Supporting Information

Unexpected Formation of Pyrazoline-Fused Metallofullerenes from Multi-Component Cascade Reaction of $Sc_3N@I_h$-C_{80} with Tetrazines, Water, and Oxygen

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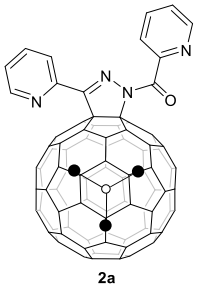
1. General Information

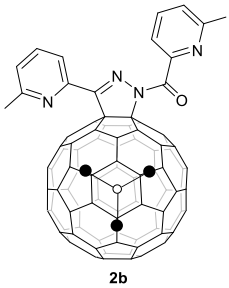
3,6-Di(pyridin-2-yl)-1,2,4,5-tetrazine (**1a**) was obtained commercially and used without further purification. 3,6-Bis(6-methylpyridin-2-yl)-1,2,4,5-tetrazine (**1b**) was synthesized by the literature procedure and and its ^{1}H NMR data were consistent with those reported in the literature.[1] ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker ASCEND III–400 spectrometer at room temperature. ^{1}H NMR and ^{13}C NMR chemical shifts were determined relative to TMS. Abbreviations for signal couplings are: s, singlet; d, doublet; t, triplet; m, multiplet. Compound **4a** is known, and its ^{1}H NMR data were consistent with those reported in the literature.[2] High-resolution mass spectra (HRMS) were obtained on a Bruker UltrafleXtreme MALDI-TOF/TOF instrument. UV-vis-NIR/UV-vis spectra were obtained on a SHIMADZU UV-3600PLUS instrument. IR spectra were obtained on a Thermo Scientific Nicolet 6700 instrument.

2. Synthesis and Spectral Data of Compounds 2a, 2b, 3a, and 4a



2a

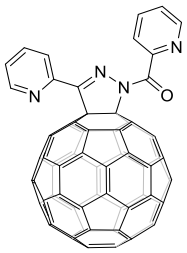
***Synthesis and Spectral Data of Compound 2a*:** a mixture of $Sc_3N@I_h$-C_{80} (5.1 mg, 4.6 μmol) and **1a** (54.3 mg, 230 μmol) was dissolved in 1,2-dichlorobenzene (1,2-$C_6H_4Cl_2$) (10 mL). Then, the solution was stirred in an oil bath at 180 °C for 36 h. The resulting solution was evaporated in vacuo and subsequently separated on a silica gel column (300–400 mesh) with CS_2/ethyl acetate (10:1 v/v) as the eluent to afford unreacted $Sc_3N@I_h$-C_{80} (2.0 mg, 39%) and product **2a** (2.2 mg, 36%) as amorphous brown solid. ^{1}H NMR (400 MHz, $C_2D_2Cl_4$) δ 8.75 (d, J = 4.6 Hz, 1H), 8.69 (d, J = 4.5 Hz, 1H), 7.96–7.86 (m, 3H), 7.72 (td, J = 7.8, 1.8 Hz, 1H), 7.51–7.44 (m, 1H), 7.34 (dd, J = 6.8, 4.9 Hz, 1H); UV-vis-NIR (CS_2) λ_{max}/nm 476, 584, 950; HRMS (MALDI) m/z: $[M]^-$ Calcd for $C_{92}H_8N_5OSc_3$ 1332.9412; Found 1332.9410.



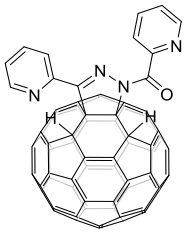
2b

***Synthesis and Spectral Data of Compound 2b*:** a mixture of $Sc_3N@I_h$-C_{80} (5.0 mg, 4.5 μmol) and **1b** (59.5 mg, 225 μmol) was dissolved in 1,2-$C_6H_4Cl_2$ (10 mL). Then, the solution was stirred in an oil bath at 180 °C for 36 h. The resulting solution was evaporated in vacuo and subsequently separated on a silica gel column (300–400

mesh) with CS_2/ethyl acetate (10:1 v/v) as the eluent to afford unreacted $Sc_3N@I_h$-C_{80} (2.1 mg, 42%) and product **2b** (2.1 mg, 34%) as amorphous brown solid. ^{1}H NMR (400 MHz, $C_2D_2Cl_4$) δ 7.80–7.74 (m, 3H), 7.61 (t, J = 7.8 Hz, 1H), 7.32 (dd, J = 6.7, 2.0 Hz, 1H), 7.18 (d, J = 7.6 Hz, 1H), 2.66 (s, 3H), 2.57 (s, 3H); UV-vis-NIR (CS_2) λ_{max}/nm 474, 578, 950; HRMS (MALDI) m/z: $[M]^-$ Calcd for $C_{94}H_{12}N_5OSc_3$ 1360.9725; Found 1360.9742.



3a



4a

***Synthesis and Spectral Data of Compounds 3a and 4a*:** a mixture of C_{60} (36.0 mg, 0.05 mmol) and **1a** (12.1 mg, 0.05 mmol) was dissolved in 1,2-$C_6H_4Cl_2$ (10 mL) and degassed with argon for 30 min. Then, the solution was stirred in an oil bath at 180 °C for 24 h. The resulting solution was evaporated in vacuo and subsequently separated on a silica gel column (300–400 mesh) with CS_2/ethyl acetate (10:1 v/v) as the eluent to afford unreacted C_{60} (17.8 mg, 49%), **3a** (2.8 mg, 6%) and **4a**[2] (14.7 mg, 31%) as amorphous brown solids.

***Compound 3a*:** ^{1}H NMR (400 MHz, 1:1 CS_2/$CDCl_3$) δ 8.86 (d, J = 4.7 Hz, 1H), 8.54 (d, J = 4.6 Hz, 1H), 8.16 (d, J = 8.0 Hz, 1H), 8.01–7.93 (m, 2H), 7.78 (td, J = 7.8, 1.5 Hz, 1H), 7.56–7.51 (m, 1H), 7.31 (dd, J = 7.6, 4.7 Hz, 1H); ^{13}C NMR (101 MHz, CS_2 with DMSO-d_6 as the external deuterium lock, all 2C unless indicated) δ 164.4 (1C, *C*=*O*), 152.9 (1C, aryl *C*), 149.8 (1C, aryl *C*), 147.8, 147.7 (1C, aryl *C*), 147.5 (1C, aryl *C*), 146.6 (1C), 146.4, 146.2 (1C), 146.0, 145.9 (1C), 145.4, 145.3, 145.1, 144.9, 144.8, 144.7, 144.4, 144.10, 144.08, 143.3, 143.2, 142.5, 141.8, 141.7 (4C), 141.6, 141.5, 141.1, 140.85, 140.78, 140.7, 138.2, 137.8, 135.11 (1C, aryl *C*), 135.06, 135.0 (1C, aryl *C*), 134.8, 123.8 (1C, aryl *C*), 123.2 (1C, aryl *C*), 122.8 (1C, aryl *C*), 122.7 (1C, aryl *C*), 86.3 (1C, sp^3-*C* of C_{60}), 77.6 (1C, sp^3-*C* of C_{60}); FT-IR ν/cm^{-1} (KBr) 1672, 1579, 1431, 1387, 1306, 995, 883, 846, 798, 778, 741, 687, 618, 570, 527; UV-vis ($CHCl_3$) λ_{max}/nm 312, 426; HRMS (MALDI) m/z: $[M]^-$ Calcd for $C_{72}H_8N_4O$ 944.0704; Found 944.0709.

***Compound 4a*:** ^{1}H NMR (400 MHz, 1:1 CS_2/$CDCl_3$) δ 8.89 (d, J = 4.7 Hz, 1H), 8.77 (d, J = 4.4 Hz, 1H), 8.19 (d, J = 8.0 Hz, 1H), 8.01–7.93 (m, 2H), 7.81 (td, J = 7.8, 1.5 Hz, 1H), 7.59–7.52 (m, 1H); 7.40 (dd, J = 6.8, 5.0 Hz, 1H), 6.62 (d, J = 1.7 Hz, 1H), 6.58 (d, J = 1.7 Hz, 1H).

***Synthesis of Compound 3a from 4a*: 4a** (49.0 mg, 0.05 mmol) was dissolved in 1,2-$C_6H_4Cl_2$ (10 mL) and degassed with argon for 30 min. Then, the solution was stirred in an oil bath at 180 °C for 36 h. The resulting solution was evaporated in vacuo and subsequently separated on a silica gel column (300–400 mesh) with CS_2/ethyl acetate (10:1 v/v) as the eluent to afford C_{60} (3.8 mg, 10%), **3a** (18.6 mg,

38%) and unreacted **4a** (13.4 mg, 27%).

3. HPLC Profiles

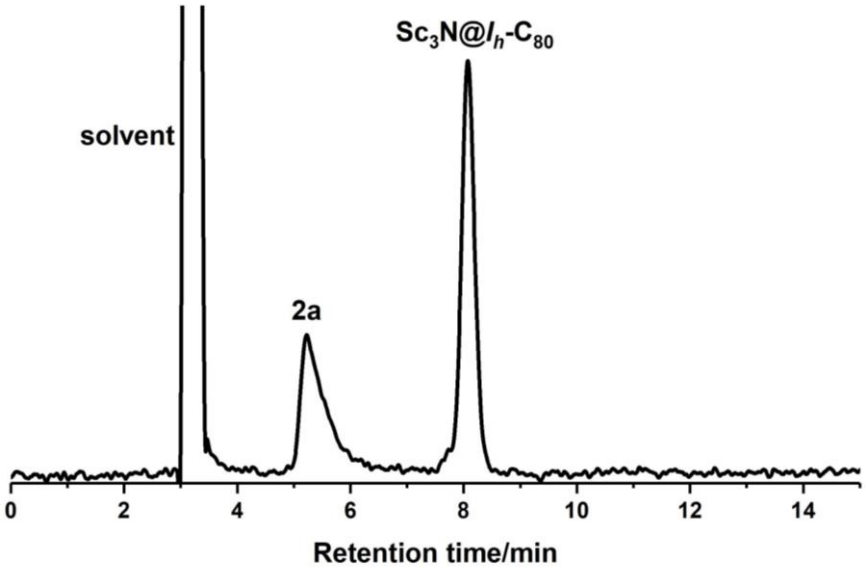


Figure S1. HPLC trace of the crude reaction mixture obtained from the reaction of $Sc_3N@I_h$-C_{80} with **1a**. HPLC column: Cosmosil Buckyprep column (4.6 ×250 mm; chlorobenzene, 1 mL/min; 326 nm; 25 ^oC).

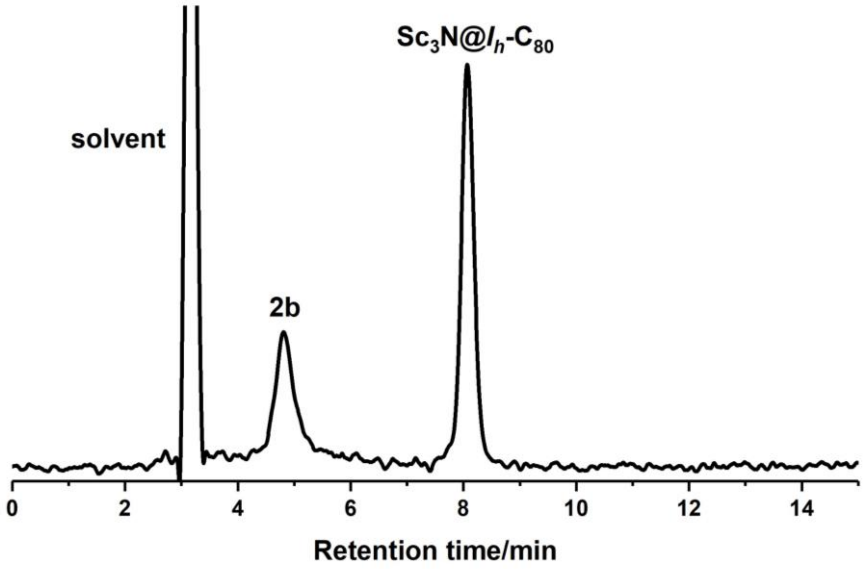


Figure S2. HPLC trace of the crude reaction mixture obtained from the reaction of $Sc_3N@I_h$-C_{80} with **1b**. HPLC column: Cosmosil Buckyprep column (4.6 ×250 mm; chlorobenzene, 1 mL/min; 326 nm; 25 ^oC).

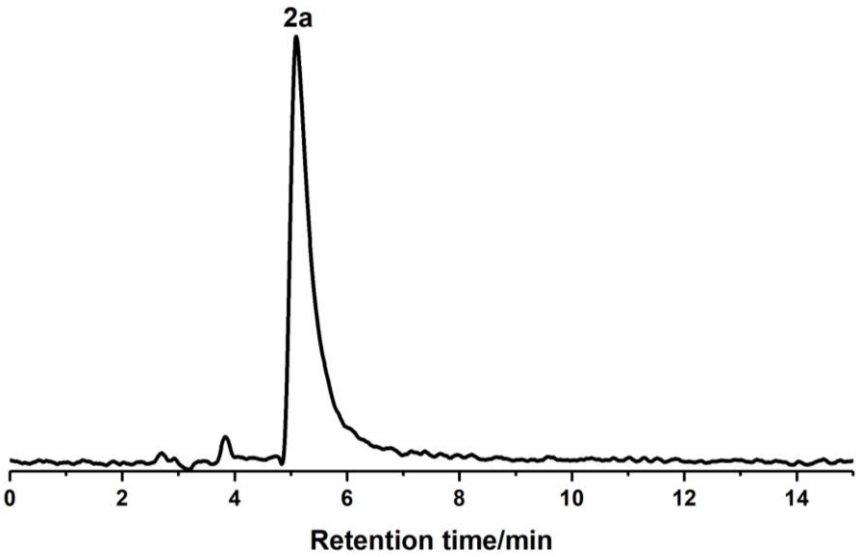


Figure S3. HPLC profile of **2a**. HPLC column: Cosmosil Buckyprep column (4.6 ×250 mm; chlorobenzene, 1 mL/min; 326 nm; 25 ºC).

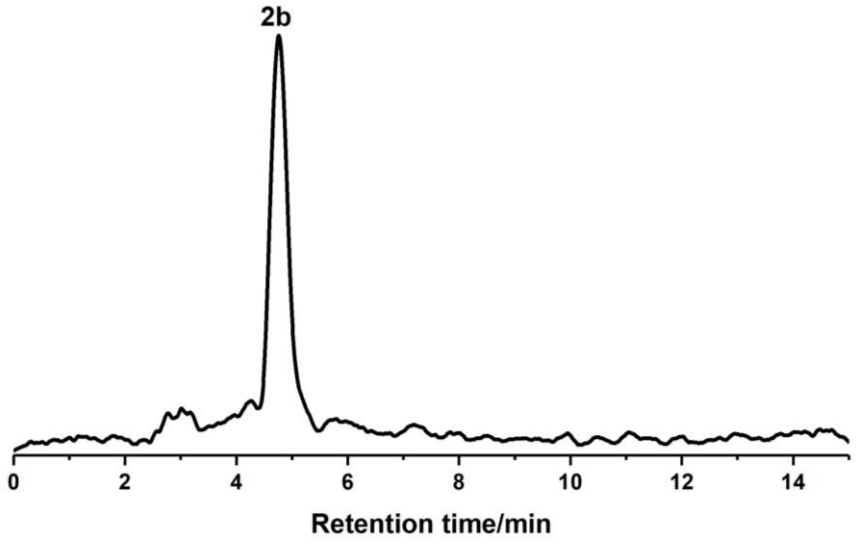


Figure S4. HPLC profile of **2b**. HPLC column: Cosmosil Buckyprep column (4.6 ×250 mm; chlorobenzene, 1 mL/min; 326 nm; 25 ºC).

4. X-Ray Data of Compound 2a

Black block crystals of **2a** were obtained by slow volatilization of a toluene solution of decapyrrylcorannulene (DCP) host and **2a** in a glass tube at 4 ^{o}C. Single-crystal X-ray diffraction data collection was performed at 100(2) K in beamline station BL17B at the Shanghai Synchrotron Radiation Facility in the scan range $1.456° < 2\theta < 48.212°$. The structure was solved with direct methods using SHELXT and refined with full-matrix least-squares refinement using the SHELXL program within OLEX2. Crystallographic data have been deposited in the Cambridge Crystallographic Data Centre as deposition number CCDC 2109051.

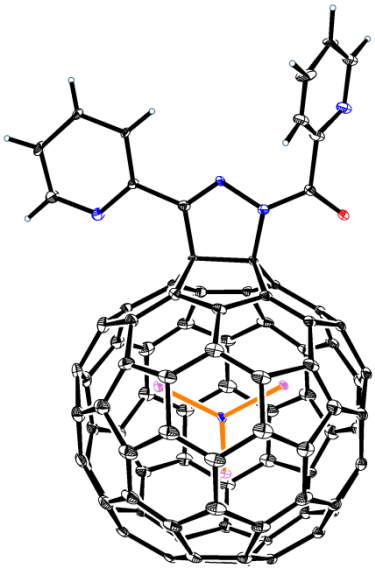


Figure S5. ORTEP diagram of **2a** with 10% thermal ellipsoids. The major occupancy for the scandium sites and cage orientation in **2a** are presented, and toluene molecule and DCP hosts are omitted for clarity.

Table S1. Crystal Data for 2a

Identification code	2109051
Empirical formula	$C_{219}H_{96}N_{25}OSc_3$
Formula weight	3228.08
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1
a/Å	14.454
b/Å	19.974
c/Å	30.098
α/°	105.76
β/°	101.60
γ/°	99.45
Volume/Å^3	7968.3
Z	2
ρ_{calc}g/cm^3	1.345
μ/mm^{-1}	0.195
F(000)	3312.0
Crystal size/mm^3	0.08 × 0.06 × 0.06
Radiation	synchrotron (λ = 0.71073)
2θ range for data collection/°	1.456 to 48.212
Reflections collected	22705
Independent reflections	18042 [R_{int} = 0.057, R_{sigma} = 0.0747]
Data/restraints/parameters	18042/2634/3267
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.1123, wR_2 = 0.3087
Final R indexes [all data]	R_1 = 0.1290, wR_2= 0.3235
Largest diff. peak/hole / e Å^{-3}	1.17/-0.56

5. Electrochemical Properties of Compounds 2a and 2b

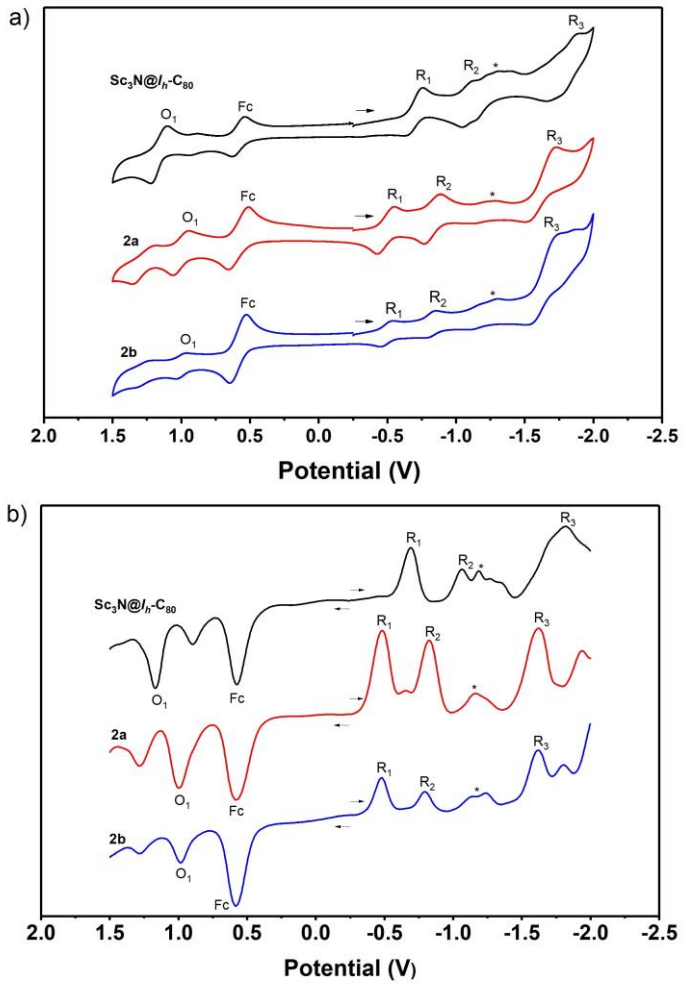


Figure S6. (a) CVs and (b) DPVs of $Sc_3N@I_h$-C_{80} (black), **2a** (red), and **2b** (blue).

Table S2. Redox Potentials of $Sc_3N@I_h$-C_{80}, 2a, and 2b[a]

Compound	$^{ox}E_1$	$^{red}E_1$	$^{red}E_2$	$^{red}E_3$
$Sc_3N@I_h$-C_{80}	0.60	–1.27	–1.64	–2.39
2a	0.42	–1.06	–1.41	–2.20
2b	0.41	–1.07	–1.38	–2.20

[a]Values obtained by DPV (V). Versus ferrocene/ferrocenium. Conditions: reference electrode: saturated calomel electrode; working electrode: Pt disc; auxiliary electrode: Pt wire; supporting electrolyte: 0.05 M *n*-Bu_4NPF_6 in 1,2-$C_6H_4Cl_2$. CV: scan rate: 50 mV s^{-1}. DPV: pulse amplitude: 50 mV; pulse width: 50 ms; pulse period: 200 ms.

6. MALDI-TOF HRMS Spectra of Compound 2a, 2b, and 3a

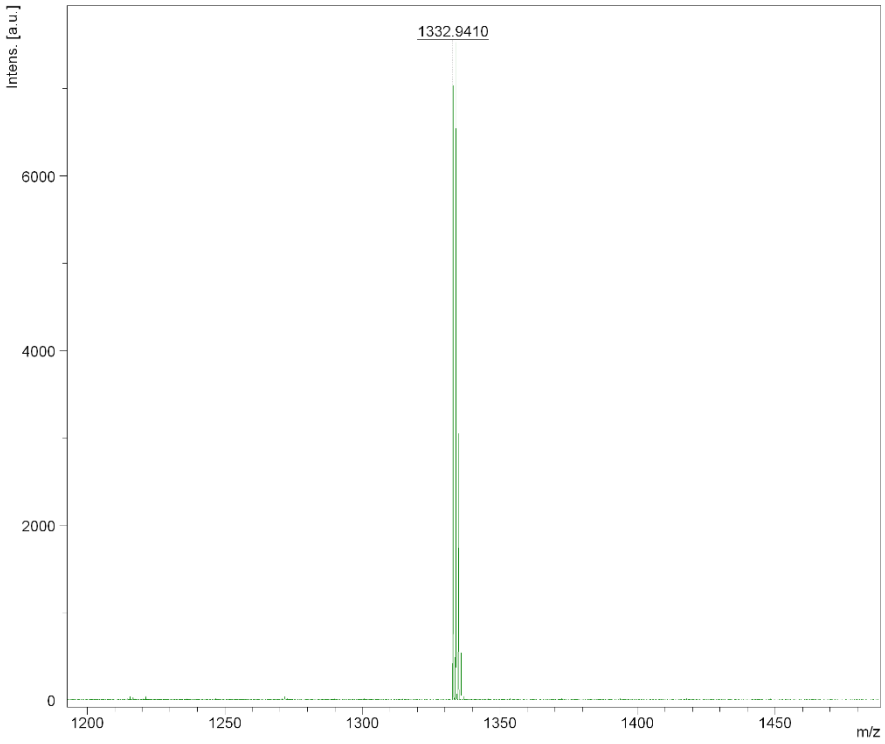


Figure S7. MALDI-TOF HRMS of **2a**.

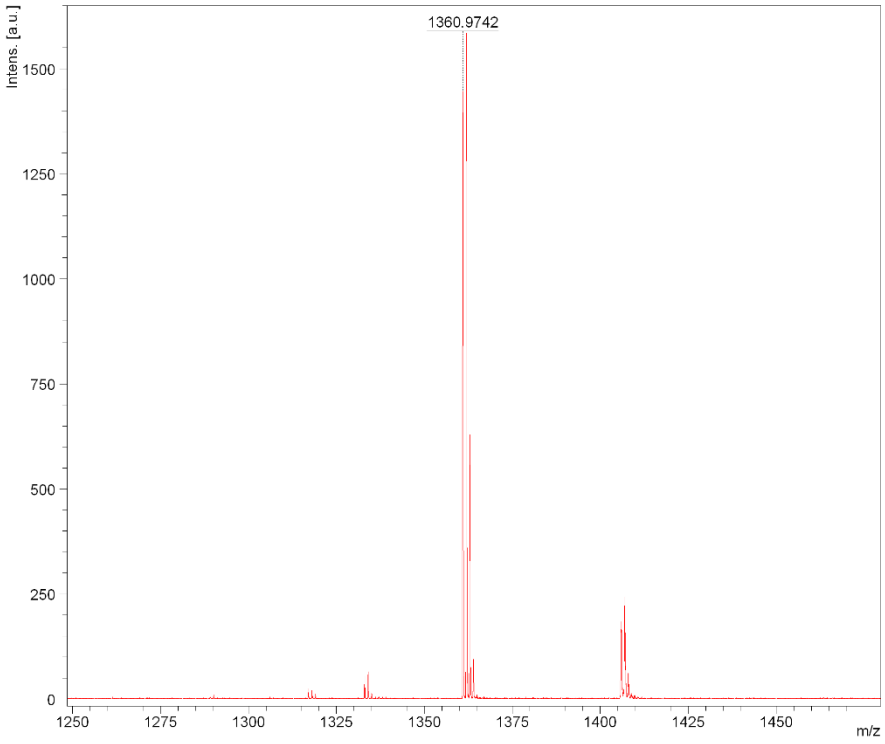


Figure S8. MALDI-TOF HRMS of **2b**.

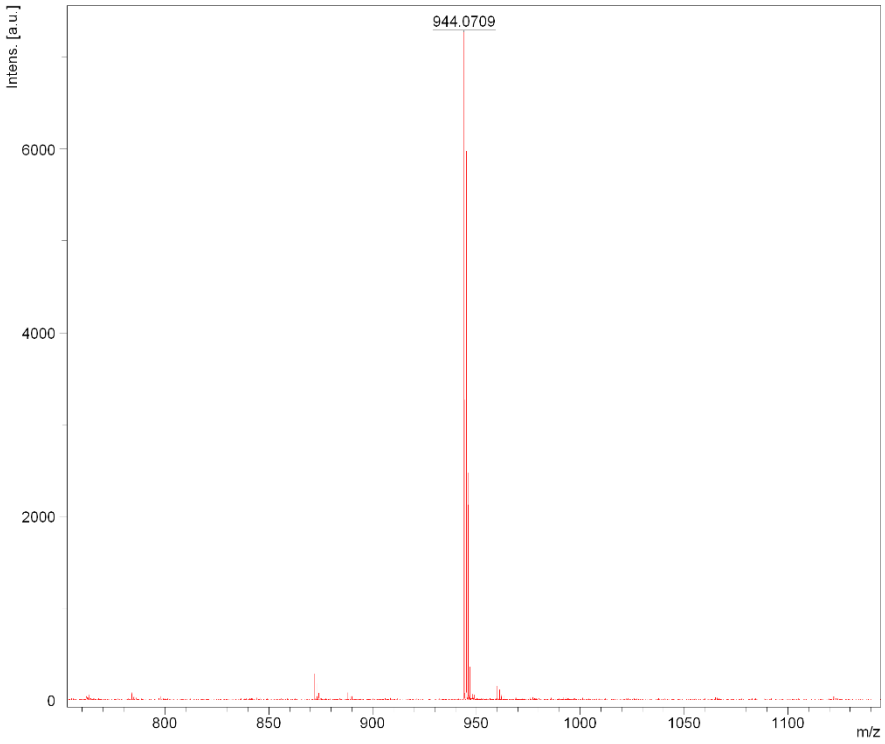


Figure S9. MALDI-TOF HRMS of **3a**.

7. UV-vis-NIR/UV-vis Spectra of Compounds 2a, 2b, and 3a

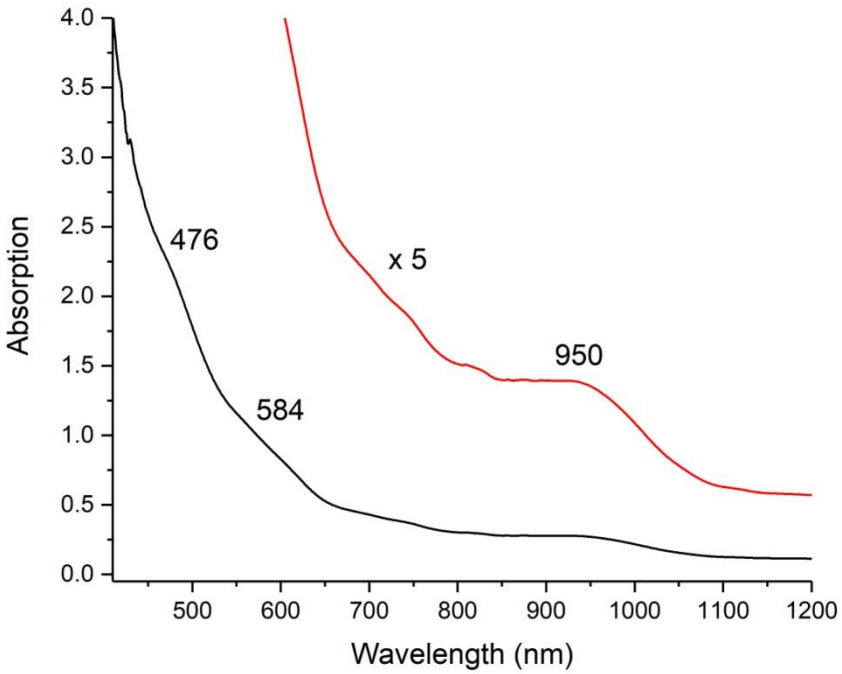


Figure S10. UV-vis-NIR absorption of **2a** in CS_2.

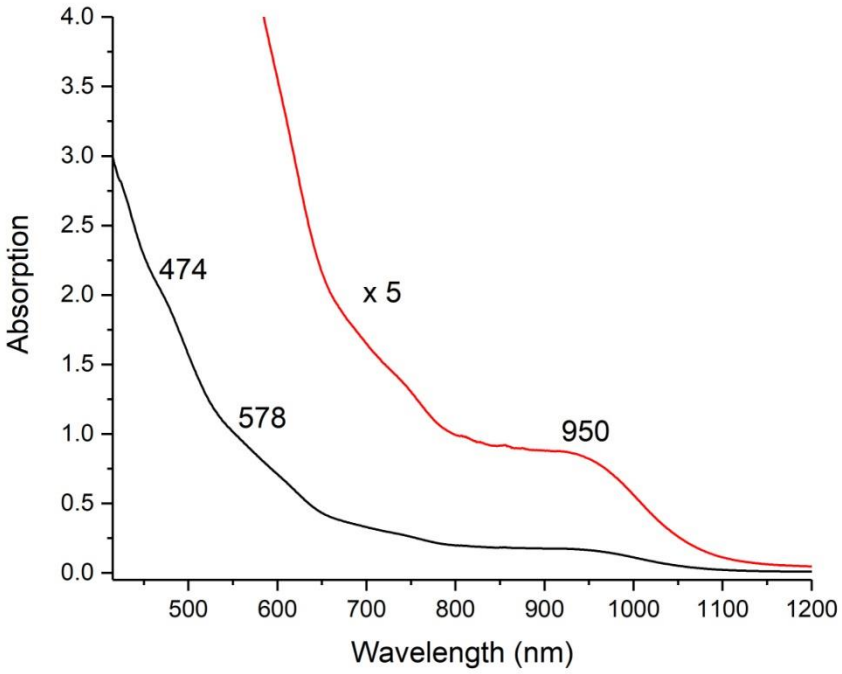


Figure S11. UV-vis-NIR absorption of **2b** in CS_2.

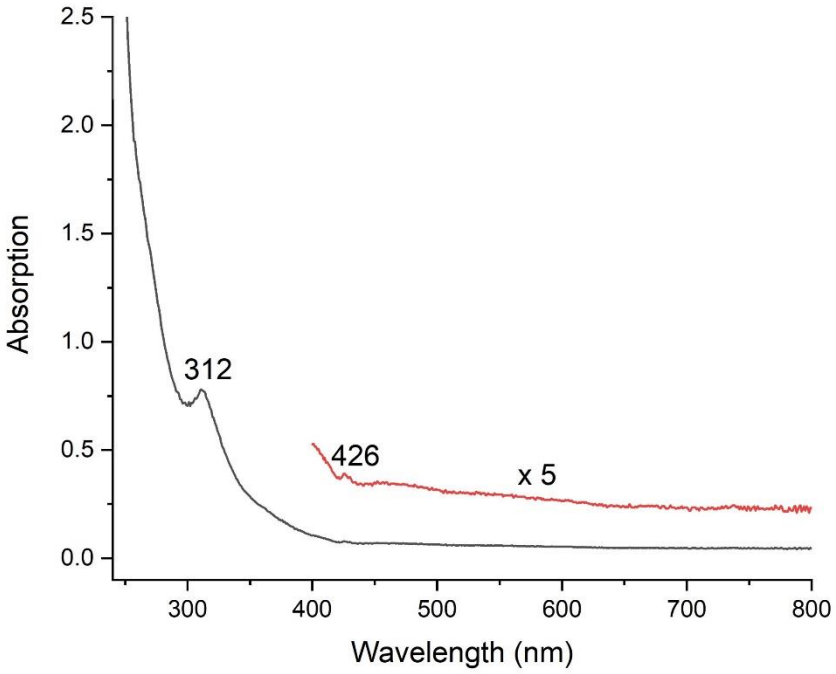


Figure S12. UV-vis absorption of **3a** in $CHCl_3$.

8. NMR Spectra of Compounds 1b, 2a, 2b, 3a, and 4a

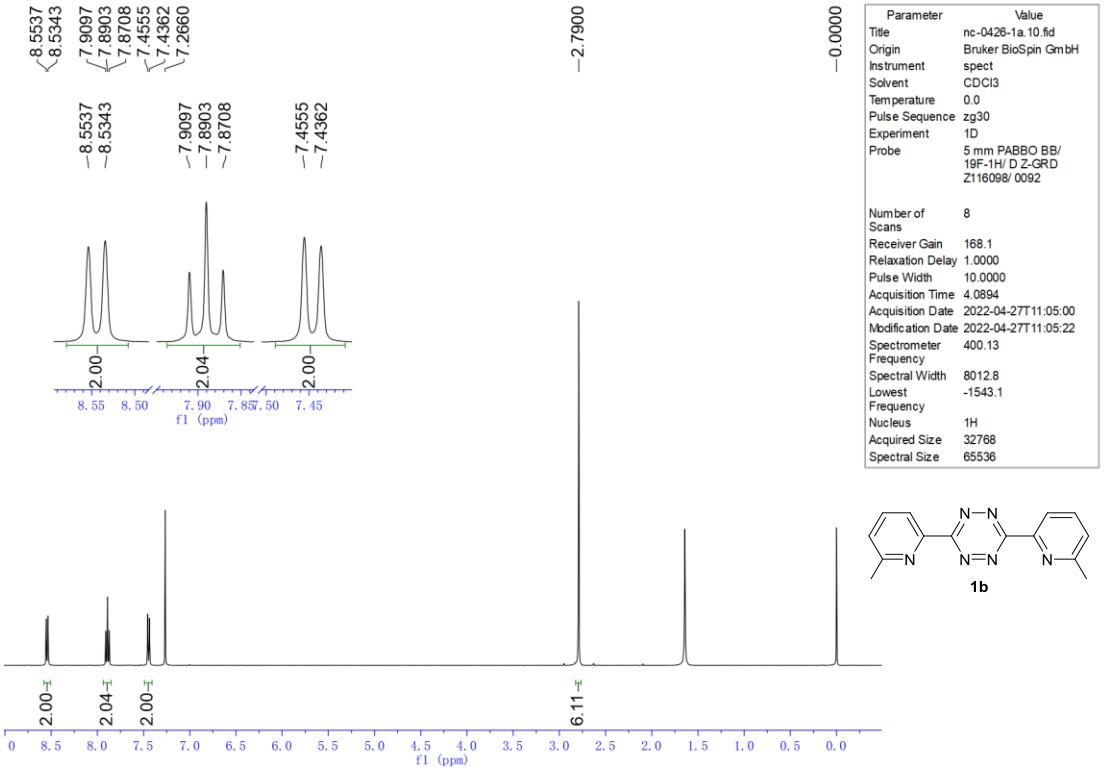


Figure S13. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1b**[1].

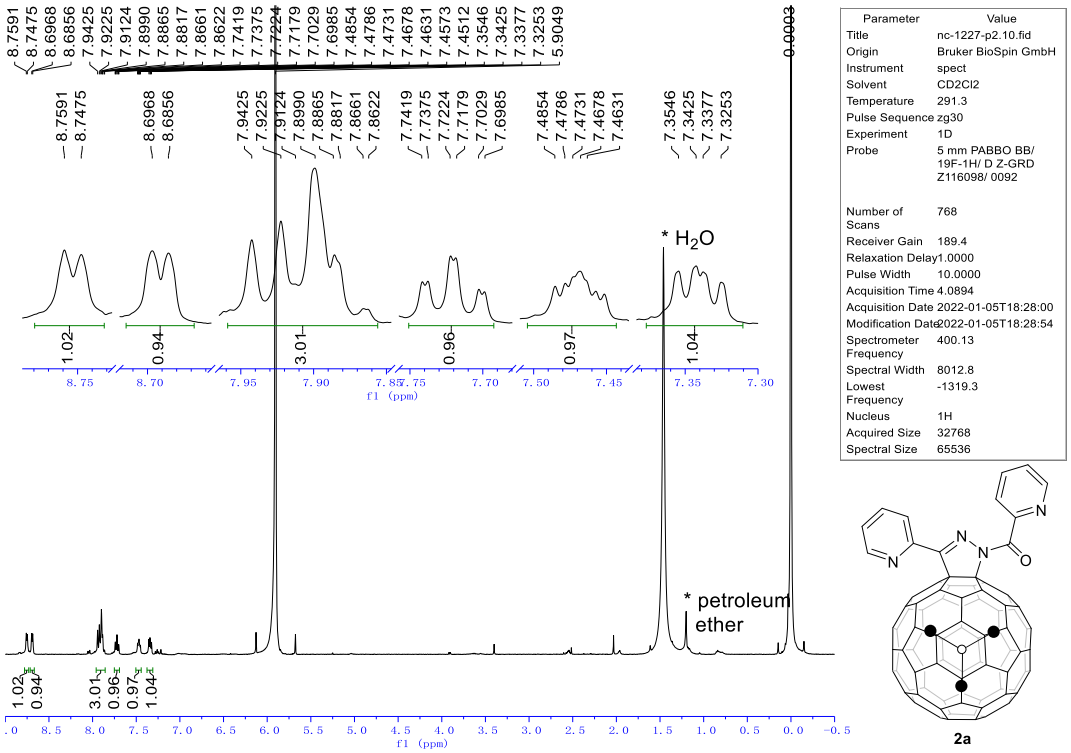
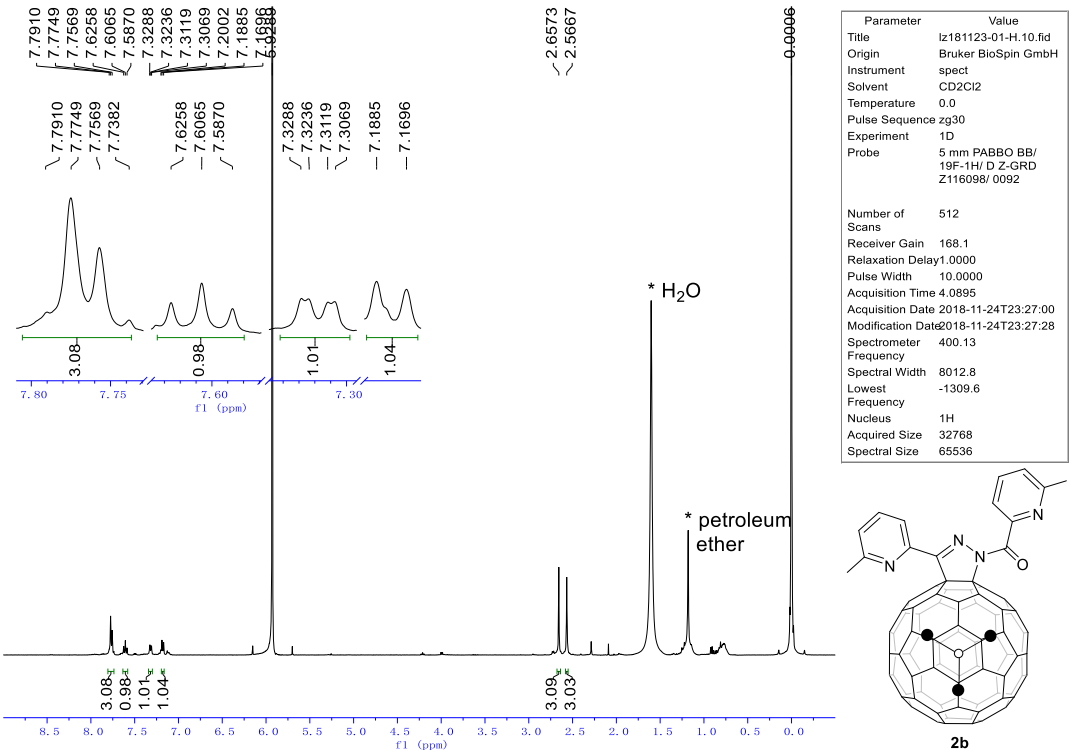


Figure S14. ^{1}H NMR (400 MHz, $C_2D_2Cl_4$) of compound **2a**.



Parameter	Value
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Instrument	spect
Solvent	CD2Cl2
Temperature	0.0
Pulse Sequence	zg30
Experiment	1D
Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z116098/ 0092
Number of Scans	512
Receiver Gain	168.1
Relaxation Delay	1.0000
Pulse Width	10.0000
Acquisition Time	4.0895
Acquisition Date	2018-11-24T23:27:00
Modification Date	2018-11-24T23:27:28
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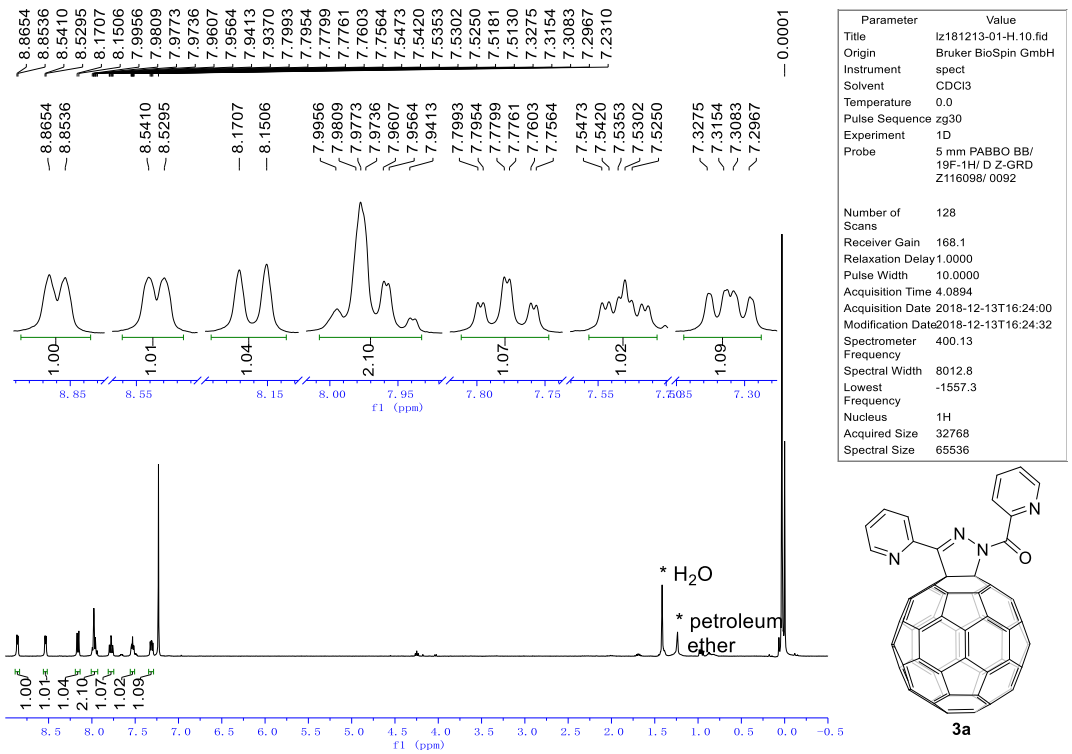
Spectral Width	8012.8
Lowest Frequency	-1309.6
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

Figure S15. ^{1}H NMR (400 MHz, $C_2D_2Cl_4$) of compound **2b**.



Parameter	Value
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Origin	Bruker BioSpin GmbH
Instrument	spect
Solvent	CDCl3
Temperature	0.0
Pulse Sequence	zg30
Experiment	1D
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Receiver Gain	168.1
Relaxation Delay	1.0000
Pulse Width	10.0000
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Spectral Width	8012.8
Lowest Frequency	-1557.3
Nucleus	1H
Acquired Size	32768
Spectral Size	65536

Figure S16. ^{1}H NMR (400 MHz, 1:1 CS_2/$CDCl_3$) of compound **3a**.

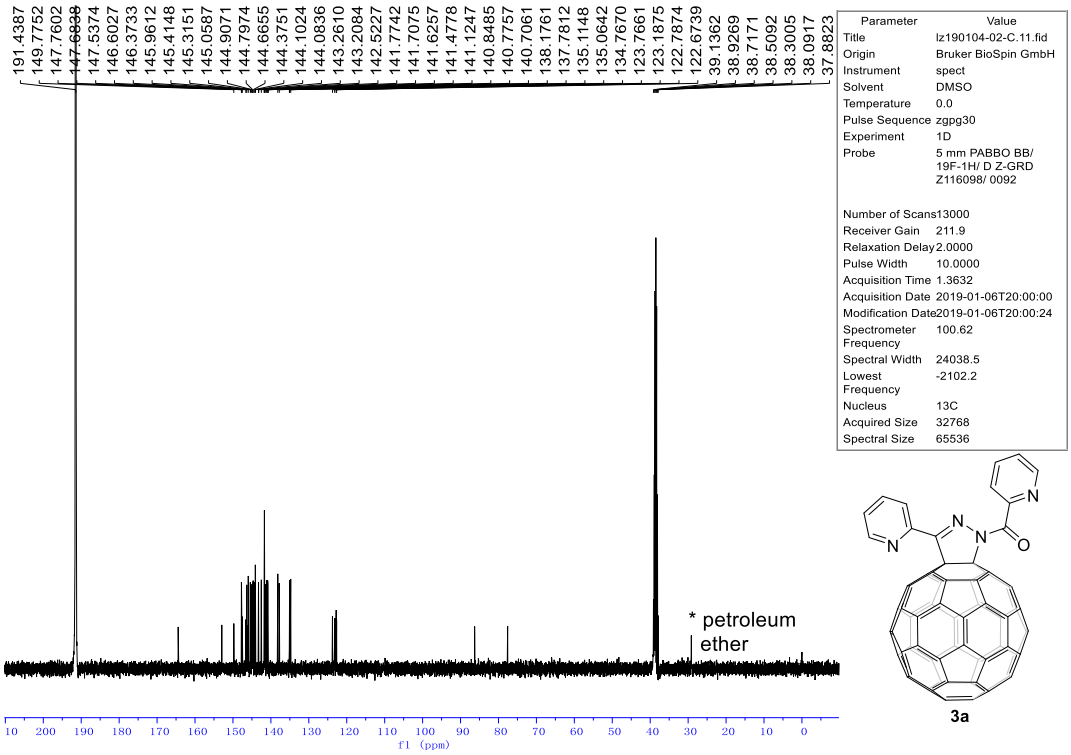

Figure S17. ^{13}C NMR (101 MHz, CS_2/DMSO-d_6) of compound **3a**.

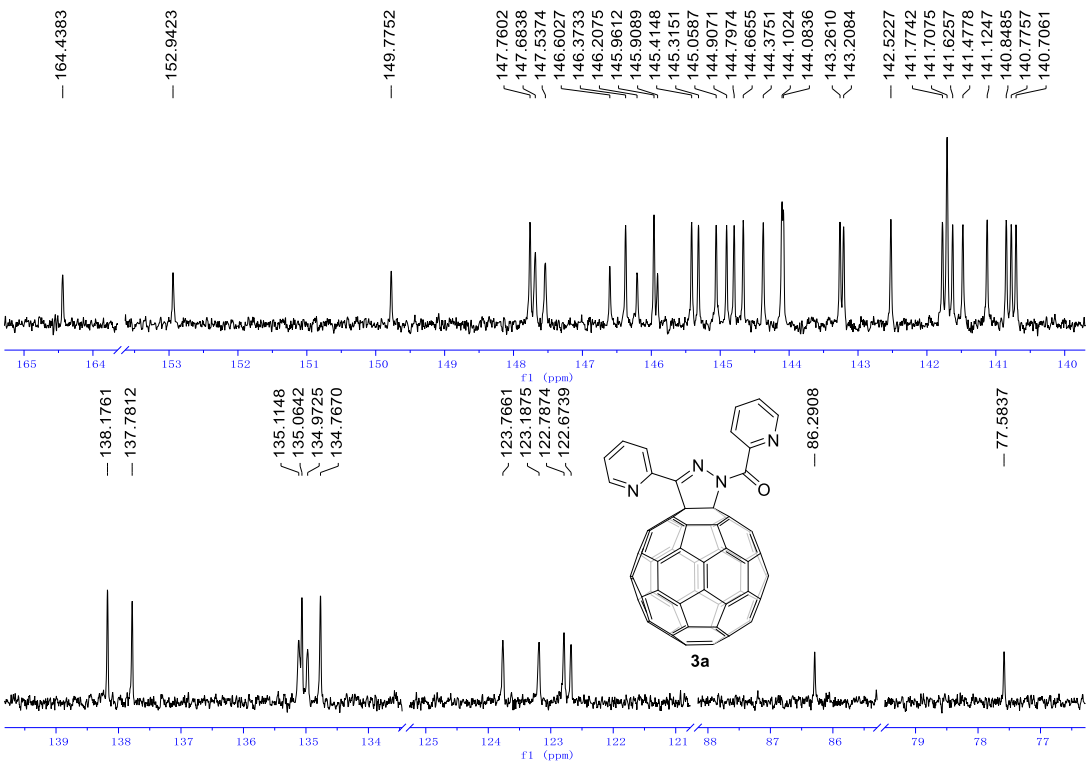

Figure S18. Expanded ^{13}C NMR (101 MHz, CS_2/DMSO-d_6) of compound **3a**.

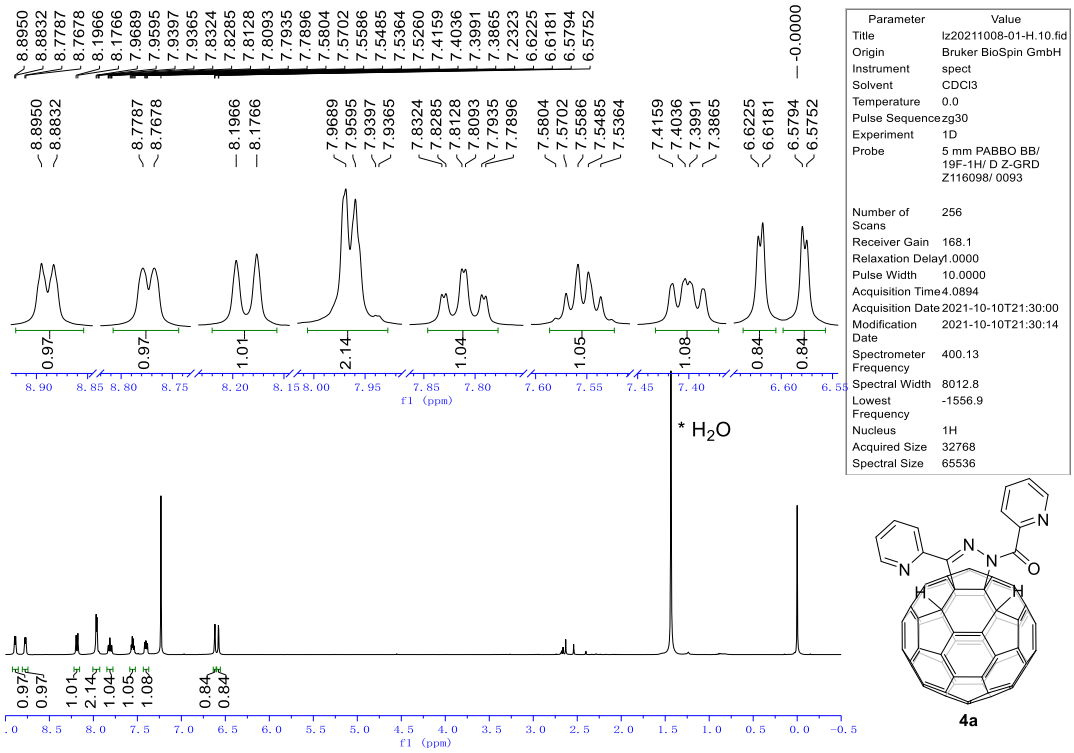

Figure S19. ^{1}H NMR (400 MHz, 1:1 CS_2/$CDCl_3$) of compound **4a**[2].

9. Computational Study on the Key Processes from III to V

To better understand the mechanism of the reaction, we performed the theoretical calculations for the processes from **III** to **V**. The partial natural bond orbital (NBO) charge distribution of the optimized intermediate **III** (Figure S20) was computed at the B3LYP/6-31G*/LANL2DZ(Sc) level. Among the nonfunctionalized I_h-C_{80} carbon atoms, C1 (−0.036), C10 (−0.127), and C12 (−0.024) were the three most negatively charged carbon atoms and were more prone to be protonated. Theoretical calculations on the relative energies of **IV**, **IV'**, and **IV''** arising from the protonation at the most negatively charged carbons in **III** showed that the relative energy of the protonated intermediate **IV** was more stable than those of **IV'** and **IV''** (Figure S21). Thus, the most likely formed intermediate should be **IV** rather than **IV'** and **IV''**. Furthermore, **IV** could undergo an intramolecular cyclization to the neighboring [6,6]-bond or [5,6]-bond of the fullerene cage to attain the ring-fused fullerenyl anion by nucleophilic attack of nitrogen atom at either C12 or C3 position (Figure S22). Calculations showed that C12 (0.035) was a positively charged carbon atom, whereas C3 (−0.074) was negatively charged one. Therefore, the nucleophilic intramolecular cyclization of **IV** preferably took place at C12 and fused at the [6,6]-bond to generate fullerenyl anion **V**.

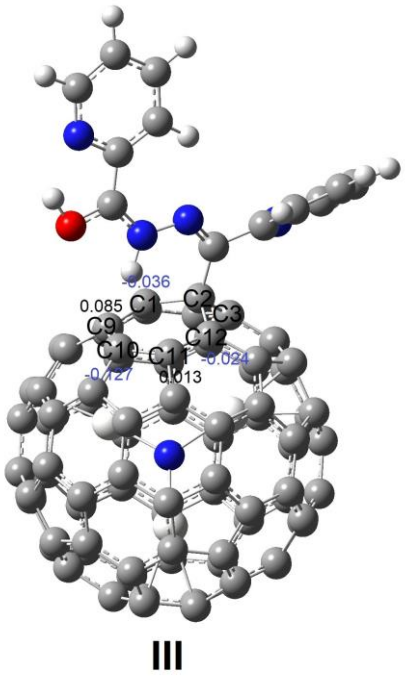

Figure S20. Partial NBO charge distributions for **III**.

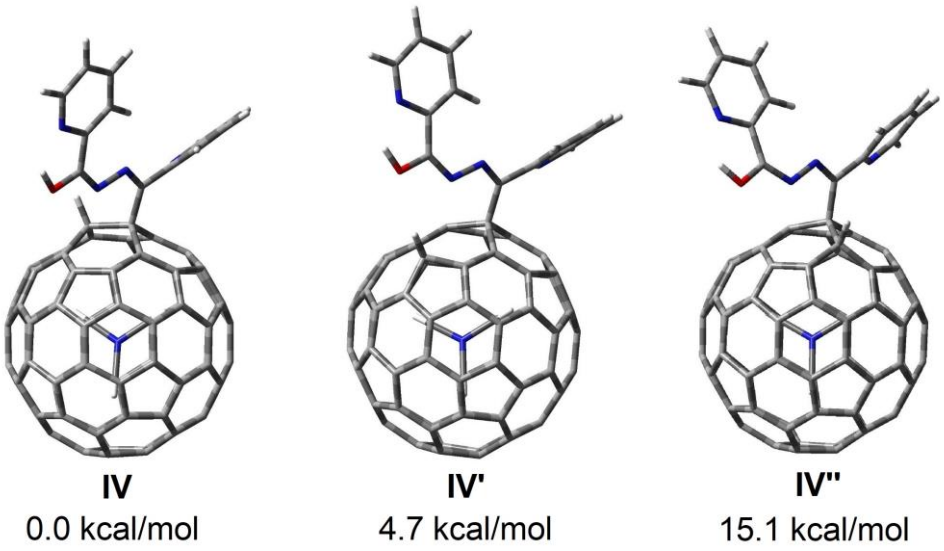

Figure S21. Optimized structures and relative energies of **IV**, **IV'**, and **IV''**.

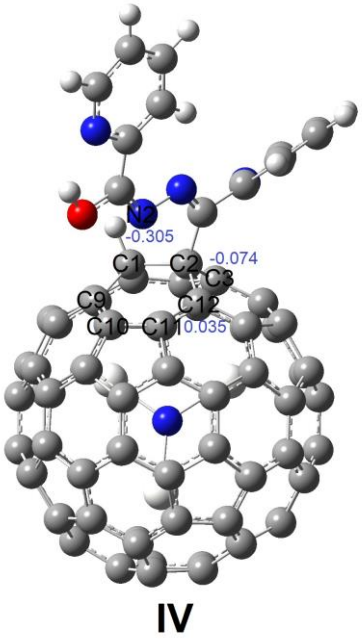

Figure S22. Partial NBO charge distributions for **IV**.

Optimized xyz Coordinates

III

Sc	-0.87826800	-1.31972600	1.46879300
Sc	-2.97614400	-0.46921700	-1.22629000
N	-1.38708500	-0.12763700	-0.05076000
N	5.42044800	0.19094100	-0.17045800
N	5.14712400	-1.15095500	-0.27134200
C	4.46886300	1.03319900	0.08679800
C	2.95999600	0.72781300	0.24223000
C	8.23509700	-0.65223400	0.12911400
H	7.68005900	0.27017600	0.22237600
C	4.94629000	2.45177200	0.07775400
N	4.60036700	3.19887300	1.13672400
C	-5.37164500	0.36129500	-1.05039300
C	5.74031500	2.93507300	-0.97099800
H	5.98719100	2.29012500	-1.80703600
C	-5.42577000	-0.77004300	-0.17082000
C	2.22576400	-1.74410500	0.57855000
C	2.59818000	-0.50241600	1.12179000
C	2.11589700	1.82339900	0.91910100
C	2.39952200	0.54065700	-1.17195600
N	8.21449700	-3.04095200	-0.25992700

C	7.56299000	-1.85643000	-0.13637200
C	6.12149300	-2.05105500	-0.31453300
C	6.18594800	4.25497100	-0.91371600
H	6.79253700	4.66611800	-1.71585200
C	-5.10480100	1.67816000	-0.51492700
C	10.29144600	-1.91531500	0.13147200
H	11.36958800	-1.98175000	0.23236900
C	9.53664900	-3.06443700	-0.12990200
H	10.01387800	-4.03564300	-0.23705900
C	-4.97948200	-1.92703200	-0.90120300
C	-3.78446300	2.09661800	-2.58729800
C	-4.93130400	-0.08785100	-2.35870100
C	-5.28278300	-0.64184600	1.25446800
C	9.62145300	-0.69739100	0.26037200
H	10.17268500	0.21541000	0.46579600
C	5.83479100	5.03453500	0.18705900
C	1.40171900	-2.61130800	1.38290700
C	2.16639500	-1.93804200	-0.84749200
C	0.91116800	-2.24556900	2.68750700
C	1.97147900	-0.03945600	2.32606400
C	-1.93666200	3.85314900	1.16412400
C	1.80653700	1.64779300	-1.85859500
C	5.04564700	4.45702000	1.18586600
C	-2.25227000	0.08172700	4.04772800
C	-4.19100600	-2.88863700	1.21695200
C	-0.34460200	-2.96509100	2.92433600
C	0.36392300	3.49619700	0.94709500
C	1.47966700	2.90465800	0.25185000
C	-4.68137000	-1.73923500	1.93944800
C	-2.29070500	3.61968500	-1.64682400
C	-0.11376500	2.40129900	-2.95374000
C	1.21121300	-2.85825300	-1.43024600
C	-0.64380200	-0.19408200	-4.00018100
C	1.33537800	-1.00437600	-2.81725600
C	1.69759100	1.36780700	2.21591100
C	-3.01212500	-3.35749200	1.88528500
C	-4.33121300	2.55481300	-1.32998700
C	-2.52225900	2.76846700	-2.78423200
C	0.04371500	-0.25922200	3.83050400
C	-3.24503100	3.55588700	0.66887800
C	0.16270800	3.32602100	-1.88084800
C	-3.23747700	-3.64333600	-0.90611900
C	2.19402700	-0.76652500	-1.68715900
C	-0.20528800	1.14866800	3.74955300

C	1.40237000	2.89395300	-1.21312100
C	-5.01466900	1.81379700	0.89593100
C	-4.02448200	0.77990600	-3.09257800
C	-4.68864200	-1.53641800	-2.26879300
C	-4.28374400	-2.98486100	-0.20338500
C	-4.08845500	2.74663000	1.48313800
C	-1.44313000	2.11250400	-3.43463800
C	-2.68507800	-1.26894500	-3.69561500
C	1.11038700	-0.87956100	3.11028600
C	-0.60432800	-3.73307400	1.70813300
C	-2.77342900	-2.50326500	3.03437900
C	-0.94586000	-3.98889200	-1.13010600
C	-3.55860900	-0.17662200	3.52294300
C	0.35290300	-3.67034200	-0.63869600
C	-1.46147900	-2.27041300	3.55977100
C	-1.93034900	-3.95222000	1.17435400
C	0.64521000	0.06247800	-3.44518100
C	-2.93644600	0.15420900	-3.79117200
C	-0.60350700	-2.52989100	-3.11373000
C	-4.24809300	0.90281500	2.90101800
C	-0.04628200	3.06566700	2.25931600
C	-2.84154800	-3.19361700	-2.22381300
C	-2.27924000	2.41099000	3.16502900
C	0.48380100	-3.53577700	0.79067700
C	0.72972600	-2.29722200	-2.66152200
C	-0.81733800	3.98195600	0.26890000
C	-5.10534100	0.66927800	1.77049900
C	0.89793200	1.38275100	-2.94695700
C	-1.26241900	-1.47471000	-3.82150500
C	-1.45963800	3.29208400	2.39197900
C	-1.22623800	-0.93346400	4.03068700
C	-3.61024400	2.18024500	2.71648300
C	-1.62209700	1.35731500	3.87616200
C	-3.81758300	-1.50210700	3.05571100
C	0.59293600	1.96565700	2.89444000
C	-0.96758600	3.85071300	-1.14907800
C	-2.06920200	-4.13786800	-0.23383000
C	-3.51899700	-2.13239200	-2.90402200
C	-3.41112300	3.48658400	-0.75086100
C	-1.66930500	0.81568500	-3.98105200
C	-1.42239600	-3.42128300	-2.35745200
Sc	-0.17314500	1.43854000	-0.55007600
H	6.15665100	6.06782400	0.27292900
H	4.75473500	5.03119300	2.06315800

O	5.71889100	-3.29209400	-0.53511900
H	6.56238300	-3.82242100	-0.53931900
H	4.21185300	-1.51073900	-0.51872300

IV

Sc	-0.70998200	-0.66464000	1.80625500
Sc	-2.93282900	-0.97695500	-0.93757700
N	-1.36594500	-0.11344000	-0.03098900
N	5.48161200	0.14454600	-0.00525300
N	5.09348500	-1.17840100	-0.00344600
C	4.52298700	1.00057100	0.13539500
C	3.02115200	0.64089600	0.26346100
C	8.26134200	-0.67920500	-0.04123600
H	7.72431700	0.25249900	0.05947700
C	4.97202400	2.42403300	0.14113800
N	4.46326800	3.21758900	1.09852100
C	-5.25894500	0.15855100	-1.41070400
C	5.91797900	2.87727000	-0.79125800
H	6.29282300	2.19973200	-1.55016800
C	-5.46038600	-0.67107300	-0.25647200
C	2.10216800	-1.65132400	1.28250200
C	2.75724800	-0.30538800	1.56077700
C	2.10751700	1.84647700	0.52804900
C	2.51959800	0.04072500	-1.06285600
N	8.17502200	-3.07204500	-0.23920400
C	7.54999000	-1.88260800	-0.12150100
C	6.05215800	-2.04745100	-0.07056500
C	6.34468400	4.20124600	-0.72184100
H	7.06798500	4.58388900	-1.43687000
C	-4.97202700	1.56398400	-1.28074900
C	10.29553600	-1.96161000	-0.22326300
H	11.37745500	-2.03666600	-0.26724300
C	9.50590700	-3.11107100	-0.29032800
H	9.95567300	-4.09667300	-0.38654500
C	-5.06295900	-2.01483900	-0.58932800
C	-3.52948700	1.32874900	-3.30436800
C	-4.73622400	-0.66118100	-2.47336200
C	-5.38454200	-0.13081600	1.07634500
C	9.65489300	-0.73098200	-0.09451500
H	10.23191800	0.18734800	-0.03280300
C	5.82345900	5.02605600	0.27527700
C	1.20625200	-2.19725500	2.26344000

C	2.03404000	-2.16926700	-0.00376100
C	0.67763400	-1.47440800	3.41509100
C	1.78862500	0.50258900	2.42521100
C	-1.81488500	4.03695900	-0.09340300
C	1.97012200	0.91582400	-2.06280800
C	4.88911300	4.48322900	1.15940100
C	-2.48618800	1.27995000	3.74356000
C	-4.41695400	-2.32334500	1.77471600
C	-0.67052300	-2.00561300	3.67137800
C	0.47353600	3.55611500	-0.03868500
C	1.58283600	2.73469600	-0.45116700
C	-4.88229900	-0.99592200	2.09310400
C	-2.00581600	2.99519300	-2.72551300
C	0.17180900	1.38819000	-3.47894700
C	1.11317300	-3.21009800	-0.37766800
C	-0.42748000	-1.38741100	-3.75830000
C	1.43777100	-1.86016600	-2.24351900
C	1.54768300	1.77200400	1.83676600
C	-3.31264500	-2.62656500	2.64613100
C	-4.12032900	2.14055300	-2.26869800
C	-2.22236500	1.86039000	-3.59197000
C	-0.19745500	0.80115300	3.80204400
C	-3.10413100	3.64588500	-0.56951000
C	0.44443500	2.58613500	-2.71554200
C	-3.36970200	-3.67280500	0.02801700
C	2.23697100	-1.31779200	-1.17915200
C	-0.38334500	2.12756900	3.26814200
C	1.60160200	2.31067600	-1.84769800
C	-4.96217200	2.10351600	0.03342000
C	-3.77209200	-0.07447900	-3.37985000
C	-4.63142900	-2.03783800	-1.98722400
C	-4.43830800	-2.82015000	0.43784000
C	-4.03498700	3.14012600	0.38867300
C	-1.14174300	1.01058000	-3.94748600
C	-2.53361600	-2.24931800	-3.28019600
C	0.91041700	-0.03292100	3.41075900
C	-0.91179600	-3.06813500	2.71698100
C	-3.09150000	-1.47933900	3.49666800
C	-1.09981900	-4.15090800	0.08319400
C	-3.76772400	0.91759200	3.22522800
C	0.18222700	-3.72938800	0.55406400
C	-1.79134900	-1.13273400	3.98279800
C	-2.21736300	-3.41442100	2.20440800
C	0.83999200	-1.01660800	-3.21138400

C	-2.69833100	-0.91190000	-3.80899500
C	-0.55333100	-3.34720800	-2.21551600
C	-4.36270500	1.79115000	2.26462400
C	-0.04083300	3.53305000	1.30834000
C	-2.87494600	-3.65098800	-1.33234000
C	-2.34333700	3.24744100	2.21441600
C	0.24589300	-3.19770900	1.87800200
C	0.75358800	-3.02634100	-1.75535700
C	-0.63610000	3.86503800	-0.90959800
C	-5.16507900	1.26762600	1.19565200
C	1.11767200	0.37858300	-3.09249900
C	-1.11639900	-2.53162700	-3.24913500
C	-1.44200000	3.84200500	1.27520400
C	-1.51096200	0.27273600	4.09272700
C	-3.65742600	2.94069400	1.76321800
C	-1.78719500	2.42684100	3.24693200
C	-4.07216300	-0.47605200	3.15390800
C	0.48236800	2.62838600	2.26428600
C	-0.70320900	3.34221100	-2.24601400
C	-2.27540200	-3.99086100	0.90051800
C	-3.46091100	-2.82525200	-2.34804900
C	-3.18715600	3.16824800	-1.91358900
C	-1.39861500	-0.38363000	-4.11207600
C	-1.46053400	-3.94601100	-1.28401400
Sc	-0.19849800	1.28180900	-0.92679200
H	6.12608100	6.06471900	0.36620200
H	4.46109000	5.09162700	1.95397800
O	5.66662700	-3.32590400	-0.09230200
H	6.50344700	-3.84828700	-0.16423000
H	3.71850500	-0.46005800	2.06082000

E = -4000.248649 a.u.

IV'

Sc	-0.86771300	-1.31852000	1.47317400
Sc	-3.05620200	-0.47625900	-1.10343300
N	-1.39800600	-0.11673800	-0.04521900
N	5.46243600	0.20818500	-0.49707200
N	5.10755600	-1.09850600	-0.72655800
C	4.51305400	1.03433400	-0.21486000
C	2.99578400	0.68845500	-0.09328800
C	8.12018400	-0.67706900	0.24680600

H	7.57217000	0.25372500	0.27043900
C	4.98690200	2.44536900	-0.06295500
N	4.55203600	3.13553900	1.00293400
C	-5.42598600	0.31935300	-0.83847000
C	5.89347200	2.98317800	-0.99068400
H	6.21639600	2.38584500	-1.83571600
C	-5.42401800	-0.72465000	0.14676300
C	2.27357900	-1.72258600	0.52176000
C	2.64503600	-0.45046200	0.90044100
C	2.16143100	1.83413100	0.51996900
C	2.37478200	0.36144900	-1.46264600
N	8.12311000	-3.03583100	-0.21768700
C	7.48106000	-1.85027300	-0.17157700
C	6.04846300	-1.97768300	-0.60978100
C	6.35381500	4.28358400	-0.79997900
H	7.04774200	4.72982800	-1.50722300
C	-5.10590700	1.67311600	-0.43986600
C	10.12435400	-1.97977300	0.56379900
H	11.16763000	-2.07459800	0.84780100
C	9.40535000	-3.09891800	0.13914100
H	9.87321400	-4.07922500	0.08420600
C	-5.02609300	-1.94582400	-0.49759200
C	-3.91439800	1.87985300	-2.61860500
C	-5.07709800	-0.25331500	-2.12861900
C	-5.19050400	-0.46966700	1.54317500
C	9.46429000	-0.75367700	0.61434600
H	9.98623600	0.14087300	0.94187400
C	5.90624000	5.00151900	0.30940700
C	1.46915500	-2.49324400	1.43305100
C	2.30378600	-2.16094200	-0.93295900
C	1.04909000	-2.00176100	2.71817200
C	2.11844900	0.12981500	2.11565800
C	-1.82360900	3.94887600	0.83527400
C	1.69677700	1.41277200	-2.17927500
C	5.00924600	4.37925000	1.17926800
C	-1.98835400	0.46672800	4.07175900
C	-4.11348800	-2.71779200	1.64179200
C	-0.17328600	-2.69771700	3.11450600
C	0.46333400	3.56038500	0.51318900
C	1.52786500	2.88505700	-0.19085900
C	-4.55234300	-1.50632500	2.28600800
C	-2.34938700	3.45911000	-1.91165600
C	-0.27286200	2.09956500	-3.22883200
C	1.10310200	-3.03828600	-1.32693100

C	-0.88763800	-0.56900300	-3.99735400
C	1.16294300	-1.28081800	-2.85234900
C	1.82336500	1.50754900	1.87411200
C	-2.89428700	-3.13750200	2.27840100
C	-4.37794300	2.46144400	-1.37712900
C	-2.66040100	2.51302400	-2.95289300
C	0.28997600	0.08064800	3.75043600
C	-3.16163600	3.62522500	0.45076400
C	0.08163000	3.11263800	-2.26719400
C	-3.30978500	-3.68513400	-0.45295400
C	2.11395700	-0.95249800	-1.84392400
C	0.04542600	1.47416600	3.55628700
C	1.34982100	2.72024100	-1.63495200
C	-4.92470900	1.93586800	0.94588200
C	-4.20911200	0.53028100	-2.99608800
C	-4.82182600	-1.68667400	-1.91021500
C	-4.30217600	-2.94884600	0.24969300
C	-3.95874600	2.90630400	1.38766900
C	-1.62912000	1.78784800	-3.60341300
C	-2.91490200	-1.58249200	-3.47496900
C	1.29810000	-0.61488200	3.01668800
C	-0.49999200	-3.59476300	2.00080000
C	-2.58875300	-2.19228300	3.33442800
C	-1.03718100	-4.07286600	-0.78365600
C	-3.32591400	0.17739900	3.65500200
C	0.30131400	-3.73787700	-0.41183400
C	-1.24235200	-1.92586700	3.74505200
C	-1.86541200	-3.81907100	1.56516000
C	0.43434500	-0.27899700	-3.54026600
C	-3.16427600	-0.17261900	-3.69135800
C	-0.81297300	-2.80863000	-2.89966000
C	-4.04593800	1.20410900	2.97747500
C	0.12194300	3.24075800	1.87864600
C	-3.00073500	-3.36909900	-1.82767000
C	-2.05242700	2.70081500	2.98194800
C	0.52780900	-3.48268800	1.00135800
C	0.54616100	-2.54958500	-2.52966800
C	-0.75728900	3.98859400	-0.13497800
C	-4.97428900	0.87979900	1.92836400
C	0.72439300	1.06840300	-3.17967800
C	-1.50218600	-1.81559900	-3.66315400
C	-1.27655200	3.49706400	2.07859800
C	-0.97085700	-0.55752100	4.07594400
C	-3.41125700	2.45001600	2.63803700

C	-1.36235600	1.71388700	3.75081300
C	-3.62083600	-1.18050800	3.32517000
C	0.78805300	2.19402800	2.57578300
C	-0.99666200	3.72727000	-1.52329700
C	-2.10107200	-4.12252200	0.18892800
C	-3.69990300	-2.35683500	-2.55386700
C	-3.41697800	3.43003600	-0.94377500
C	-1.90175500	0.44990200	-4.01270500
C	-1.58625500	-3.61422500	-2.02044900
Sc	-0.23908100	1.45355600	-0.64757400
H	6.23771600	6.01816300	0.49738900
H	4.63900300	4.90136800	2.05963300
O	5.70088200	-3.23673600	-0.91160500
H	6.52096400	-3.77235800	-0.77265200
H	3.26075000	-2.65566400	-1.15423900

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IV''

Sc	-0.55769300	-1.05918600	1.54682100
Sc	-3.07648500	-0.72622100	-0.87885100
N	-1.37528800	-0.09186100	-0.00844900
N	5.47290800	0.29356100	-0.71647500
N	5.07249600	-0.95961200	-1.09343500
C	4.54196300	1.13272400	-0.40143600
C	3.02318700	0.77686900	-0.36808000
C	7.85422100	-0.89095800	0.43744800
H	7.37824400	0.07903500	0.44986300
C	5.05054600	2.51370400	-0.13620800
N	4.50906600	3.20908200	0.87551400
C	-5.43300100	0.21011900	-0.59801900
C	6.09794600	3.02681800	-0.92180700
H	6.50490400	2.42985100	-1.72945800
C	-5.37527600	-0.79380800	0.42373800
C	2.35328200	-1.63808000	0.35515600
C	2.73607700	-0.33257500	0.67534000
C	2.17250500	1.91818400	0.22321000
C	2.58819000	0.40434100	-1.88820400
N	7.78752100	-3.19557000	-0.24306100
C	7.22950000	-1.96846900	-0.20186500
C	5.90222100	-1.93334700	-0.90732200
C	6.58555700	4.29984400	-0.64107500

H	7.38739300	4.72403900	-1.23934300
C	-5.12992500	1.58793000	-0.28529300
C	9.66976700	-2.37731100	0.99032100
H	10.63123200	-2.58196900	1.45052400
C	8.97106400	-3.39401200	0.33592100
H	9.37439100	-4.40228500	0.27468600
C	-5.01404800	-2.04316200	-0.19362000
C	-4.08404800	1.72879900	-2.54027700
C	-5.13896600	-0.41315300	-1.87249100
C	-5.06394600	-0.47131500	1.79303900
C	9.09619500	-1.10831000	1.03567300
H	9.60526400	-0.29000400	1.53685400
C	6.02424000	5.02139500	0.41342500
C	1.63357600	-2.38772700	1.37000900
C	2.05637000	-1.97497400	-1.01870400
C	1.30227700	-1.86636500	2.67519600
C	2.23151300	0.26748100	1.86940100
C	-1.83795500	3.97975400	0.69438500
C	1.53419900	1.36968100	-2.41516900
C	4.99113700	4.42763800	1.13907500
C	-1.73736100	0.62980500	4.07875100
C	-3.94918600	-2.70194500	1.92674100
C	0.07927300	-2.53580600	3.14310100
C	0.43476700	3.61606700	0.24763900
C	1.46076600	2.91543000	-0.48745500
C	-4.36809500	-1.46404800	2.54188800
C	-2.50199000	3.34998000	-1.98279000
C	-0.49221000	1.97125700	-3.36841200
C	1.08141000	-3.00650400	-1.34571200
C	-1.08897400	-0.74013300	-4.00520700
C	1.04651000	-1.38156600	-2.98393000
C	1.89086900	1.63875800	1.58865000
C	-2.68926900	-3.07252900	2.50241700
C	-4.48705700	2.35335900	-1.29936700
C	-2.86259400	2.34956000	-2.96541500
C	0.52268600	0.26259200	3.62783300
C	-3.18757200	3.61585300	0.40740200
C	-0.09424500	3.05191100	-2.49476600
C	-3.23947300	-3.72738800	-0.17654100
C	2.04633100	-1.00822000	-2.03227000
C	0.23675600	1.64679800	3.38609500
C	1.20219000	2.67534200	-1.91245500
C	-4.87775200	1.91334900	1.07630100
C	-4.34133500	0.34749000	-2.81858500

C	-4.88798900	-1.83854800	-1.63071200
C	-4.21028100	-2.98694000	0.55337900
C	-3.91357600	2.92086200	1.42132000
C	-1.86087000	1.61803100	-3.65332400
C	-3.06429500	-1.76400600	-3.31130500
C	1.51020700	-0.45431500	2.87886300
C	-0.31377800	-3.44748300	2.07769000
C	-2.32899600	-2.06862800	3.48596100
C	-0.99036500	-4.09807100	-0.62866500
C	-3.09291500	0.29975800	3.75604000
C	0.34633200	-3.68963800	-0.35095600
C	-0.96822900	-1.76176300	3.80277500
C	-1.69050000	-3.75263500	1.75257800
C	0.24987800	-0.42028000	-3.65750100
C	-3.34284800	-0.36121400	-3.55836500
C	-0.90706500	-2.92655300	-2.82543600
C	-3.87085000	1.28400100	3.08220300
C	0.17939600	3.35192900	1.64414400
C	-3.01346300	-3.46244400	-1.58457400
C	-1.91249900	2.81711100	2.89938200
C	0.65541600	-3.37349900	1.02170500
C	0.46310500	-2.63998500	-2.58026700
C	-0.82769000	3.99864400	-0.34388100
C	-4.84928100	0.89801900	2.10297200
C	0.51962100	0.95790200	-3.32304500
C	-1.66961000	-1.98723100	-3.58936900
C	-1.20990300	3.59202900	1.91919900
C	-0.70222700	-0.37529300	4.07022000
C	-3.28329600	2.52752100	2.65342000
C	-1.15645900	1.87144500	3.66110900
C	-3.37972300	-1.07616600	3.50276800
C	0.89975900	2.34099900	2.33434900
C	-1.13988700	3.68765400	-1.70792900
C	-1.99271700	-4.12580100	0.40942100
C	-3.79098800	-2.51060000	-2.32130000
C	-3.51751700	3.35068300	-0.95891200
C	-2.12500400	0.26429500	-3.99775500
C	-1.61758000	-3.69727300	-1.85226300
Sc	-0.41754300	1.50382300	-0.83007600
H	6.37175000	6.01833400	0.66653900
H	4.52688500	4.95188100	1.97244100
O	5.52557900	-3.12134000	-1.39114900
H	6.25830800	-3.74065300	-1.15529100
H	3.49945700	0.50471700	-2.48975500

E = -4000.224632 a.u.

10. References

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