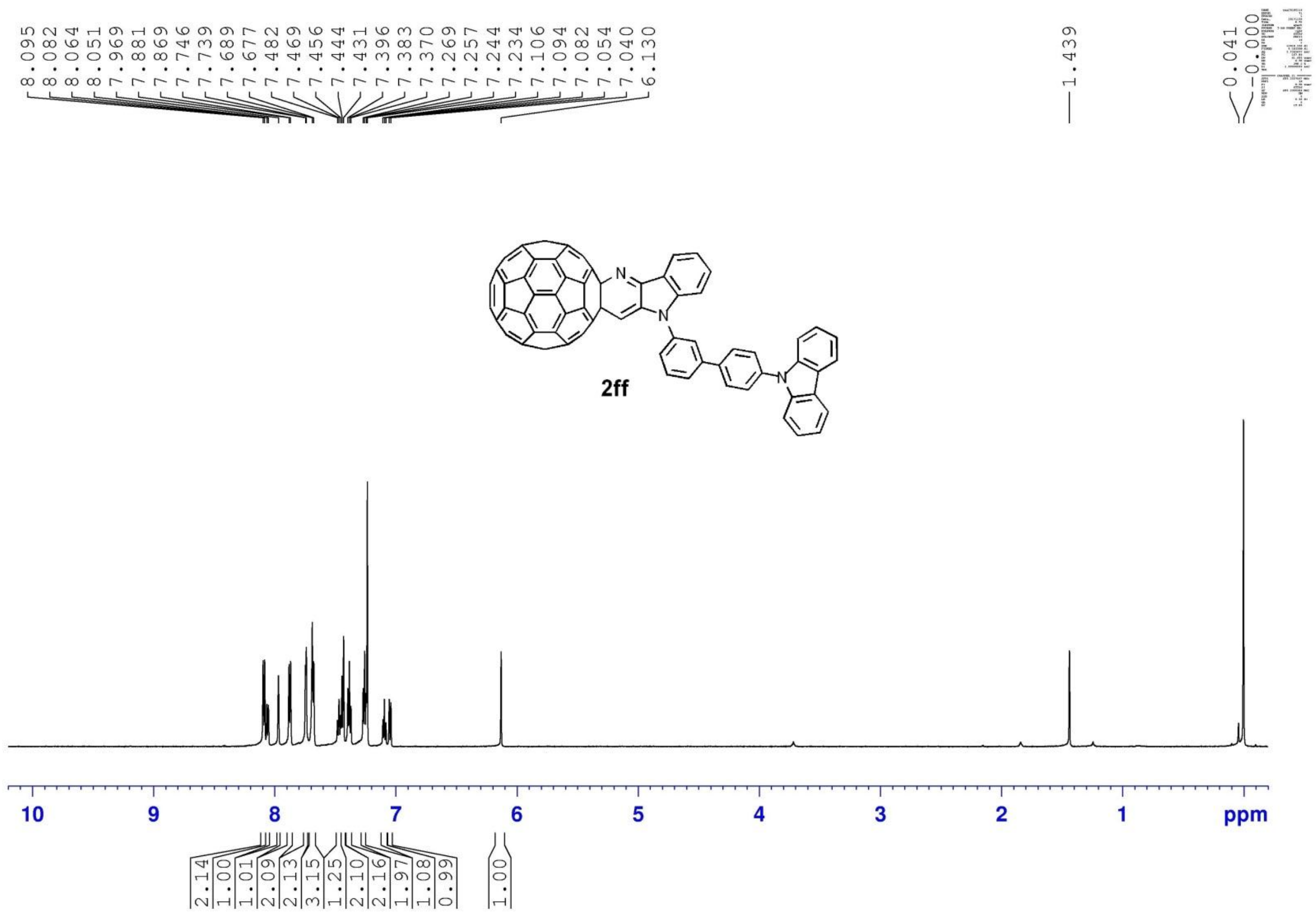
2ee



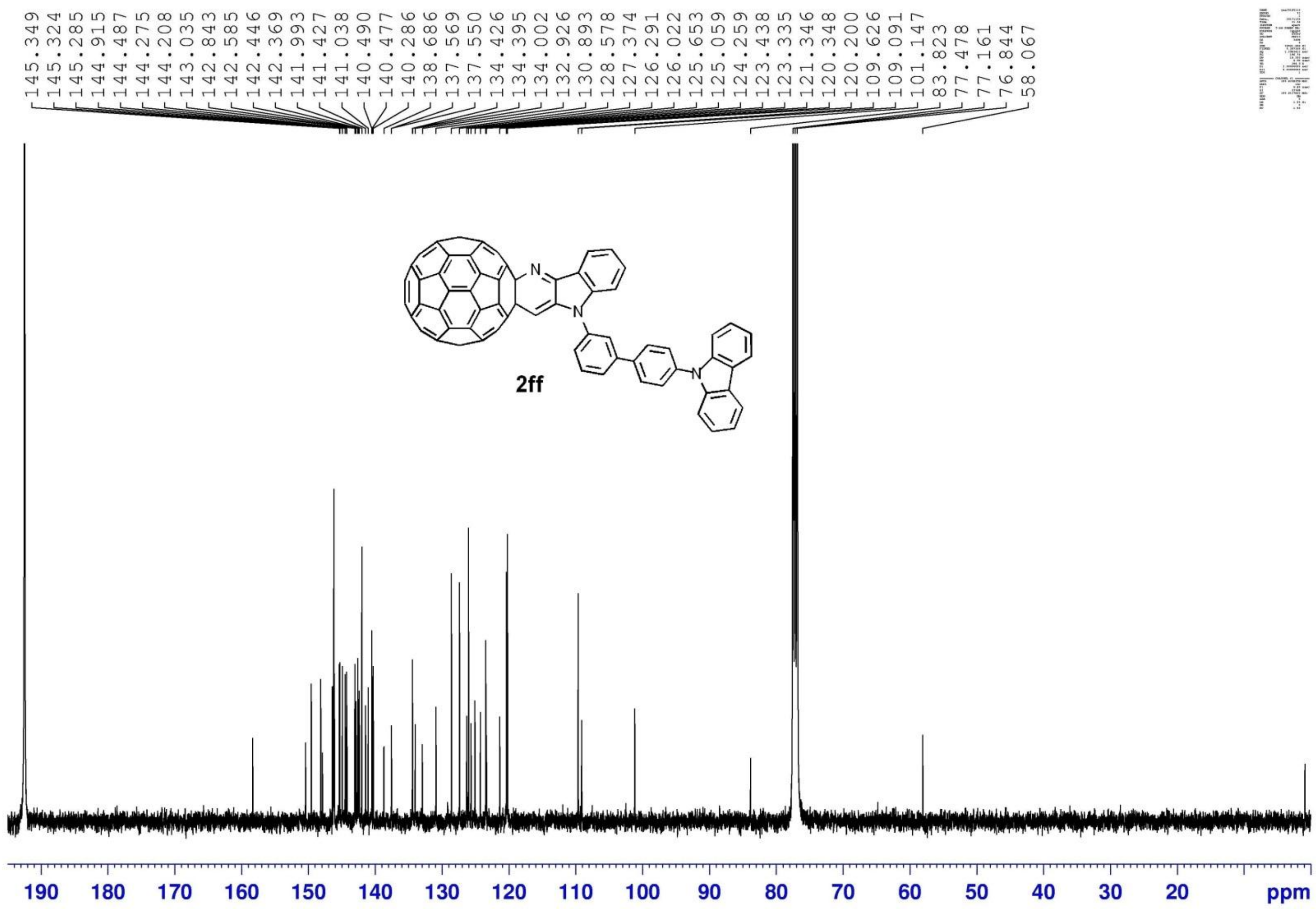
^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 2ee



^{1}H NMR (600 MHz, $CDCl_3/CS_2$) of compound 2ff



^{13}C NMR (100 MHz, $CDCl_3/CS_2$) of compound 2ff



10. Optimized Cartesian Coordinates

1

6	-0.307708	0.442917	-0.007579
6	-0.550986	-0.956766	0.000958
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6	-2.649199	0.893430	-0.001458
6	-1.345687	1.377825	-0.005995
6	1.689403	-0.608654	-0.002303
6	0.733477	-1.593288	0.004735
1	-2.090280	-2.478224	0.009372
1	-3.940157	-0.832608	0.006409
1	-3.476951	1.593577	-0.000255
1	-1.151439	2.444349	-0.006153
7	1.062409	0.635402	-0.016119
6	1.701997	1.935865	0.014955
1	1.306636	2.573827	-0.780278
1	1.541785	2.436308	0.976074
1	2.773299	1.823859	-0.141246
6	3.176740	-0.748581	-0.002477
1	3.440138	-1.806729	0.009719
1	3.634083	-0.303321	-0.892919
1	0.933483	-2.653971	0.008716
1	3.637177	-0.280971	0.874630

NO^+

7	0.000000	0.000000	-0.565291
8	0.000000	0.000000	0.494630

I

6	-0.611835	-0.536083	0.576955
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8	1.095307	-2.783615	-1.074789
6	1.188825	2.480116	-0.549251
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1	2.269225	2.586771	-0.468530
1	0.894439	2.564404	-1.598730

II

6	-0.496132	-0.619354	0.000027
6	-0.672115	0.782156	0.000026

6	-1.930322	1.378179	0.000006
6	-3.035942	0.530608	-0.000013
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1	-4.031998	0.958030	-0.000032
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1	-1.495873	-2.526295	0.000021
7	0.593530	1.385496	0.000021
6	3.018534	0.709376	-0.000002
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1	3.315918	1.280930	0.885055
7	1.696162	-1.983921	0.000004
8	1.066806	-3.047300	-0.000033
6	0.797307	2.824486	-0.000030
1	1.862277	3.044791	0.000204
1	0.346881	3.272878	-0.889400
1	0.346481	3.272962	0.889091
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TS1-1

Frequencies **-283.9613**

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6	-2.800140	-1.252034	-0.051804
6	-1.477644	-1.664106	-0.129818

6	0.964644	-0.721405	-0.141444
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1	-2.415424	2.140292	0.176208
1	-4.174094	0.401165	0.124904
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7	0.346549	1.427273	-0.016174
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1	3.008984	1.734542	-0.996695
1	3.140665	1.572887	0.760933
7	1.765497	-1.912015	-0.385724
8	2.109429	-2.491122	0.616483
6	0.397966	2.865781	0.168945
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1	-0.308231	3.355273	-0.505688
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1	3.527096	0.207188	-0.283274

II′

6	-0.520234	-0.750642	0.000026
6	-0.885076	0.610161	-0.000028
6	-2.214341	1.030900	-0.000053
6	-3.192527	0.041407	-0.000020
6	-2.847720	-1.321029	0.000029
6	-1.519186	-1.729543	0.000048
6	0.925359	-0.785814	0.000020
6	1.380988	0.544414	0.000009
1	-2.484781	2.080149	-0.000085
1	-4.237861	0.327628	-0.000033
1	-3.635712	-2.065375	0.000057

1	-1.253542	-2.779277	0.000087
7	0.290300	1.368340	-0.000036
6	2.776922	1.070467	0.000127
1	2.968275	1.686717	-0.884961
1	2.967586	1.688247	0.884282
7	1.612222	-1.990284	0.000110
8	2.846338	-1.951650	-0.000202
6	0.298309	2.822776	-0.000021
1	1.322416	3.187299	-0.000499
1	-0.211061	3.203585	-0.888965
1	-0.210278	3.203624	0.889361
1	3.471640	0.235628	0.001023

TS2-1

Frequencies **-1573.4641**

6	0.565579	-0.766599	0.130604
6	0.886479	0.599275	0.006684
6	2.199507	1.039874	-0.109022
6	3.205763	0.071424	-0.090727
6	2.901642	-1.288742	0.029960
6	1.579221	-1.719344	0.139546
6	-0.888378	-0.832173	0.195230
6	-1.379891	0.531871	0.203179
1	2.444760	2.089403	-0.216712
1	4.240393	0.382818	-0.176315
1	3.704656	-2.016391	0.034201
1	1.339114	-2.772004	0.226802
7	-0.305783	1.354189	0.023963
6	-2.761661	0.837993	0.146092
1	-3.343670	0.533323	1.017970

1	-3.052772	1.815285	-0.230725
7	-1.625897	-1.857377	-0.201028
8	-2.914115	-1.655793	-0.254919
6	-0.356872	2.799428	-0.098316
1	-0.266480	3.116464	-1.141661
1	-1.305291	3.158067	0.300123
1	0.454709	3.245490	0.479410
1	-3.089081	-0.421830	-0.333664

III

6	-0.513868	-0.742905	-0.057136
6	-0.895209	0.605426	0.052956
6	-2.238758	0.968074	0.085967
6	-3.190682	-0.053094	0.015839
6	-2.818211	-1.396316	-0.080511
6	-1.468282	-1.750040	-0.113227
6	0.951783	-0.780374	-0.042698
6	1.401013	0.648213	-0.059342
1	-2.552370	2.001779	0.160238
1	-4.242570	0.209091	0.036628
1	-3.580323	-2.164444	-0.132153
1	-1.159209	-2.785680	-0.186428
7	0.246356	1.412863	0.127951
6	2.631169	1.159516	-0.285281
1	3.477700	0.540696	-0.538556
1	2.796401	2.227968	-0.318815
7	1.599274	-1.888425	0.053183
8	2.971392	-1.822920	0.192407
6	0.244811	2.857229	0.066952
1	1.010845	3.260875	0.733511

1	0.434538	3.224545	-0.949938
1	-0.720453	3.233370	0.401303
1	3.222286	-0.930287	0.485901

TS1-2

Frequencies **-740.1112**

6	-0.746691	0.459772	-0.102315
6	-0.986386	-0.948514	-0.081365
6	-2.294654	-1.421939	0.138898
6	-3.314745	-0.507777	0.332547
6	-3.057795	0.879201	0.307056
6	-1.779872	1.379981	0.088789
6	1.221615	-0.572498	-0.483080
6	0.261829	-1.576982	-0.309490
1	-2.494066	-2.487626	0.156444
1	-4.326773	-0.855436	0.503954
1	-3.877669	1.572067	0.458395
1	-1.604169	2.448552	0.064048
7	0.598947	0.661421	-0.334105
6	1.272392	1.949630	-0.388852
1	0.685808	2.683025	0.163497
1	2.250147	1.872724	0.088055
1	1.391163	2.299173	-1.419548
6	2.628617	-0.713414	-0.709901
1	3.237818	-0.423941	0.306701
1	2.940845	-1.725651	-0.954095
1	0.463081	-2.635970	-0.365674
1	3.101289	0.036485	-1.343873
8	3.888802	-0.034234	1.250523
1	3.703624	-0.704230	1.922933

VI

6	0.823729	0.625199	0.045334
6	0.512720	-0.706400	-0.270325
6	1.505518	-1.664396	-0.365207
6	2.836127	-1.284659	-0.152072
6	3.140061	0.041935	0.152141
6	2.143953	1.018006	0.254065
6	-1.444585	0.631527	-0.312471
6	-0.977162	-0.819331	-0.432179
1	1.256519	-2.694195	-0.596795
1	3.628515	-2.019452	-0.225161
1	4.173358	0.329801	0.311204
1	2.405077	2.043115	0.485137
7	-0.344769	1.387182	0.101693
6	-0.399235	2.818147	0.291765
1	0.474010	3.146817	0.854415
1	-0.430154	3.359214	-0.662986
1	-1.289495	3.077960	0.869057
6	-2.678021	1.079856	-0.579803
1	-3.454978	0.384377	-0.865121
1	-2.947962	2.124053	-0.495183
1	-1.290300	-1.269679	-1.378200
7	-1.575962	-1.695026	0.642282
8	-2.732263	-2.095800	0.588539

TS2-2

Frequencies	**-440.4091**		
6	0.807865	0.631284	0.046057
6	0.533065	-0.687952	-0.377280

6	1.558022	-1.621959	-0.485498
6	2.861770	-1.229799	-0.186364
6	3.124232	0.082424	0.225651
6	2.108787	1.031586	0.348724
6	-1.421451	0.584152	-0.429470
6	-0.911053	-0.800579	-0.563013
1	1.342080	-2.638947	-0.792784
1	3.675498	-1.939728	-0.270776
1	4.143692	0.373511	0.453309
1	2.337664	2.042351	0.662613
7	-0.373685	1.361541	0.078641
6	-0.481864	2.771235	0.380555
1	0.321883	3.062064	1.056802
1	-0.426118	3.391823	-0.522529
1	-1.430357	2.966828	0.884298
6	-2.657549	1.015947	-0.752228
1	-3.395891	0.309914	-1.105057
1	-2.959329	2.049440	-0.647443
1	-1.325130	-1.427451	-1.343422
7	-1.570107	-1.715675	0.839089
8	-2.726048	-2.046113	0.744759

VII

6	-0.733837	0.696797	-0.043475
6	-0.481838	-0.644343	0.293306
6	-1.516064	-1.556222	0.404084
6	-2.830314	-1.118066	0.195137
6	-3.074733	0.215489	-0.127153
6	-2.035315	1.144859	-0.249336
6	1.535267	0.595875	0.301232

6	1.007649	-0.823363	0.429005
1	-1.315080	-2.592130	0.654833
1	-3.654778	-1.814629	0.285189
1	-4.094744	0.548206	-0.284311
1	-2.252659	2.177621	-0.491645
7	0.468824	1.402462	-0.107689
6	0.592121	2.829532	-0.294284
1	-0.285309	3.208372	-0.816819
1	0.692584	3.360162	0.661405
1	1.469953	3.046199	-0.907836
6	2.798989	0.980431	0.528702
1	3.537557	0.252210	0.834037
1	3.125870	2.005398	0.416611
1	1.345906	-1.348654	1.323304
7	1.497082	-1.617160	-0.791271
8	2.012226	-2.658224	-0.500670

TS2-2′

Frequencies	**-323.5190**		
6	-1.052666	0.473479	0.069387
6	-1.190672	-0.946677	0.135690
6	-2.455968	-1.527599	-0.080135
6	-3.533497	-0.704433	-0.349850
6	-3.378112	0.697708	-0.406419
6	-2.147008	1.303382	-0.197500
6	0.972990	-0.389510	0.547537
6	0.092922	-1.467442	0.427029
1	-2.577457	-2.604100	-0.035464
1	-4.513531	-1.134933	-0.518998
1	-4.242808	1.317145	-0.615680

1	-2.049024	2.381446	-0.236986
7	0.265735	0.789288	0.306887
6	0.823803	2.130306	0.327877
1	0.250761	2.769899	-0.343411
1	0.800682	2.563636	1.333355
1	1.851408	2.103917	-0.033746
6	2.362966	-0.427394	0.814279
1	2.770816	-1.388299	1.099913
1	2.844874	0.431767	1.262497
1	0.369882	-2.503827	0.545423
7	3.347978	-0.233987	-0.897222
8	4.528732	-0.334334	-0.756490

VII′

6	-1.019428	0.474393	0.037008
6	-1.083386	-0.940376	0.160767
6	-2.322189	-1.584958	0.012769
6	-3.450032	-0.822439	-0.247963
6	-3.367393	0.579182	-0.362971
6	-2.157533	1.245568	-0.221585
6	1.055035	-0.276254	0.471338
6	0.248064	-1.387748	0.429590
1	-2.393241	-2.663551	0.101073
1	-4.412389	-1.307471	-0.364753
1	-4.267009	1.149776	-0.563720
1	-2.108062	2.324829	-0.305247
7	0.295080	0.860904	0.217092
6	0.762484	2.236220	0.204237
1	0.235585	2.792187	-0.572875
1	0.591775	2.730596	1.166862

1	1.824084	2.264809	-0.035087
6	2.524029	-0.233836	0.716617
1	2.881305	-1.179649	1.127837
1	2.812952	0.592041	1.376972
1	0.578037	-2.404087	0.581016
7	3.245929	0.045907	-0.588507
8	4.041498	-0.798208	-0.888876

XII

6	0.725849	-0.494473	-0.843153
6	0.578625	0.648272	-0.012674
6	1.661037	1.226586	0.655012
6	2.908962	0.637960	0.486523
6	3.075517	-0.498963	-0.326087
6	1.997756	-1.069089	-0.989235
6	-0.576313	-0.794136	-1.357226
6	-1.452935	0.139663	-0.852937
1	1.541248	2.101505	1.283556
1	3.769269	1.062216	0.991653
1	4.063167	-0.932906	-0.433630
1	2.136100	-1.944568	-1.614411
1	-0.844841	-1.599681	-2.023267
7	-0.756248	1.017396	-0.030358
6	-2.919638	0.270774	-1.099512
1	-3.245890	-0.527013	-1.767152
1	-3.499920	0.186736	-0.174904
1	-3.173576	1.226446	-1.570536
7	-1.710105	-1.980644	1.230863
8	-0.924457	-1.692505	2.023074
6	-1.293645	2.157514	0.687477

1	-0.879146	3.095050	0.303008
1	-2.375566	2.187033	0.574787
1	-1.062009	2.083294	1.753641

TS1-3

Frequencies **-277.2536**

6	-1.297088	-0.491892	-0.043579
6	-0.651489	0.747488	-0.040888
6	-1.410046	1.909215	-0.058087
6	-2.802702	1.796831	-0.092389
6	-3.426163	0.546267	-0.111305
6	-2.675559	-0.632548	-0.086560
6	0.914824	-0.971585	0.006413
6	0.817627	0.503932	-0.022555
1	-0.929988	2.880107	-0.039912
1	-3.411171	2.693544	-0.104415
1	-4.507575	0.485832	-0.141901
1	-3.161226	-1.600648	-0.099117
7	-0.297484	-1.512607	0.008482
6	-0.635279	-2.929934	0.072705
1	-1.262415	-3.114608	0.947282
1	-1.179315	-3.222475	-0.827773
1	0.272396	-3.521143	0.154540
1	1.453856	0.871701	-0.895042
7	1.567511	1.079403	1.157801
8	2.744777	1.428491	0.884576
6	2.198171	-1.711365	0.055425
1	2.456074	-1.939065	1.097155
1	2.158416	-2.648904	-0.502543
1	2.973345	-1.062182	-0.359328

8	3.065886	0.929564	-1.404151
1	3.568339	1.747375	-1.311407

TS1-3′

Frequencies	**-623.3153**		
6	0.757713	0.547399	0.178003
6	0.754873	-0.779970	-0.253684
6	1.915296	-1.533328	-0.330648
6	3.111772	-0.900295	0.023882
6	3.131044	0.431119	0.438536
6	1.945714	1.170361	0.518722
6	-0.664555	1.040014	0.155465
6	-1.437149	-0.189945	-0.276676
1	1.912476	-2.569877	-0.642487
1	4.038507	-1.460027	-0.023848
1	4.072334	0.895560	0.706816
1	1.957940	2.204430	0.842228
1	-1.049238	1.351060	1.131133
7	-0.580266	-1.166055	-0.562020
6	-2.873342	-0.254665	-0.290551
1	-3.331200	0.711067	-0.499112
1	-3.307205	-1.055981	-0.884166
7	-0.886371	2.154263	-0.825208
8	-0.508265	3.296733	-0.589886
6	-0.959599	-2.550043	-0.806687
1	-1.090403	-3.059722	0.151841
1	-1.893831	-2.582547	-1.362941
1	-0.185366	-3.039981	-1.395082
8	-1.997111	-0.654131	2.051438
1	-1.919919	-0.850004	2.991998

1	-2.985230	-0.486121	0.863624

DMSO

16	-0.000001	0.242942	-0.439557
8	-0.000010	1.508261	0.387017
6	1.363360	-0.822141	0.180111
1	1.331841	-1.796845	-0.316569
1	2.300234	-0.314040	-0.060802
1	1.275980	-0.932770	1.265094
6	-1.363350	-0.822157	0.180111
1	-2.300229	-0.314063	-0.060799
1	-1.331824	-1.796861	-0.316570
1	-1.275965	-0.932786	1.265093

I-D

6	1.631805	-0.719944	-0.008107
6	2.504788	0.308091	-0.381293
6	3.748707	0.081365	-0.945112
6	4.118063	-1.255011	-1.126179
6	3.265668	-2.297197	-0.756388
6	2.009826	-2.042882	-0.195275
6	0.432313	-0.083990	0.580750
6	0.686243	1.367603	0.452558
1	4.413132	0.884688	-1.237161
1	5.082592	-1.481766	-1.563440
1	3.581258	-3.321554	-0.912331
1	1.353719	-2.858919	0.078387
1	-0.573851	-0.346605	0.203016
7	1.876957	1.561327	-0.079568
6	-0.273553	2.387993	0.917067
1	-0.399507	2.271950	2.001797

1	0.017233	3.412605	0.698367
1	-1.250440	2.163219	0.476372
7	0.166233	-0.398053	2.183939
8	0.505387	-1.467960	2.500630
6	2.538754	2.838120	-0.358817
1	2.740489	2.910549	-1.428247
1	1.905075	3.664127	-0.052457
1	3.478906	2.880510	0.192669
16	-3.650892	-0.678876	-0.604925
8	-2.405053	0.106525	-0.156748
6	-4.911833	-0.390400	0.680640
1	-5.856177	-0.830164	0.355659
1	-4.564099	-0.890092	1.583972
1	-5.011803	0.681686	0.852663
6	-4.411857	0.307587	-1.936734
1	-3.726268	0.279717	-2.782772
1	-5.362329	-0.149773	-2.216460
1	-4.552211	1.332399	-1.591550

TS1

Frequencies **-657.0782**

6	1.133413	-0.584764	0.543533
6	2.166342	-0.251734	-0.343779
6	3.088819	-1.176132	-0.814022
6	2.961780	-2.483287	-0.344354
6	1.948319	-2.833122	0.554523
6	1.017908	-1.894208	1.003005
6	0.356880	0.658825	0.759516
6	1.092291	1.699827	0.050968
1	3.879982	-0.907787	-1.502742

1	3.665111	-3.236516	-0.677580
1	1.886353	-3.854284	0.910970
1	0.239622	-2.172231	1.700238
1	-0.744414	0.545316	0.083568
7	2.093297	1.143711	-0.617434
6	0.750678	3.144642	0.045496
1	0.127060	3.366965	0.911243
1	1.640508	3.775650	0.074335
1	0.179230	3.399569	-0.854066
7	-0.234664	1.076292	2.032701
8	-0.538841	0.169688	2.765048
6	3.027562	1.813317	-1.524106
1	2.966988	1.351238	-2.510459
1	2.773608	2.865943	-1.607938
1	4.043194	1.713523	-1.138393
16	-2.959759	-0.599315	-0.329843
8	-1.875237	0.501875	-0.620874
6	-4.419506	0.345191	0.190171
1	-5.259617	-0.344821	0.285214
1	-4.184871	0.778236	1.161851
1	-4.622859	1.125634	-0.542815
6	-3.489622	-1.115761	-1.986134
1	-2.653502	-1.651810	-2.432968
1	-4.346504	-1.783023	-1.880094
1	-3.740726	-0.231853	-2.572034

I-D1

6	1.302242	-0.529112	-0.057714
6	2.704552	-0.659690	-0.008529
6	3.355600	-1.884314	-0.036688

6	2.558579	-3.025427	-0.119565
6	1.165248	-2.924783	-0.173154
6	0.525199	-1.686238	-0.143169
6	1.046068	0.908547	-0.007257
6	2.319030	1.563372	0.066394
1	4.434813	-1.963422	0.001747
1	3.027996	-4.001215	-0.144333
1	0.570322	-3.827629	-0.240014
1	-0.552797	-1.647732	-0.188579
1	-1.930979	-0.074647	-0.060637
7	3.278259	0.632464	0.066570
6	2.570246	3.027168	0.133756
1	1.618873	3.553641	0.108229
1	3.095406	3.294830	1.055566
1	3.181220	3.361359	-0.710017
7	-0.031313	1.692344	-0.016627
8	-1.190861	1.172735	-0.076383
6	4.719999	0.857604	0.129570
1	5.196030	0.452972	-0.765474
1	4.924061	1.922965	0.190575
1	5.131812	0.364183	1.011683
16	-4.020001	0.199540	0.464487
8	-2.783478	-0.683380	-0.074892
6	-4.470493	1.223786	-0.959891
1	-5.377304	1.773959	-0.701706
1	-3.638941	1.914121	-1.103030
1	-4.616615	0.591390	-1.835054
6	-5.304360	-1.068301	0.427590
1	-5.062338	-1.788464	1.207910
1	-6.255757	-0.582142	0.647685

1	-5.311169	-1.540978	-0.553812

I-D2+DMSO

6	1.150321	0.446901	0.018780
6	2.494398	0.862835	0.038297
6	2.881673	2.190352	0.086048
6	1.862155	3.144740	0.114938
6	0.521402	2.759192	0.096098
6	0.146083	1.414219	0.047737
6	1.199773	-1.021468	-0.036442
6	2.611819	-1.391752	-0.046237
1	3.922058	2.489226	0.100208
1	2.120551	4.195889	0.152760
1	-0.249452	3.519756	0.120162
1	-0.902919	1.151215	0.036614
7	3.335794	-0.286484	-0.000991
6	3.164659	-2.768620	-0.096115
1	3.780463	-2.973732	0.784775
1	2.346955	-3.484485	-0.128070
7	0.382515	-2.041746	-0.080814
8	-0.916955	-1.929882	-0.075783
6	4.795873	-0.193470	0.008928
1	5.229352	-1.188824	-0.020962
1	5.129110	0.372364	-0.862387
1	5.120002	0.315055	0.918125
1	3.790640	-2.905924	-0.982914
1	-1.377606	-1.015386	-0.014465
16	-4.011481	-0.477150	-0.219422
8	-2.564039	-0.008349	0.090670
6	-4.904984	-0.304974	1.355500
1	-5.964838	-0.495613	1.179189

1	-4.500822	-1.057502	2.031374
1	-4.739742	0.696459	1.753145
6	-4.758837	0.913840	-1.120647
1	-4.254879	0.974288	-2.084345
1	-5.819025	0.702890	-1.269609
1	-4.612385	1.831410	-0.550624

I-D3

1	-3.875486	-2.370608	-0.647026
16	4.443272	-0.383359	-0.276172
8	2.984802	-0.013718	0.035765
6	4.812662	0.354082	-1.903795
1	5.871734	0.212386	-2.125378
1	4.207810	-0.178568	-2.636614
1	4.548920	1.412110	-1.888499
6	5.477404	0.724512	0.740525
1	5.314315	0.444452	1.780569
1	6.525361	0.570947	0.477730
1	5.174921	1.758455	0.571238
6	-2.777606	-0.105635	-0.131091
6	-1.976069	0.994604	0.219793
6	-2.414046	2.302470	0.134426
6	-3.716793	2.509253	-0.331772
6	-4.531244	1.437250	-0.693354
6	-4.072463	0.121165	-0.597175
6	-1.942847	-1.285962	0.123202
6	-0.653083	-0.797448	0.630110
1	-1.790318	3.140121	0.417462
1	-4.096156	3.520511	-0.411051
1	-5.535735	1.624287	-1.051594

1	-4.745445	-0.677760	-0.887515
7	-0.700389	0.519426	0.660957
6	0.491430	-1.623526	1.059467
1	0.615232	-1.543496	2.146154
1	0.309736	-2.665922	0.807566
7	-2.078143	-2.568775	0.011766
8	-3.228633	-3.068764	-0.441274
6	0.376916	1.410497	1.110547
1	0.359021	2.309846	0.497312
1	0.212709	1.679537	2.156406
1	1.341119	0.920525	0.978271
1	1.424730	-1.265356	0.603419

TS2

Frequencies **-864.1852**

1	0.713906	-2.811783	-0.569124
16	-3.639433	-0.032619	-0.010243
8	-2.470611	0.848759	0.612697
6	-3.400458	-1.665606	0.735081
1	-4.266193	-2.279199	0.479358
1	-2.501408	-2.085296	0.286194
1	-3.293676	-1.555382	1.813946
6	-5.082542	0.555256	0.910628
1	-5.266175	1.580000	0.590923
1	-5.932336	-0.076812	0.648185
1	-4.867852	0.515074	1.978020
6	2.002307	-0.666569	-0.193363
6	2.456137	0.621437	0.151820
6	3.683865	0.833060	0.754584
6	4.487473	-0.286559	0.997566

6	4.072502	-1.567759	0.639240
6	2.827550	-1.767608	0.039093
6	0.660311	-0.474630	-0.754052
6	0.416041	0.998810	-0.799025
1	4.023629	1.821993	1.033391
1	5.454121	-0.149337	1.466945
1	4.720314	-2.415602	0.821873
1	2.557234	-2.776386	-0.253739
7	1.493541	1.587280	-0.232999
6	-0.754707	1.602462	-1.241234
1	-0.793369	2.683226	-1.312229
1	-1.281728	1.064896	-2.024457
7	-0.321290	-1.247494	-1.060802
8	-0.162866	-2.595905	-0.927029
6	1.684163	3.022299	-0.065145
1	1.389869	3.342059	0.937765
1	2.732555	3.269567	-0.229859
1	1.087754	3.556161	-0.802381
1	-1.699512	1.209835	-0.180833

III′+DMSO-H

1	-0.388261	-2.655061	0.458755
16	3.500807	-0.091826	0.088258
8	2.553877	0.881146	-0.804140
6	3.387254	-1.663680	-0.794119
1	4.199112	-2.293958	-0.425689
1	2.426156	-2.105122	-0.536078
1	3.482576	-1.476231	-1.863201
6	5.121282	0.501111	-0.454287
1	5.242995	1.506566	-0.053605

1	5.874955	-0.163998	-0.029547
1	5.162287	0.507096	-1.542969
6	-1.910343	-0.671790	0.233514
6	-2.514878	0.539923	-0.171922
6	-3.817594	0.570834	-0.650434
6	-4.520364	-0.634891	-0.714036
6	-3.947892	-1.838344	-0.299350
6	-2.639690	-1.862441	0.181250
6	-0.546656	-0.321591	0.634592
6	-0.468100	1.173867	0.613081
1	-4.291996	1.493609	-0.957358
1	-5.539771	-0.628998	-1.081327
1	-4.524880	-2.753359	-0.336169
1	-2.243436	-2.804174	0.546505
7	-1.623906	1.610865	0.004786
6	0.549920	1.928125	1.098849
1	0.523195	3.008686	1.075548
1	1.273789	1.457480	1.751496
7	0.541841	-0.981041	0.817983
8	0.494895	-2.360209	0.733043
6	-1.969897	3.015146	-0.142691
1	-1.114853	3.564469	-0.539238
1	-2.787173	3.114846	-0.853907
1	-2.269901	3.457144	0.813083
1	1.808322	1.246333	-0.235719

DMSO-H

16	-0.000089	-0.080527	-0.495591
8	0.001510	-1.452601	0.401906
6	-1.411387	0.785439	0.231502

1	-1.417888	1.802267	-0.173707
1	-2.313839	0.255473	-0.081872
1	-1.315408	0.791411	1.319992
6	1.410272	0.787382	0.231247
1	2.313392	0.259280	-0.083331
1	1.414931	1.804857	-0.172286
1	1.314818	0.791222	1.319800
1	0.000026	-2.232197	-0.190892

C_{60}

6	2.204963	2.206471	-1.718229
6	2.446865	2.567273	-0.324888
6	3.100936	1.671532	0.525368
6	3.541486	0.375063	0.020067
6	3.310016	0.029752	-1.314051
6	2.627097	0.965230	-2.201972
6	0.898186	2.732628	-2.100011
6	0.332375	3.418264	-0.942619
6	1.289614	3.316134	0.154423
6	0.835057	3.137318	1.463891
6	2.625883	1.484702	1.892670
6	3.339375	-0.612772	1.075110
6	2.914354	-1.904163	0.751272
6	2.672956	-2.265057	-0.642092
6	2.866289	-1.318831	-1.652355
6	1.908672	-1.216885	-2.749033
6	1.760919	0.194803	-3.088441
6	0.509632	0.698512	-3.453649
6	0.068671	1.994899	-2.949127
6	-1.038431	3.336666	-0.683501

6	-1.904739	2.566980	-1.570486
6	-1.363186	1.910518	-2.679085
6	-1.806697	0.561691	-3.016593
6	-0.649285	-0.186999	-3.495585
6	-0.508005	-1.538733	-3.170786
6	0.798673	-2.064984	-2.789536
6	0.596476	-3.052548	-1.734213
6	1.512944	-3.149907	-0.683800
6	2.773181	0.073080	2.232173
6	-0.898186	-2.732628	2.100011
6	-0.068671	-1.994899	2.949127
6	-0.509632	-0.698512	3.453649
6	-1.760919	-0.194803	3.088442
6	-2.627097	-0.965230	2.201972
6	-2.446865	-2.567273	0.324888
6	-1.289614	-3.316134	-0.154423
6	-0.332375	-3.418264	0.942619
6	1.038431	-3.336666	0.683501
6	1.904739	-2.566980	1.570486
6	1.363186	-1.910518	2.679085
6	0.649285	0.186999	3.495585
6	0.508005	1.538733	3.170786
6	-0.798673	2.064984	2.789536
6	-1.908672	1.216885	2.749033
6	-2.866289	1.318831	1.652355
6	-3.310016	-0.029752	1.314051
6	-3.541486	-0.375063	-0.020067
6	-3.100936	-1.671532	-0.525368
6	-0.835057	-3.137318	-1.463891
6	-1.517707	-2.201939	-2.351921

6	-2.625883	-1.484702	-1.892670
6	-2.773181	-0.073080	-2.232173
6	-3.339375	0.612772	-1.075109
6	-2.914354	1.904163	-0.751272
6	-2.672956	2.265057	0.642092
6	-1.512944	3.149907	0.683800
6	-0.596476	3.052548	1.734213
6	1.806697	-0.561691	3.016593
6	1.517707	2.201939	2.351921
6	-2.204963	-2.206471	1.718229

TS3

Frequencies **-379.6039**

6	1.806933	0.879235	1.170864
6	1.866026	-0.582989	1.241709
6	1.833128	-1.314613	0.054696
6	1.839218	-0.667463	-1.240632
6	1.915411	0.778329	-1.351521
6	1.767339	1.522819	-0.058395
6	0.977378	1.344238	2.265783
6	0.515283	0.183136	3.005568
6	1.061301	-1.005339	2.368480
6	0.285466	-2.168943	2.291225
6	1.036801	-2.526895	-0.027408
6	0.963524	-1.438085	-2.101069
6	0.123287	-0.821404	-3.027037
6	0.073771	0.639652	-3.075947
6	0.875701	1.398026	-2.234916
6	0.325530	2.565091	-1.588384
6	0.873179	2.640527	-0.244968

6	0.081337	3.109785	0.808309
6	0.133460	2.444844	2.092047
6	-0.774711	0.163837	3.538241
6	-1.655542	1.305921	3.349904
6	-1.210490	2.424072	2.643334
6	-2.094611	3.082816	1.695655
6	-1.295370	3.508034	0.559502
6	-1.820757	3.436003	-0.730143
6	-0.993388	2.962866	-1.829475
6	-1.826143	2.176294	-2.713572
6	-1.301332	1.032232	-3.320094
6	0.492605	-2.601427	-1.367544
6	-3.866614	-1.355586	-2.153663
6	-3.019740	-2.451338	-1.970785
6	-2.971698	-3.123141	-0.681385
6	-3.767283	-2.671131	0.372178
6	-4.645797	-1.529307	0.181459
6	-4.741016	0.567359	-1.117320
6	-3.941250	0.994312	-2.251448
6	-3.397513	-0.194198	-2.890021
6	-2.103228	-0.174679	-3.411978
6	-1.221794	-1.316909	-3.225847
6	-1.677331	-2.437262	-2.521285
6	-1.596520	-3.520275	-0.434231
6	-1.070989	-3.450556	0.856602
6	-1.897968	-2.977856	1.953698
6	-3.219204	-2.596456	1.716737
6	-3.758882	-1.407883	2.355714
6	-4.639470	-0.748407	1.406810
6	-4.687826	0.645509	1.348932

6	-4.738995	1.316673	0.060890
6	-3.172018	2.155912	-2.166229
6	-3.168571	2.935292	-0.938982
6	-3.937187	2.524663	0.151769
6	-3.389187	2.599687	1.496167
6	-3.851895	1.437457	2.235251
6	-3.002008	0.804427	3.144332
6	-2.954260	-0.647724	3.206019
6	-1.579158	-1.043466	3.454293
6	-1.058604	-2.183686	2.838053
6	-0.797836	-3.091346	-1.571819
6	0.276132	-2.944107	1.065724
6	-4.692596	-0.885070	-1.055887
6	5.919031	-0.639234	-0.051513
6	6.138767	0.698413	0.365487
6	7.022766	1.004780	1.400838
6	7.704574	-0.049838	2.008159
6	7.526613	-1.375033	1.586316
6	6.640681	-1.676842	0.552934
6	4.962220	-0.562087	-1.154118
6	4.678899	0.839834	-1.369218
1	7.179232	2.025926	1.732981
1	8.393475	0.165311	2.820014
1	8.086082	-2.172983	2.064451
1	6.547724	-2.701945	0.207749
7	4.278474	-1.455150	-1.837865
6	3.643383	1.303166	-2.191206
1	3.483502	0.727653	-3.096699
1	3.512104	2.375039	-2.311099
7	5.381622	1.562435	-0.423774

6	5.358462	3.007053	-0.289219
1	5.210942	3.461070	-1.272389
1	6.317888	3.352646	0.102611
1	4.556345	3.338723	0.379919
8	4.422410	-2.760443	-1.407756
1	4.636197	-2.749214	-0.452525

IV

6	1.611117	1.005224	1.488471
6	1.720566	-0.469244	1.523642
6	1.877525	-1.180934	0.355176
6	2.243888	-0.564027	-1.013143
6	2.117231	1.048555	-1.050379
6	1.655630	1.664938	0.282506
6	0.655603	1.397616	2.501539
6	0.175560	0.197725	3.163694
6	0.833049	-0.947786	2.560292
6	0.127731	-2.144389	2.391425
6	1.121486	-2.389720	0.163504
6	1.222368	-1.294603	-1.905305
6	0.440833	-0.679788	-2.855584
6	0.328128	0.795676	-2.895764
6	0.997029	1.562803	-1.970325
6	0.324492	2.674396	-1.357322
6	0.731585	2.738152	0.033917
6	-0.178756	3.155709	1.011341
6	-0.220138	2.465531	2.277552
6	-1.154222	0.107756	3.575249
6	-2.066208	1.213192	3.328266
6	-1.607264	2.369086	2.692994

6	-2.425731	3.010724	1.676300
6	-1.540505	3.499896	0.633846
6	-1.932174	3.436393	-0.702623
6	-0.979809	3.026282	-1.722184
6	-1.677356	2.228255	-2.699836
6	-1.032298	1.121946	-3.264245
6	0.714897	-2.456360	-1.230004
6	-3.588411	-1.410759	-2.417250
6	-2.717931	-2.475671	-2.174798
6	-2.767530	-3.177416	-0.901857
6	-3.684275	-2.785223	0.075891
6	-4.589551	-1.679037	-0.179759
6	-4.651518	0.444881	-1.439466
6	-3.765976	0.936175	-2.476973
6	-3.102161	-0.209956	-3.077832
6	-1.762261	-0.118653	-3.455182
6	-0.854682	-1.222829	-3.202850
6	-1.328088	-2.382842	-2.581188
6	-1.405729	-3.512976	-0.524994
6	-1.015052	-3.451046	0.810994
6	-1.967599	-3.046583	1.829705
6	-3.276147	-2.718714	1.469647
6	-3.929111	-1.571270	2.074111
6	-4.742106	-0.928729	1.055329
6	-4.847079	0.462677	1.020040
6	-4.804680	1.163781	-0.252025
6	-3.067374	2.131154	-2.292795
6	-3.226309	2.880094	-1.056539
6	-4.077393	2.405581	-0.056497
6	-3.668432	2.471633	1.337508

6	-4.144274	1.271120	2.001912
6	-3.357870	0.655547	2.978132
6	-3.248573	-0.795691	3.015474
6	-1.888820	-1.133869	3.387295
6	-1.259160	-2.238030	2.808706
6	-0.520607	-3.016246	-1.567492
6	0.277865	-2.885308	1.163441
6	-4.541914	-1.006383	-1.402813
6	5.880011	-0.673913	-0.115493
6	6.494385	0.550791	0.295872
6	7.703778	0.567083	1.000634
6	8.313247	-0.651481	1.275025
6	7.736256	-1.866614	0.853423
6	6.532886	-1.889479	0.162098
6	4.673673	-0.278545	-0.782617
6	4.606899	1.087023	-0.781646
1	8.156704	1.500588	1.322116
1	9.254226	-0.665996	1.817887
1	8.245985	-2.801342	1.069849
1	6.111855	-2.828497	-0.181108
7	3.638726	-0.975818	-1.452034
6	3.473216	1.739984	-1.480179
1	3.582390	1.606584	-2.565069
1	3.385081	2.813023	-1.288358
7	5.710913	1.612012	-0.124950
6	5.962465	3.005142	0.179573
1	5.345075	3.636333	-0.462660
1	7.012035	3.247847	-0.015104
1	5.734901	3.241593	1.227102
8	3.793362	-2.378334	-1.360426

1	3.747431	-2.607282	-0.407750

TS4

Frequencies **-525.6037**

6	-0.511218	-2.441415	1.029474
6	-0.846169	-1.270325	1.864173
6	-1.398683	-0.140017	1.302480
6	-1.976645	-0.046093	-0.129842
6	-1.586624	-1.329920	-1.053147
6	-0.725438	-2.383904	-0.325043
6	0.707820	-3.018138	1.554103
6	1.124169	-2.235776	2.703510
6	0.166171	-1.161378	2.891566
6	0.605523	0.094079	3.323596
6	-0.907575	1.154259	1.713749
6	-1.324969	1.275403	-0.589168
6	-0.687118	1.449809	-1.798265
6	-0.344028	0.287575	-2.647071
6	-0.635351	-0.983724	-2.215001
6	0.330973	-2.031310	-2.385368
6	0.277205	-2.893353	-1.220953
6	1.447729	-3.484393	-0.734663
6	1.670739	-3.547334	0.689377
6	2.479056	-2.012312	2.945861
6	3.478288	-2.555630	2.040463
6	3.081164	-3.308605	0.933876
6	3.732079	-3.107118	-0.350991
6	2.719791	-3.218166	-1.386270
6	2.770745	-2.389795	-2.506551
6	1.551698	-1.790634	-3.024735
6	1.858597	-0.457673	-3.481792

6	0.926066	0.565482	-3.280806
6	-0.865194	2.022198	0.550433
6	3.153556	2.896774	-1.475496
6	2.202804	3.424322	-0.600146
6	2.432364	3.372868	0.834391
6	3.603226	2.799211	1.333766
6	4.593230	2.257448	0.419774
6	4.708075	1.161893	-1.790549
6	3.697983	1.045300	-2.823719
6	2.731071	2.113333	-2.626108
6	1.374822	1.875759	-2.846706
6	0.382691	2.416738	-1.935105
6	0.791308	3.180315	-0.836643
6	1.161941	3.096036	1.479460
6	1.112630	2.269000	2.599046
6	2.329351	1.677958	3.126532
6	3.550845	1.935146	2.501826
6	4.508217	0.860443	2.308109
6	5.154287	1.060388	1.022253
6	5.474674	-0.038454	0.223771
6	5.251147	0.013774	-1.211104
6	3.269580	-0.215112	-3.244109
6	3.835278	-1.411569	-2.641803
6	4.804878	-1.298239	-1.644343
6	4.752135	-2.162838	-0.476242
6	5.165507	-1.383762	0.677301
6	4.540431	-1.577325	1.910264
6	4.204922	-0.431513	2.742614
6	2.933465	-0.700584	3.383486
6	2.014352	0.331559	3.576810

6	0.151383	2.975080	0.439284
6	0.053671	1.280410	2.720749
6	4.372258	2.307582	-0.957749
6	-5.667975	-1.095019	0.449722
6	-6.064921	-2.381738	0.000319
6	-7.314983	-2.927633	0.301456
6	-8.185641	-2.153704	1.061171
6	-7.812645	-0.875680	1.516554
6	-6.561181	-0.342900	1.230070
6	-4.309198	-0.928461	-0.018420
6	-3.972943	-2.062953	-0.746413
1	-7.602436	-3.915166	-0.045062
1	-9.167605	-2.544974	1.309063
1	-8.515656	-0.297257	2.108520
1	-6.277509	0.631615	1.607734
7	-3.515893	0.207646	-0.091342
6	-2.820017	-2.064202	-1.675119
1	-3.110086	-1.549511	-2.601743
1	-2.501603	-3.068236	-1.966678
7	-5.029623	-2.935208	-0.749473
6	-5.133372	-4.194255	-1.471346
1	-5.423080	-4.993800	-0.782789
1	-4.168525	-4.451707	-1.907865
1	-5.879252	-4.124532	-2.270592
8	-3.864153	1.016630	1.380772
1	-3.106904	0.880906	1.992266
16	-4.866207	3.581799	-0.610363
8	-3.991469	3.334549	0.662846
6	-5.787589	5.090210	-0.196605
1	-6.324687	5.433384	-1.085300

1	-6.498934	4.829300	0.589741
1	-5.089917	5.850729	0.162666
6	-3.708398	4.268671	-1.829630
1	-3.020419	3.465582	-2.102542
1	-4.271823	4.596043	-2.708121
1	-3.159064	5.099752	-1.380110
1	-3.911703	2.096162	1.037168

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6	2.082244	2.291608	-2.778698
6	1.013484	1.337217	-3.032518
6	-0.113412	1.308195	-2.202362
6	-0.212402	2.241414	-1.094460
6	0.806654	3.171154	-0.860886
6	1.981080	3.189636	-1.717635
6	3.344158	1.626665	-3.050462
6	3.050996	0.266775	-3.471790
6	1.609585	0.095831	-3.462261
6	1.049274	-1.113082	-3.037068
6	-0.716395	0.062427	-1.805548
6	-0.862898	1.576599	-0.003301
6	-0.462206	1.819084	1.288651
6	0.607187	2.756081	1.548177
6	1.227516	3.434229	0.492947
6	2.667824	3.612781	0.489279
6	3.135173	3.462857	-0.879362
6	4.347184	2.819469	-1.135435
6	4.453750	1.883378	-2.243089
6	3.880021	-0.780984	-3.066578
6	5.033860	-0.514082	-2.230955

6	5.315847	0.791899	-1.825883
6	5.742491	1.052311	-0.461674
6	5.142809	2.305125	-0.035191
6	4.693497	2.450783	1.278915
6	3.432897	3.114017	1.545357
6	2.787224	2.420064	2.648955
6	1.404641	2.241806	2.646477
6	-1.505364	0.263308	-0.487450
6	1.383001	-1.410760	3.069267
6	0.271553	-1.654701	2.254841
6	0.388015	-2.583527	1.147575
6	1.597005	-3.240835	0.899234
6	2.752208	-2.978927	1.741869
6	3.715680	-1.131849	3.059340
6	3.109331	0.118902	3.485290
6	1.669156	-0.061257	3.489355
6	0.830121	0.977997	3.073034
6	-0.325471	0.699878	2.248487
6	-0.618876	-0.590744	1.872807
6	-0.409668	-2.098063	0.060076
6	0.018185	-2.235789	-1.238392
6	1.276596	-2.889412	-1.510758
6	2.053233	-3.394106	-0.460703
6	3.494026	-3.225729	-0.475013
6	3.927664	-2.966953	0.888500
6	4.952642	-2.051591	1.130925
6	4.844741	-1.115806	2.238446
6	3.657792	1.334214	3.070600
6	4.832935	1.350928	2.222541
6	5.414301	0.149888	1.811913

6	5.875358	-0.002309	0.442553
6	5.587727	-1.362347	0.021728
6	5.173460	-1.614395	-1.287918
6	4.104718	-2.559785	-1.539582
6	3.299509	-2.043059	-2.636278
6	1.914779	-2.201243	-2.617917
6	-1.339777	-0.962390	0.554988
6	-0.130081	-1.119080	-2.198343
6	2.646940	-2.080967	2.802055
6	-4.825362	-2.467393	0.239999
6	-5.699690	-1.914095	-0.705762
6	-6.933047	-2.466645	-1.003328
6	-7.282232	-3.632657	-0.305283
6	-6.420179	-4.203748	0.636361
6	-5.173983	-3.628828	0.916981
6	-3.625573	-1.623945	0.225662
6	-3.904253	-0.546016	-0.733758
1	-7.606675	-2.030627	-1.732886
1	-8.240953	-4.100123	-0.506774
1	-6.721683	-5.107235	1.156832
1	-4.498547	-4.069205	1.643176
7	-5.086932	-0.737178	-1.266242
6	-3.006296	0.616334	-0.798610
7	-2.540737	-1.749293	0.890213
6	-5.805453	0.164174	-2.167828
1	-6.597776	0.669611	-1.603195
1	-5.110041	0.896732	-2.576162
1	-6.231514	-0.422292	-2.985051
8	-5.186344	0.859586	1.342138
1	-5.252071	0.771723	2.303790

1	-3.062213	1.161986	-1.744184
1	-3.400925	1.280547	-0.012883
16	-8.620149	2.452495	0.796456
8	-7.620389	1.468650	0.167724
6	-8.814515	3.825926	-0.388366
1	-9.596309	4.502428	-0.031067
1	-7.860512	4.356510	-0.427500
1	-9.064988	3.428958	-1.376130
6	-10.270025	1.705837	0.577852
1	-10.300913	0.805656	1.195672
1	-11.033893	2.411731	0.916406
1	-10.418573	1.444453	-0.473493
1	-6.089963	1.108456	1.039903

TS5

Frequencies	**-878.4877**		
6	-1.949924	1.141512	3.331831
6	-0.818421	0.227899	3.375917
6	0.353407	0.528069	2.670905
6	0.438814	1.761011	1.908488
6	-0.646513	2.645458	1.878919
6	-1.866276	2.326267	2.602789
6	-3.162666	0.343531	3.288230
6	-2.775670	-1.057461	3.305423
6	-1.326466	-1.120943	3.363125
6	-0.638062	-2.100744	2.639595
6	1.080089	-0.492317	1.966821
6	1.215896	1.506243	0.729355
6	0.860553	2.101740	-0.461001
6	-0.272141	3.000742	-0.518246

6	-1.010407	3.281942	0.637148
6	-2.458492	3.356574	0.574976
6	-2.988832	2.764524	1.792221
6	-4.151609	1.994375	1.741757
6	-4.240888	0.760292	2.505530
6	-3.483381	-1.983539	2.537009
6	-4.604587	-1.550865	1.727079
6	-4.977669	-0.205824	1.710692
6	-5.344697	0.429550	0.456816
6	-4.833393	1.789423	0.476301
6	-4.324156	2.359570	-0.692188
6	-3.112907	3.153587	-0.641700
6	-2.345032	2.873068	-1.845628
6	-0.954523	2.794287	-1.782744
6	1.941247	0.148107	0.846529
6	-0.587045	-0.546281	-3.273530
6	0.490963	-0.955137	-2.480446
6	0.397948	-2.184673	-1.715987
6	-0.762918	-2.962270	-1.778398
6	-1.885575	-2.529946	-2.595361
6	-2.930518	-0.437875	-3.376748
6	-2.413205	0.920564	-3.355817
6	-0.965252	0.845834	-3.294921
6	-0.247855	1.762074	-2.518847
6	0.877084	1.320359	-1.722472
6	1.252546	-0.003581	-1.719537
6	1.093167	-2.003374	-0.474865
6	0.594916	-2.553959	0.679701
6	-0.617364	-3.340273	0.640172
6	-1.283616	-3.555169	-0.571268

6	-2.732251	-3.491453	-0.625515
6	-3.106153	-2.856871	-1.879133
6	-4.192194	-1.981219	-1.920582
6	-4.102493	-0.747050	-2.684284
6	-3.090289	1.912845	-2.643572
6	-4.310206	1.592747	-1.929733
6	-4.806015	0.287751	-1.947268
6	-5.331334	-0.305294	-0.729326
6	-4.950809	-1.707311	-0.713212
6	-4.591617	-2.318055	0.489950
6	-3.461158	-3.223582	0.534777
6	-2.769912	-3.012965	1.797256
6	-1.377995	-3.065315	1.845353
6	1.950173	-0.712816	-0.532724
6	0.584289	-1.774615	1.939388
6	-1.799804	-1.347872	-3.328211
6	5.636682	-1.675085	-0.556745
6	6.423573	-1.342854	0.560496
6	7.755023	-1.715303	0.653773
6	8.289086	-2.451513	-0.415782
6	7.515736	-2.797784	-1.528023
6	6.172839	-2.413023	-1.606570
6	4.297071	-1.137230	-0.299412
6	4.385483	-0.438920	1.011951
1	8.372441	-1.457427	1.507638
1	9.329591	-2.758678	-0.371470
1	7.961042	-3.370960	-2.334771
1	5.556888	-2.678284	-2.460160
7	5.630685	-0.613071	1.498555
6	3.361192	0.402340	1.411665

7	3.255349	-1.198217	-1.032382
6	6.143919	-0.017467	2.722949
1	6.555572	0.980033	2.529527
1	5.334375	0.062707	3.451709
1	6.920869	-0.659808	3.141077
1	3.364254	0.799773	2.427637
1	4.044464	1.652736	0.832624
16	4.945941	3.463153	-0.518544
8	4.813085	2.510452	0.746319
6	4.552414	2.447375	-1.974092
1	4.662184	3.087391	-2.854765
1	5.291599	1.644012	-2.014204
1	3.538800	2.042474	-1.918516
6	3.514430	4.576581	-0.470792
1	3.620230	5.185760	0.429780
1	3.565764	5.217691	-1.356271
1	2.582455	4.007031	-0.448148

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6	-2.033163	0.888182	3.410703
6	-0.928069	-0.057993	3.412923
6	0.271123	0.263509	2.766035
6	0.413161	1.550261	2.108232
6	-0.647623	2.465009	2.119876
6	-1.896140	2.124869	2.782730
6	-3.264510	0.131400	3.270202
6	-2.915202	-1.277097	3.185863
6	-1.470305	-1.386540	3.278223
6	-0.786904	-2.325178	2.496874
6	0.989030	-0.718391	2.002908

6	1.219777	1.369244	0.935237
6	0.916353	2.069461	-0.213092
6	-0.192108	3.000958	-0.229199
6	-0.957495	3.209241	0.924454
6	-2.400638	3.330031	0.828858
6	-2.982260	2.658629	1.979694
6	-4.162887	1.928236	1.835324
6	-4.307415	0.640176	2.494421
6	-3.623913	-2.118063	2.326233
6	-4.709811	-1.590674	1.523837
6	-5.046708	-0.238127	1.605274
6	-5.359213	0.505106	0.396783
6	-4.812149	1.843736	0.539270
6	-4.253724	2.490325	-0.565080
6	-3.024276	3.242571	-0.417552
6	-2.228725	3.036666	-1.618472
6	-0.843022	2.914300	-1.524343
6	1.901395	-0.019316	0.960957
6	-0.520997	-0.306540	-3.266927
6	0.520601	-0.808869	-2.479297
6	0.376471	-2.093616	-1.820129
6	-0.802817	-2.829220	-1.977513
6	-1.889276	-2.299510	-2.786760
6	-2.855767	-0.123059	-3.426639
6	-2.303905	1.214370	-3.282866
6	-0.860829	1.093676	-3.188128
6	-0.142681	1.924560	-2.321716
6	0.947292	1.389210	-1.533402
6	1.280167	0.056688	-1.621654
6	1.043827	-2.031717	-0.551068

6	0.492509	-2.655794	0.540505
6	-0.739208	-3.400535	0.405094
6	-1.375082	-3.501218	-0.836963
6	-2.819087	-3.390339	-0.925096
6	-3.138811	-2.647111	-2.133008
6	-4.199891	-1.740288	-2.133941
6	-4.055173	-0.452440	-2.793254
6	-2.975433	2.166152	-2.512109
6	-4.223939	1.825261	-1.859771
6	-4.752772	0.540421	-1.995421
6	-5.329688	-0.132632	-0.844004
6	-4.986581	-1.541727	-0.929989
6	-4.679341	-2.256335	0.229440
6	-3.575142	-3.195016	0.232394
6	-2.916206	-3.105198	1.525741
6	-1.528160	-3.200622	1.606816
6	1.935344	-0.765800	-0.484750
6	0.463442	-1.980337	1.858577
6	-1.751332	-1.065986	-3.420487
6	5.652712	-1.582426	-0.577530
6	6.439719	-1.293429	0.556534
6	7.796163	-1.593629	0.587229
6	8.347219	-2.205383	-0.547512
6	7.573463	-2.505788	-1.674727
6	6.210832	-2.196650	-1.695686
6	4.289138	-1.144894	-0.268694
6	4.358021	-0.543549	1.091622
1	8.417391	-1.370732	1.448262
1	9.404786	-2.452642	-0.545643
1	8.034396	-2.984592	-2.532587

1	5.590396	-2.428990	-2.555944
7	5.637433	-0.702982	1.560616
6	3.291765	0.129698	1.594745
7	3.249240	-1.203245	-1.006532
6	6.120350	-0.213951	2.837988
1	6.457135	0.829193	2.773462
1	5.319516	-0.285797	3.578917
1	6.950469	-0.836965	3.177295
1	3.308180	0.569695	2.589775
1	4.234041	1.727688	0.880573
16	5.069826	3.309925	-0.513985
8	4.977773	2.425375	0.833654
6	4.659665	2.188380	-1.879739
1	4.782778	2.763210	-2.803193
1	5.387413	1.373442	-1.856183
1	3.637528	1.808205	-1.798061
6	3.628801	4.407343	-0.466324
1	3.773156	5.077586	0.384272
1	3.631299	4.985937	-1.395724
1	2.705644	3.830457	-0.361786

DMF

7	-0.344651	-0.018876	-0.000021
6	-1.589887	-0.764147	0.000034
1	-2.187289	-0.528954	-0.887775
1	-1.377158	-1.834385	-0.000789
1	-2.186711	-0.530156	0.888556
6	-0.423069	1.433450	-0.000008
1	0.589432	1.832665	-0.000301
1	-0.954172	1.790016	-0.889031

1	-0.953628	1.790175	0.889283
6	0.864945	-0.645931	-0.000012
8	1.951237	-0.097630	0.000028
1	0.760253	-1.746428	-0.000108

I-D′

6	1.723758	-0.739785	-0.086951
6	2.514022	0.348078	-0.475906
6	3.706810	0.212599	-1.164866
6	4.111879	-1.092680	-1.461455
6	3.342381	-2.193255	-1.079565
6	2.137129	-2.030767	-0.388350
6	0.565973	-0.196497	0.652213
6	0.736254	1.269437	0.579566
1	4.306223	1.061712	-1.467637
1	5.038451	-1.248489	-2.000069
1	3.683128	-3.190909	-1.328055
1	1.544367	-2.891588	-0.106702
1	-0.457802	-0.506966	0.394565
7	1.863851	1.550629	-0.044973
6	-0.219593	2.216321	1.186471
1	-0.256134	2.025312	2.267145
1	0.016034	3.264112	1.017228
1	-1.219649	1.984577	0.806108
7	0.518573	-0.591789	2.290134
8	1.000128	-1.623514	2.521226
6	2.440183	2.871509	-0.308156
1	2.546678	3.006911	-1.385195
1	1.797183	3.648565	0.092345
1	3.420915	2.934258	0.165349

7	-4.608603	-0.254218	-0.551942
6	-5.847815	-1.016999	-0.439744
1	-6.169019	-1.367881	-1.424090
1	-5.693514	-1.880575	0.207253
1	-6.640376	-0.396347	-0.012938
6	-4.633797	0.939666	-1.390494
1	-3.637357	1.373901	-1.415506
1	-4.941407	0.676111	-2.405882
1	-5.341415	1.670382	-0.988595
6	-3.494248	-0.628971	0.095804
8	-2.410152	-0.038407	0.071347
1	-3.630487	-1.552027	0.680161

TS1′

Frequencies	**-798.7339**		
6	-1.301981	0.691986	0.417938
6	-2.279820	0.173316	-0.441845
6	-3.222479	0.964263	-1.083549
6	-3.174634	2.333081	-0.820720
6	-2.216801	2.869637	0.046484
6	-1.264952	2.060981	0.669146
6	-0.475016	-0.460941	0.846175
6	-1.131848	-1.636350	0.283341
1	-3.968914	0.551894	-1.750627
1	-3.895271	2.988671	-1.293913
1	-2.214527	3.935871	0.237990
1	-0.529044	2.484796	1.338218
1	0.643559	-0.386453	0.171600
7	-2.129694	-1.241940	-0.494123
6	-0.729011	-3.047836	0.511878

1	-0.096380	-3.102092	1.397346
1	-1.594049	-3.698301	0.654290
1	-0.155071	-3.428917	-0.340337
7	0.096018	-0.650413	2.176166
8	0.291897	0.368610	2.791379
6	-2.996970	-2.092100	-1.311947
1	-2.945917	-1.763887	-2.350894
1	-2.669889	-3.125871	-1.248406
1	-4.025395	-2.012396	-0.956306
7	3.970774	0.245878	-0.584172
6	5.181738	0.591815	0.166116
1	5.564915	1.555605	-0.175112
1	4.956001	0.654246	1.230016
1	5.946115	-0.171693	0.007449
6	4.097640	0.128961	-2.040214
1	3.128389	-0.110835	-2.468465
1	4.457525	1.075068	-2.449707
1	4.814045	-0.659201	-2.281796
6	2.819881	0.045339	0.029764
8	1.751249	-0.263311	-0.561213
1	2.844566	0.163501	1.116845

I-D2+DMF

6	1.975315	-0.705203	-0.044250
6	3.281082	-0.192586	0.017745
6	4.407881	-0.995912	0.001506
6	4.193930	-2.375463	-0.081382
6	2.903431	-2.906669	-0.144828
6	1.776669	-2.081043	-0.127166
6	1.097471	0.458176	-0.003589

6	1.942026	1.634057	0.081831
1	5.411348	-0.592377	0.049007
1	5.047906	-3.041504	-0.097132
1	2.774727	-3.980180	-0.209291
1	0.779015	-2.493318	-0.177643
1	-1.878638	-0.246762	-0.150108
7	3.205312	1.231591	0.093254
6	1.490858	3.047137	0.144670
1	0.403797	3.080455	0.112601
1	1.830701	3.526763	1.067520
1	1.885389	3.622752	-0.697951
7	-0.197771	0.620495	-0.033933
8	-0.876202	-0.501350	-0.114466
6	4.394091	2.080479	0.167216
1	5.007612	1.923753	-0.721386
1	4.099509	3.124657	0.221874
1	4.970661	1.820702	1.056394
7	-5.547665	-0.151689	0.071335
6	-6.622579	-0.884904	0.735435
1	-7.280677	-1.343345	-0.006880
1	-6.203892	-1.668717	1.366467
1	-7.211885	-0.207191	1.358066
6	-5.932816	0.945021	-0.816574
1	-5.036431	1.386840	-1.243836
1	-6.572597	0.564809	-1.616712
1	-6.483354	1.702120	-0.252595
6	-4.268070	-0.469081	0.262488
8	-3.309122	0.114660	-0.270554
1	-4.115467	-1.312752	0.948566

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