Electronic Supplementary Information

Naphthobox: A Selective Molecular Box for Planar Aromatic Cations

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1. Experimental Section

1.1 General Method. All the reagents and guest molecules involved in this research were commercially available and used without further purification unless otherwise noted. Solvents were either employed as purchased or dried prior to use by standard laboratory procedures. ^1H, ^{13}C NMR spectra were recorded on a Bruker Avance-400 or 500 NMR spectrometer. Chemical shifts are reported in ppm with residual solvents or TMS (tetramethylsilane) as the internal standards. The following abbreviations were used for signal multiplicities: s, singlet; d, doublet; dd, doublet of doublet; m, multiplet. Electrosprayionization high-resolution mass spectrometry (ESI-HRMS) experiments were conducted on an applied Q EXACTIVE mass spectrometry system. UV−vis absorption spectra were obtained on a Hitachi U-2600 UV−vis spectrophotometer. Fluorescence spectra (FL) were obtained on a Shimadzu RF-5301pc spectrometer.

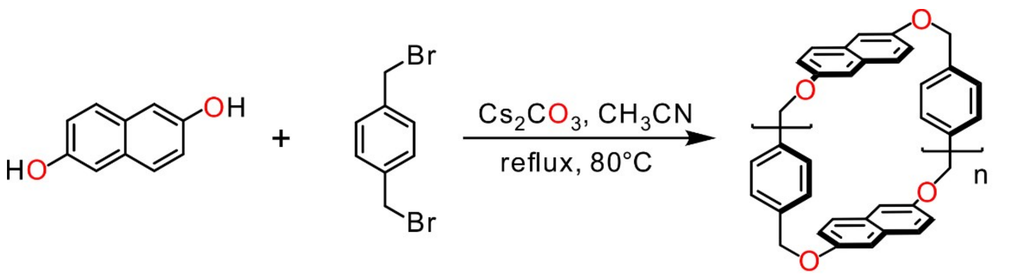
1.2 ^1H NMR Titrations

For ^1H NMR titrations, a 2×10^{-4} M solution of host was prepared in CD_2Cl_2. This solution (0.5 mL) was placed in a NMR tube. The sample was then titrated with a solution of guest. NMR titrations were performed by adding guest to the solution of host with a fixed concentration. Nonlinear curve-fitting method was then used to obtain the binding constants through the following equation:

$$\delta=\delta_0+\Delta\delta\ (0.5/[H]_0)\ ([G]+[H]_0+1/K-(([G]+[H]_0+1/K)^2-4[H]_0[G])^{0.5})$$

All of these ^1H NMR titrations were repeated three times.

1.3 Synthetic Procedures and Characterization Data of M1 and M2



M1, n=1, yields 14%
M2, n=2, yields 3%

Compound **M1** and **M2**. To a 500 ml two-necked flask, Cs_2CO_3 (8 g, 25 mmol) and CH_3CN (500 mL) were added. The solution of 2,6-dihydroxynaphthalene (0.5 g, 3.1 mmol, in 60 mL CH_3CN) and 1,4-bis(bromomethyl)-benzene (0.8 g, 3.1 mmol, in 60 mL CH_3CN) were added dropwise using two separate syringes to the flask via a double channel syringe pump during 8 h at 80°C under Ar atmosphere. Then the resulting mixture was stirred for another 24 h. The reaction mixture was filtered and the filtrate was concentrated with rotary evaporator. The solid obtained was washed with water then exacted with dichloromethane (100 mL × 3). The organic phase was collected and then dried over anhydrous $MgSO_4$. The solvent was removed under reduced pressure. The remaining residue was purified by column chromatography (SiO_2, petroleum ether : dichloromethane = 1 : 1) to afford compound **M1** (115 mg, 14%) and **M2** (37 mg, 3%).

M1. White solid (115 mg); yield, 14%; ^{1}H NMR for **M1** (400 MHz, CD_2Cl_2, 298 K) δ[ppm] = 7.39 (d, *J* = 8.6 Hz, 4H), 7.28 (s, 8H), 7.00 (dd, *J* = 8.6, 2.5 Hz, 4H), 6.98 (d, J = 2.5 Hz, 4H), 5.27 (s, 8H). ^{13}C NMR (126 MHz, CD_2Cl_2, 298 K) δ [ppm] = 153.93, 137.46, 129.89, 128.17, 127.45, 118.82, 110.28, 69.05. ESI-TOF-HRMS: m/z calcd for $[M+K]^+$ $C_{36}H_{28}KO_4^+$, 563.1619; found 563.1617 (error = -0.36 ppm).

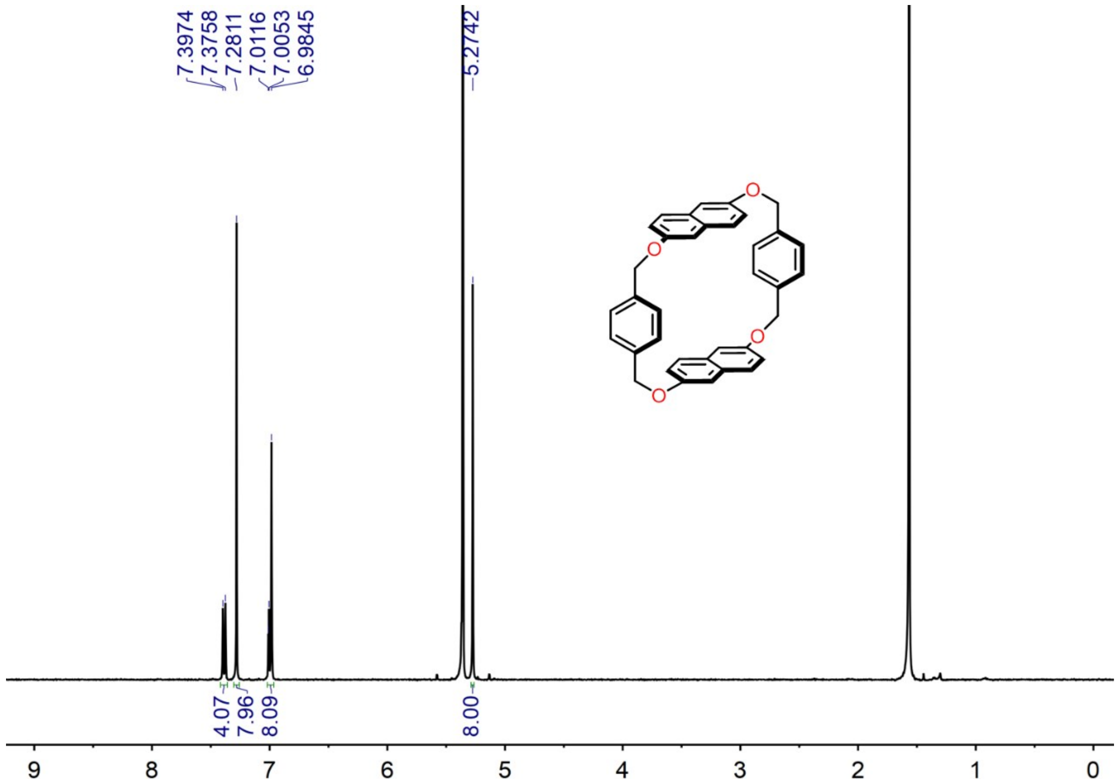


Figure S1. ^{1}H NMR spectrum (400 MHz, CD_2Cl_2, 298 K) of compound **M1**.

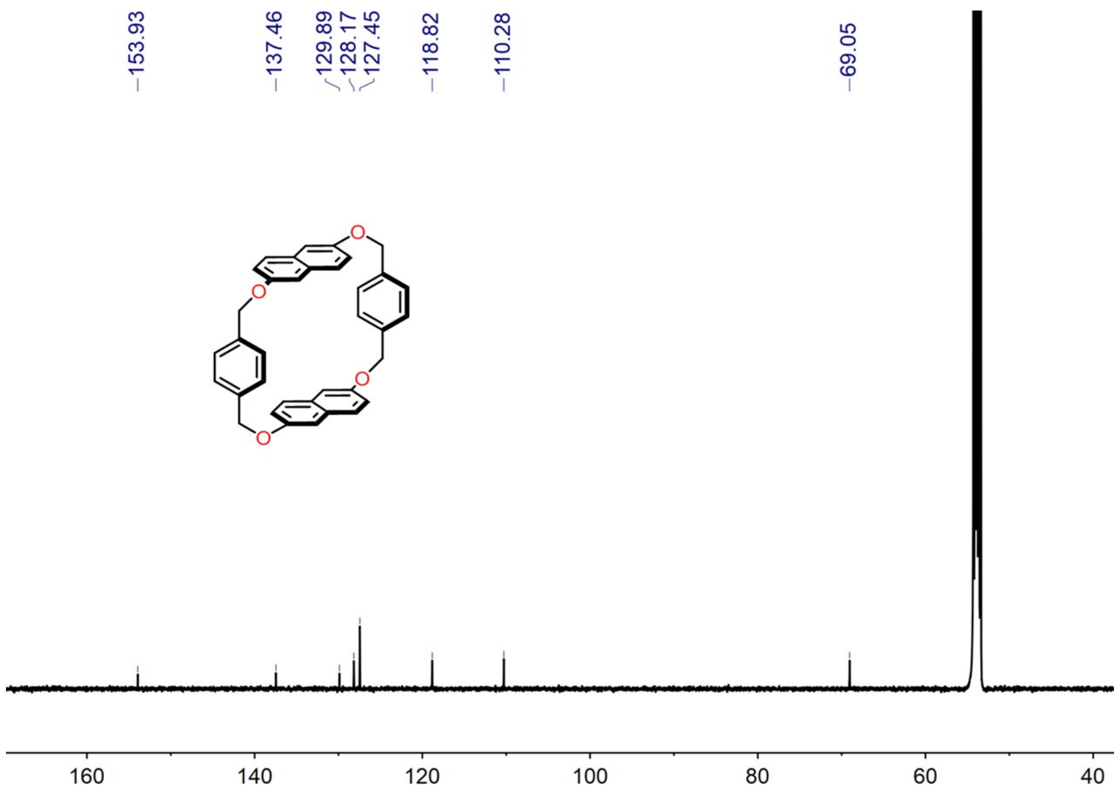


Figure S2. ^{13}C NMR spectrum (126 MHz, CD_2Cl_2, 298 K) of compound **M1**.

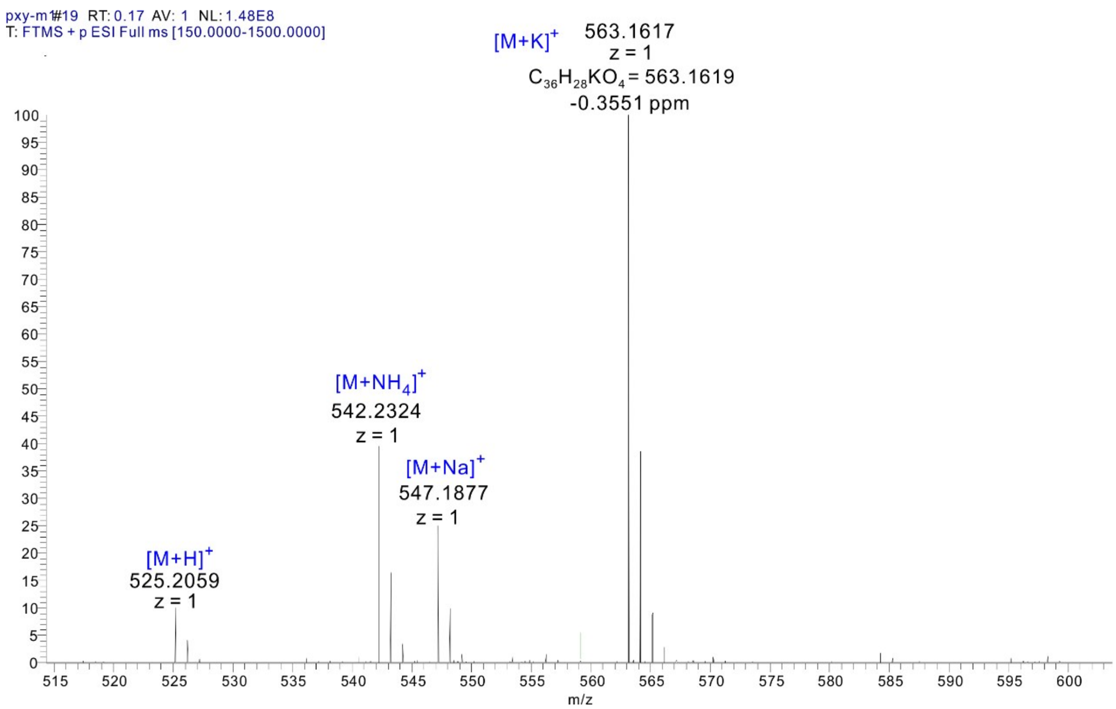


Figure S3. ESI mass spectrum of compound **M1**.

M2. White solid (37 mg); yield, 3%; ^{1}H NMR for **M2** (500 MHz, CD_2Cl_2, 298 K) δ[ppm] = 7.46 (d, J = 8.6 Hz, 6H), 7.35 (s, 12H), 7.07 (d, J = 8.6 Hz, 6H), 6.99 (s, 6H), 5.19 (s, 12H). ^{13}C NMR (101MHz, CD_2Cl_2, 298 K) δ [ppm] = 154.52, 136.80, 129.59, 128.02, 127.28, 119.25, 108.29, 69.32. ESI-TOF-HRMS: m/z calcd for $[M+K]^+$ $C_{54}H_{42}KO_6^+$, 825.2613; found 825.2607 (error = -0.73 ppm).

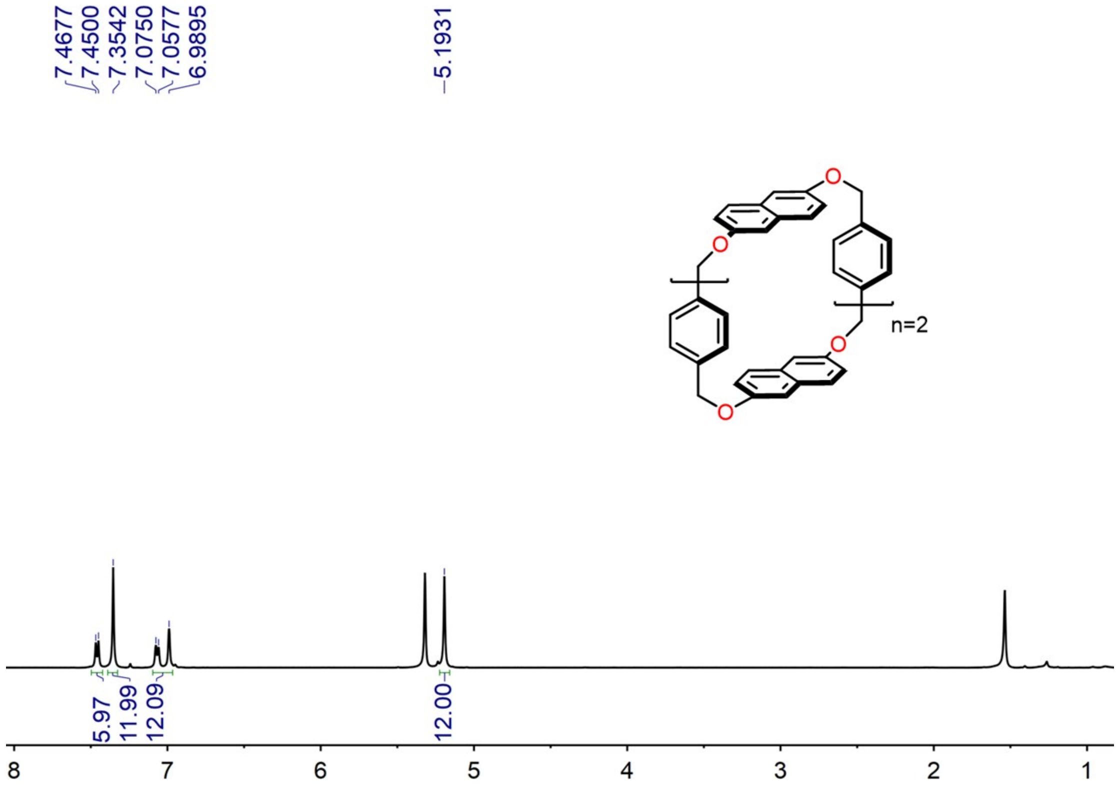


Figure S4. ^{1}H NMR spectrum (500 MHz, CD_2Cl_2, 298 K) of compound **M2**.

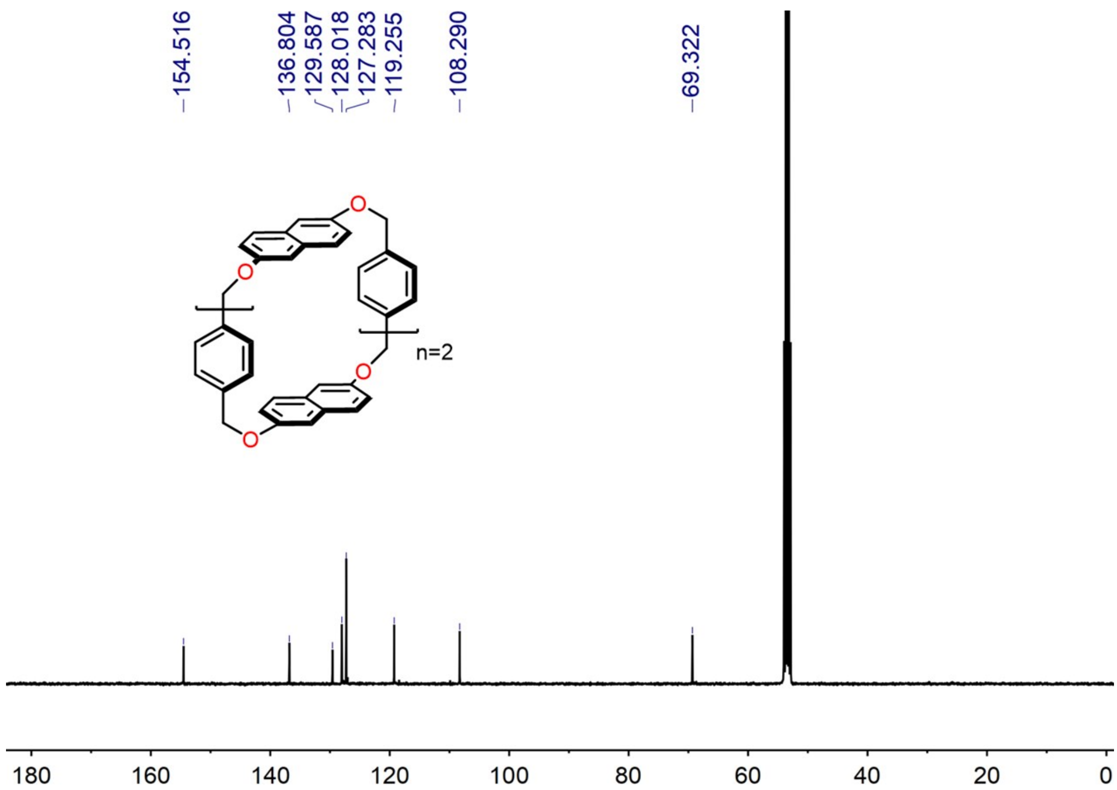


Figure S5. ^{13}C NMR spectrum (101 MHz, CD_2Cl_2, 298 K) of compound **M1**.

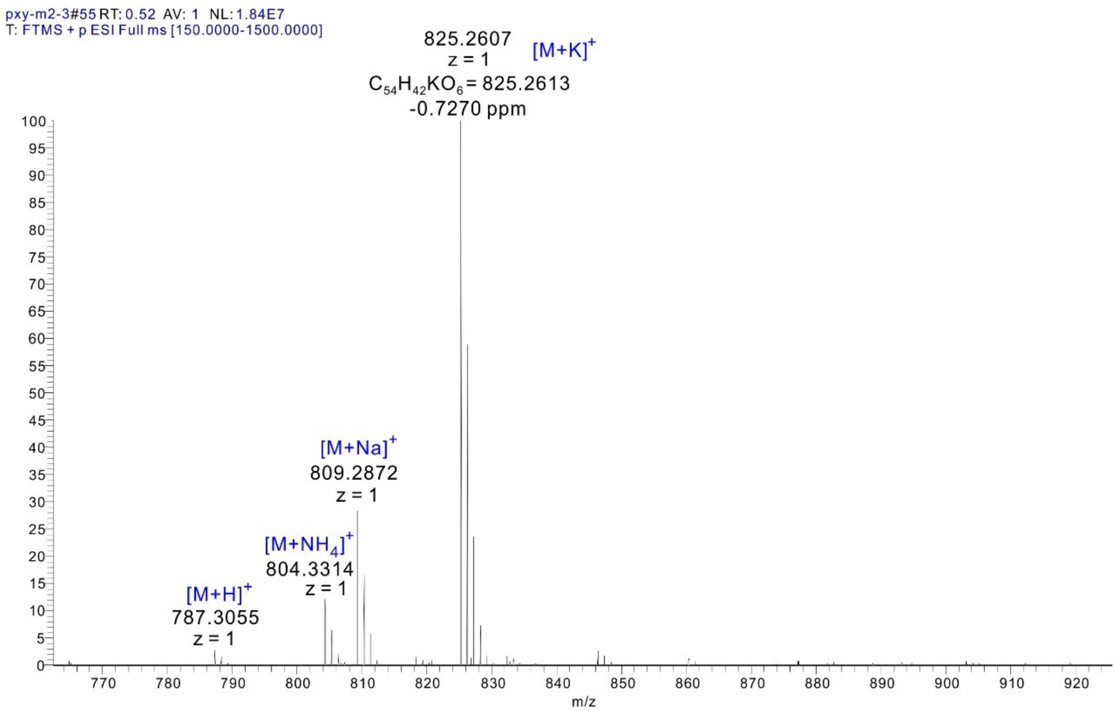


Figure S6. ESI mass spectrum of compound **M2**.

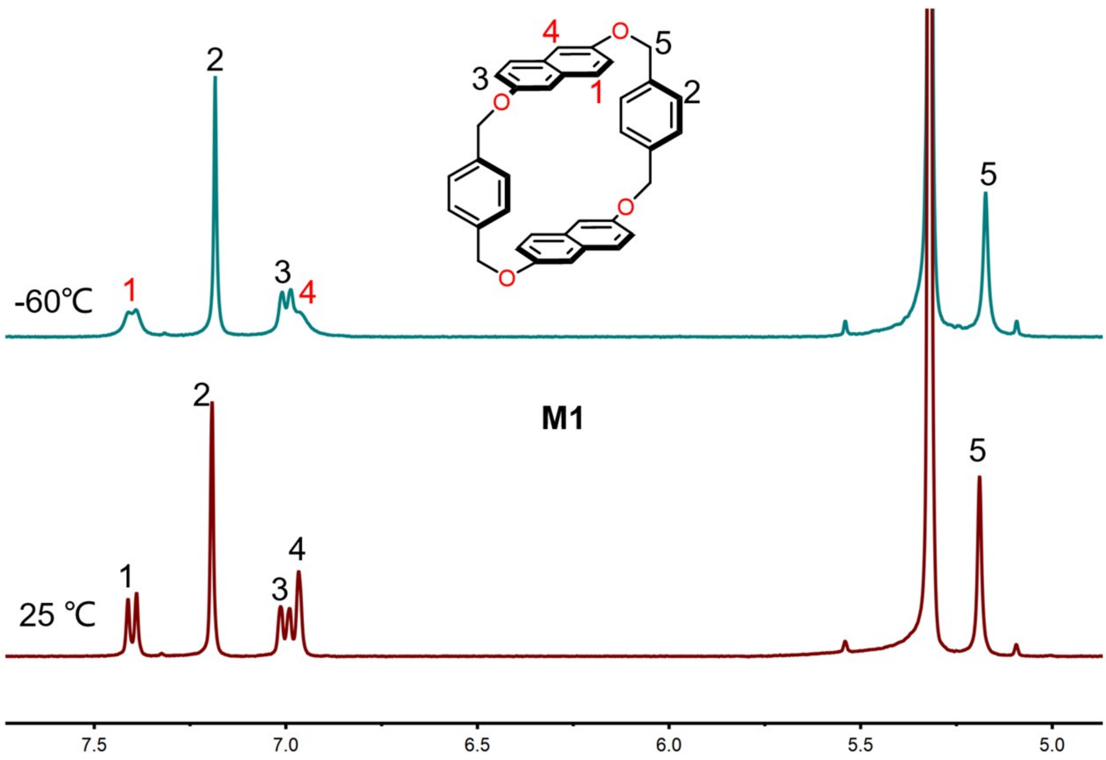


Figure S7. ^{1}H NMR spectra (400 MHz, CD_2Cl_2) of **M1** at 25℃ and -60℃. The proton signal peaks are only slightly broadened, suggesting the naphthalene flipping is very fast even at low temperatures.

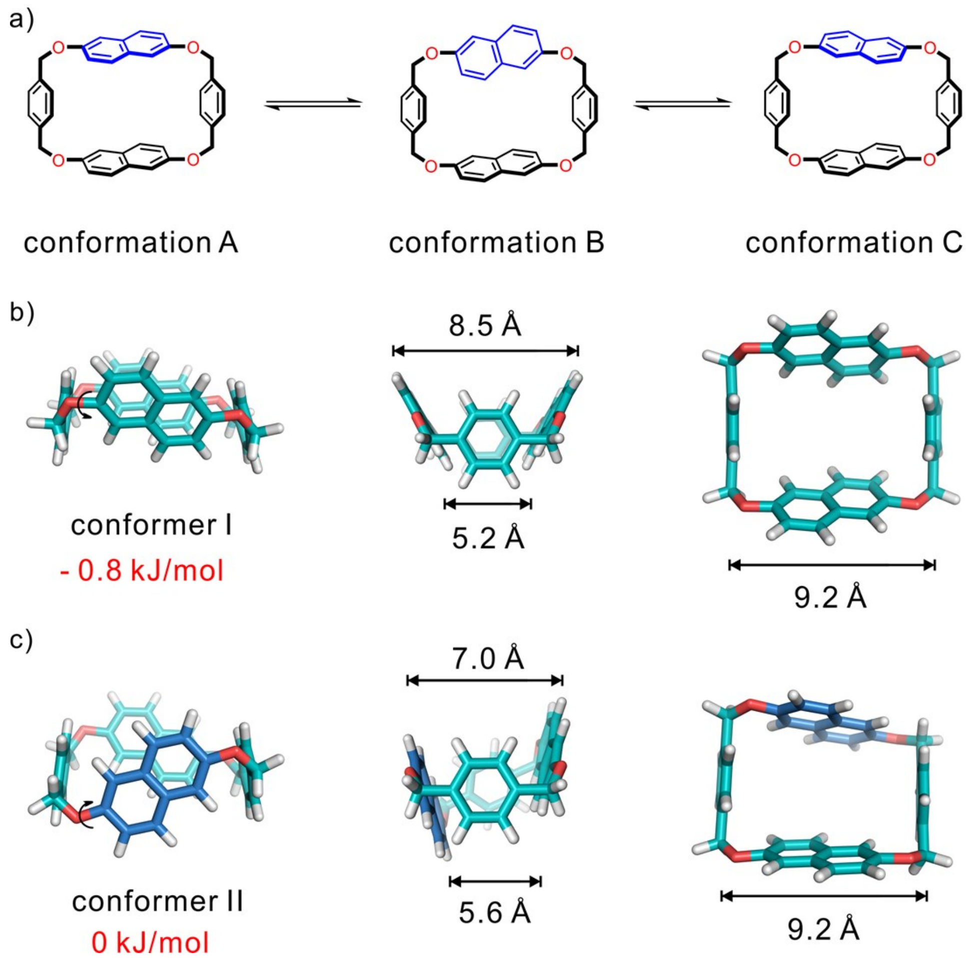


Figure S8. (a) Three limiting conformations of **M1**, (b) the top view, side view and front view of optimized conformer I, (c) the top view, side view and front view of optimized conformer II.

Due to the flipping of naphthalene units, naphthobox **M1** is conformationally flexible with many conformations, including three limiting conformations, namely conformation A, conformation B, and conformation C. Conformations A and B have a well-defined cavity, and thus are calculated by using DFT calculations at ωB97XD/6-311G(d,p) level, obtaining optimized conformer I and conformer II of **M1**, respectively.

In conformer I of **M1**, the two naphthalenes are slightly inclined into the cavity. The distance between the two naphthalenes is about 5.2 ~ 8.5 Å, and a more realistic "average" distance is about 6.8 Å according to the distance of two oxygen atoms connected to the same *p*-xylene. In addition, the distance of the two *p*-xylenes is approximately 9.2 Å. These results are consistent with related naphthol-based macrocycles.[1]

In conformer II of **M1**, the two naphthalenes are also slightly inclined into the cavity. The distance between the two naphthalenes is about 5.6 ~ 7.0 Å, and a more realistic "average" distance is about 6.8 Å according to the distance of two oxygen atoms connected to the same *p*-xylene. In addition, the distance of the two *p*-xylenes is approximately 9.2 Å. These results are consistent with the related naphthol-based macrocycles.

Conformer I is slightly more stable than conformer II by -0.8 kJ/mol according to the DFT calculations.

2. ^{1}H NMR Spectra of Host-Guest Complexes

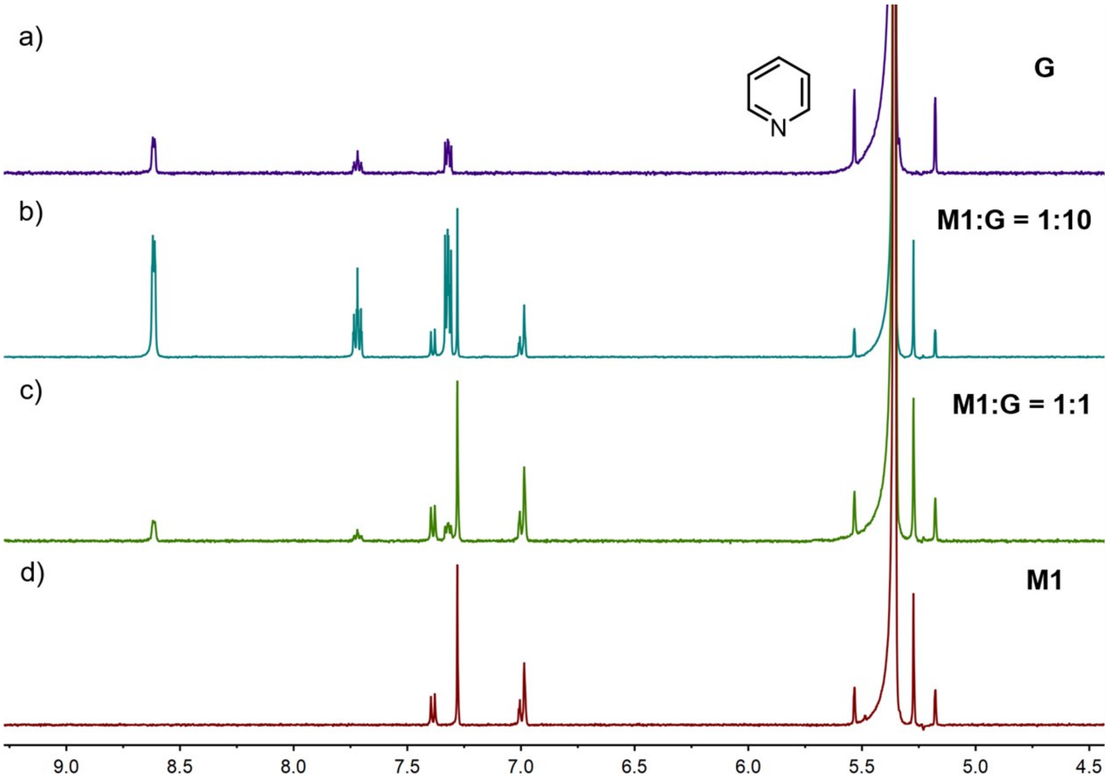
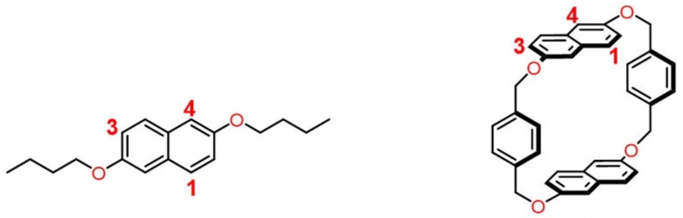


Figure S9. Partial ^{1}H NMR spectra (500 MHz, CD_2Cl_2, 0.2 mM, 298 K) of (a) pyridine, (d) **M1**, (c) their 1:1 (**M1**:pyridine) mixture, (b) their 1:10 (**M1**:pyridine) mixture. No obvious chemical shift was observed for both the host and the guest, suggesting very weak interactions between **M1** and pyridine.

Table S1. Chemical shifts (ppm) of macrocycle **M1** and acyclic compound **R** in different solvents.



R **M1**

	R			**M1**			$\Delta\delta$		
	H1	H3	H4	H1	H3	H4	H1	H3	H4
CD_2Cl_2	7.614	7.089	7.098	7.349	6.957	6.947	-0.265	-0.132	-0.151
$CDCl_3$	7.631	7.131	7.106	7.303	6.887	6.895	-0.328	-0.244	-0.211
Me_2SO-d_6	7.687	7.098	7.240	7.377	7.001	7.041	-0.310	-0.097	-0.199
Py-d_5	7.837	7.348	7.348	N/A*	6.956	7.036	N/A*	-0.392	-0.312

*：N/A: not available, the signal of the proton is buried into solvent residual signals.

The difference of chemical shifts ($\Delta\delta = \delta$(**M1**) – δ(**R**)) of **M1** and its acyclic compound **R** is obtained in different solvents, including CD_2Cl_2, $CDCl_3$, Me_2SO-d_6, and pyridine-d_5. Compared to acyclic compound **R**, the change of chemical shifts of **M1** in pyridine-d_5 is not obvious, suggesting that **M1** cannot effectively bind pyridine in pyridine-d_5 solution.

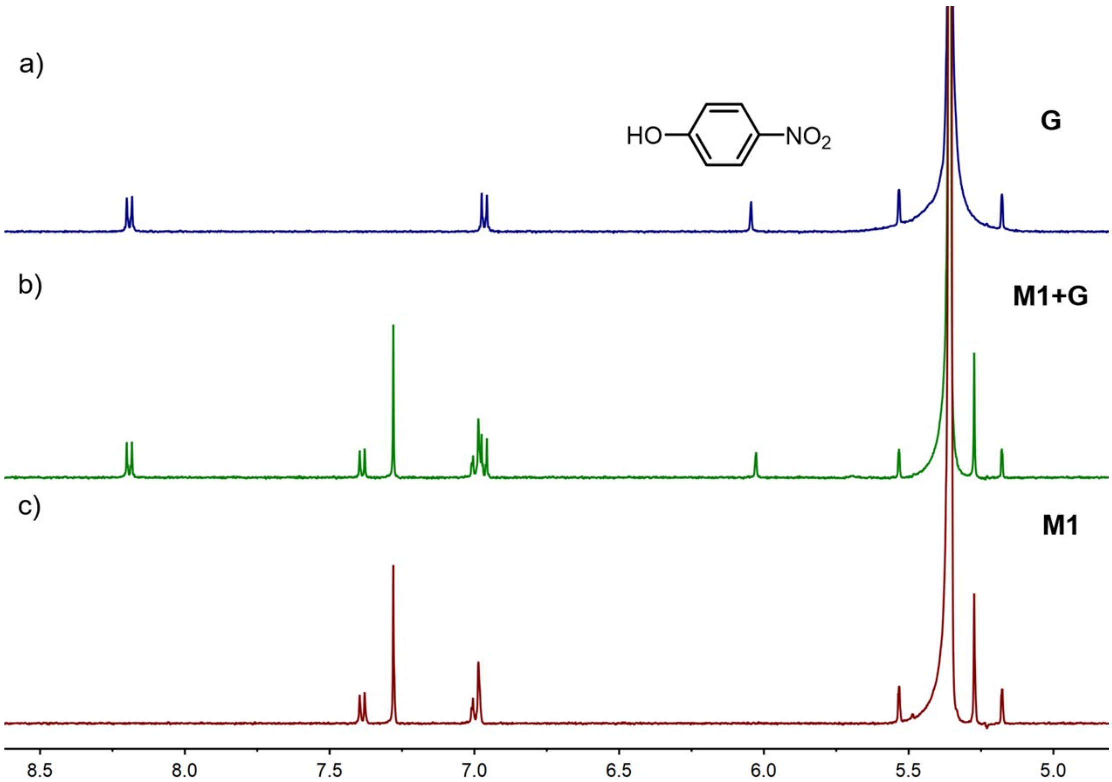


Figure S10. Partial ^{1}H NMR spectra (500 MHz, CD_2Cl_2, 0.2 mM, 298 K) of (a) *p*-nitrophenol, (c) **M1**, and (b) their equimolar mixture. No obvious chemical shift was observed for both the host and the guest, suggesting very weak interactions between **M1** and *p*-nitrophenol.

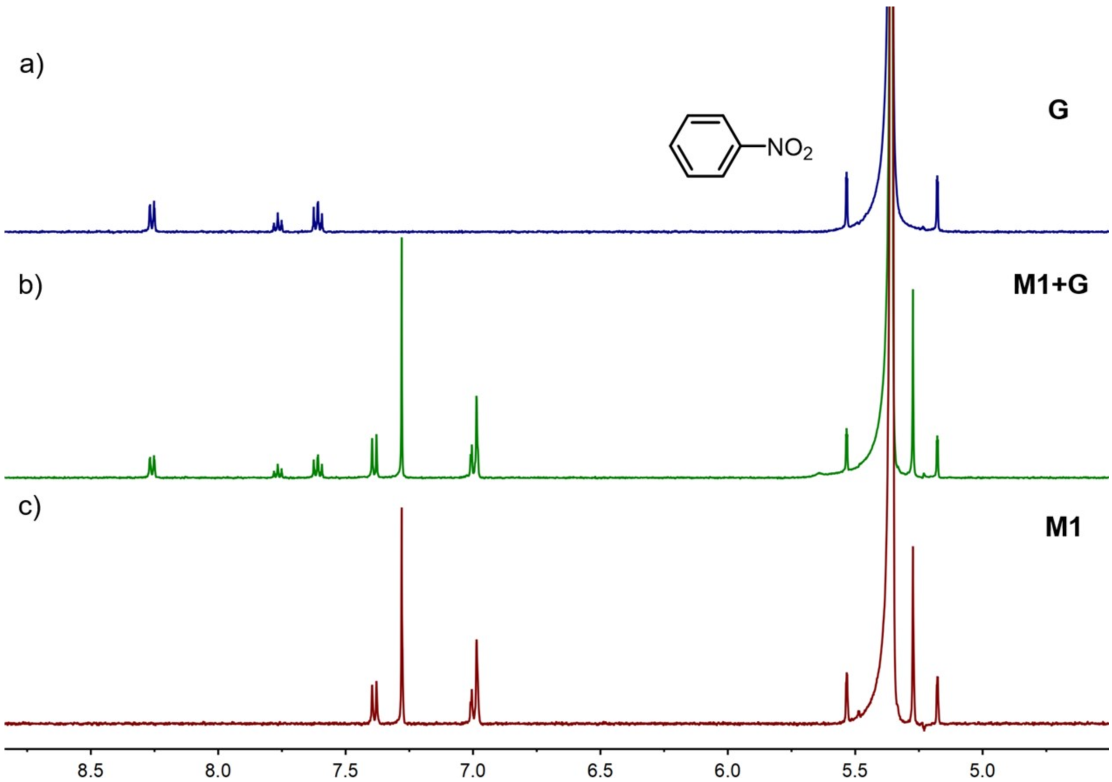


Figure S11. Partial [1]H NMR spectra (500 MHz, CD_2Cl_2, 0.2 mM, 298 K) of (a) nitrobenzene, (c) **M1**, and (b) their equimolar mixture. No obvious chemical shift was observed for both the host and the guest, suggesting very weak interactions between **M1** and nitrobenzene.

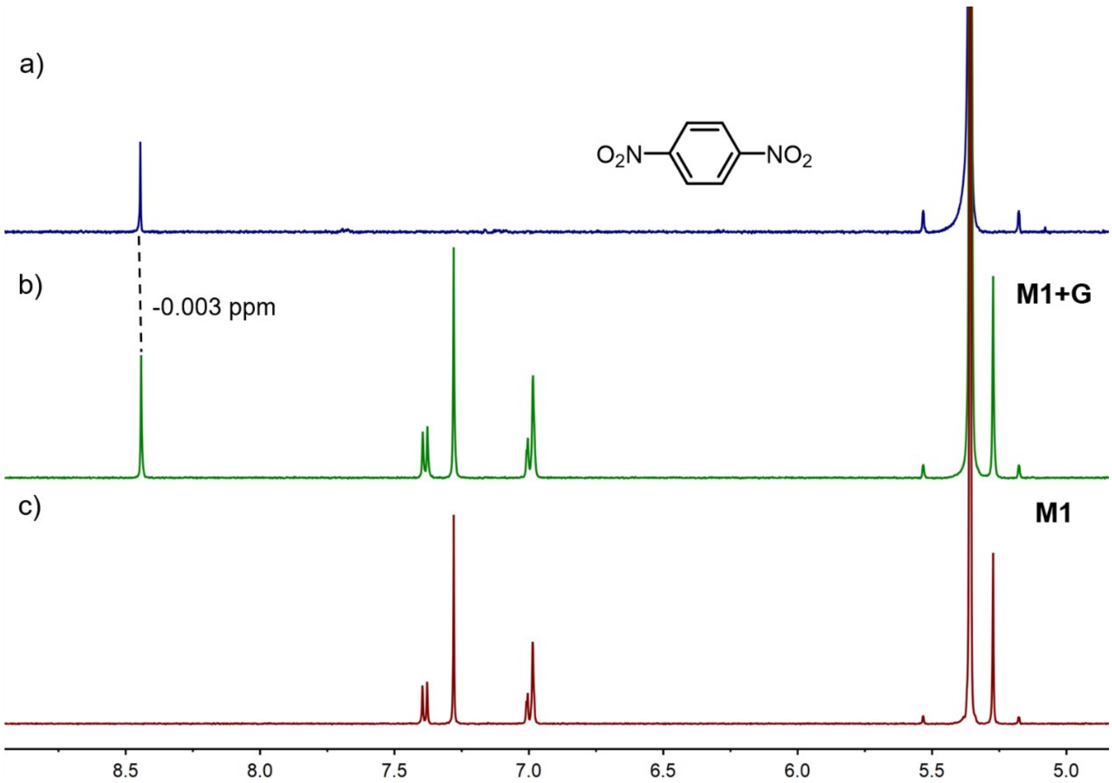


Figure S12. Partial [1]H NMR spectra (500 MHz, CD_2Cl_2, 0.2 mM, 298 K) of (a) *p*-dinitrobenzene, (c) **M1**, and (b) their equimolar mixture. The protons of the guest undergo minor shifts, suggesting very weak interactions between **M1** and *p*-dinitrobenzene.

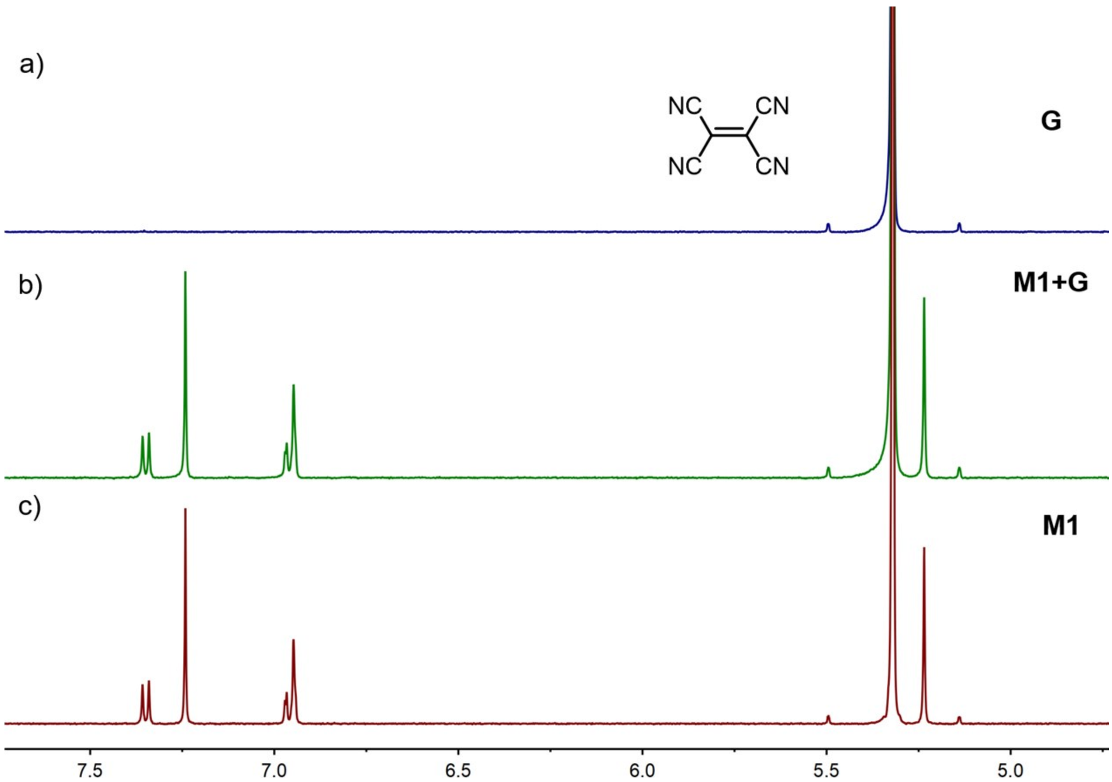


Figure S13. Partial [1]H NMR spectra (500 MHz, CD_2Cl_2, 0.2 mM, 298 K) of (a) tetracyanoethylene, (c) **M1**, and (b) their equimolar mixture. The protons of the guest undergo minor shifts, suggesting very weak interactions between **M1** and tetracyanoethylene.

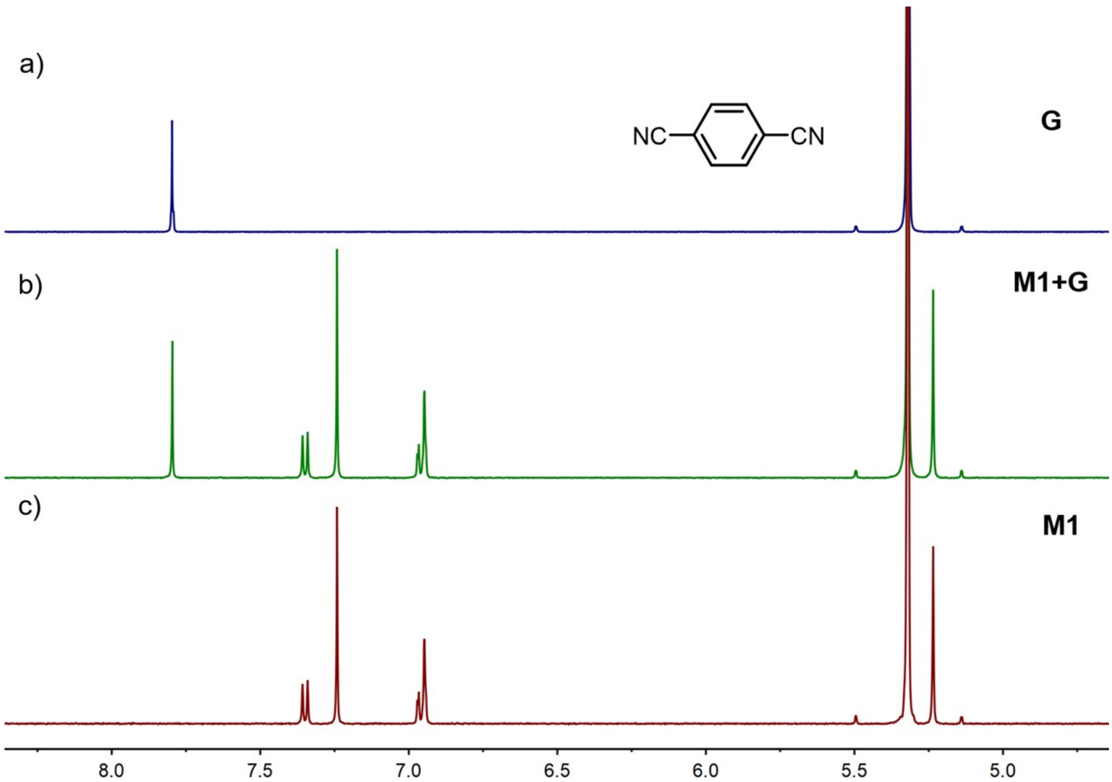


Figure S14. Partial ^{1}H NMR spectra (500 MHz, CD_2Cl_2, 0.2 mM, 298 K) of (a) *p*-dicyanobenzene, (c) **M1**, and (b) their equimolar mixture. The protons of the guest undergo minor shifts, suggesting very weak interactions between **M1** and *p*-dicyanobenzene.

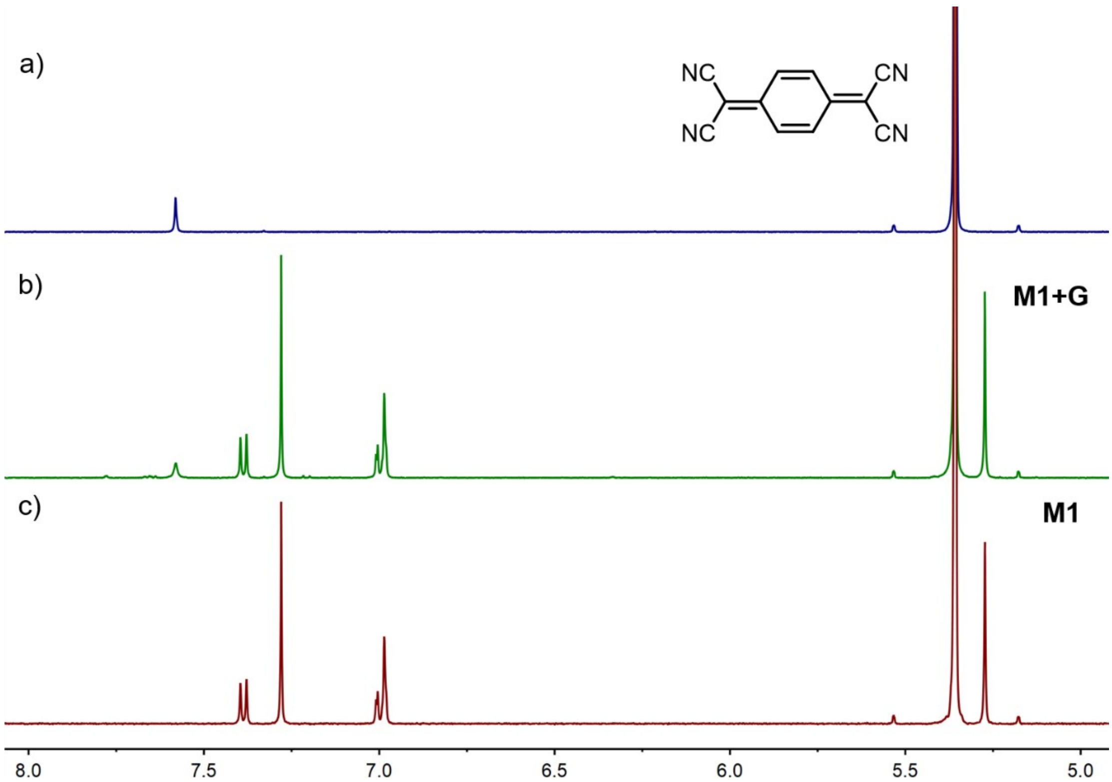


Figure S15. Partial [1]H NMR spectra (500 MHz, CD_2Cl_2, 0.2 mM, 298 K) of (a) TCNQ, (c) **M1**, and (b) their equimolar mixture. No obvious chemical shift was observed for both the host and the guest, suggesting very weak interactions between **M1** and TCNQ.

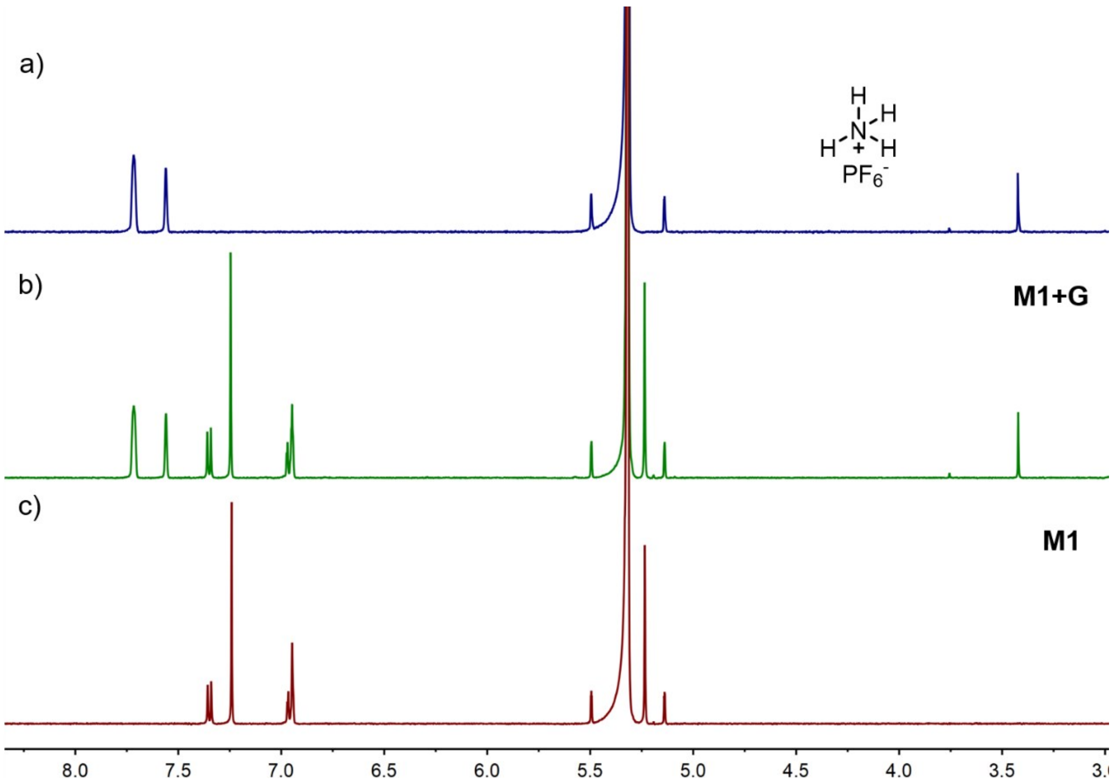


Figure S16. Partial [1]H NMR spectra (500 MHz, CD_2Cl_2, 0.2 mM, 298 K) of (a)ammonium, (c) **M1**, and (b) their equimolar mixture. No obvious chemical shift was observed for both the host and the guest, suggesting very weak interactions between **M1** and ammonium.

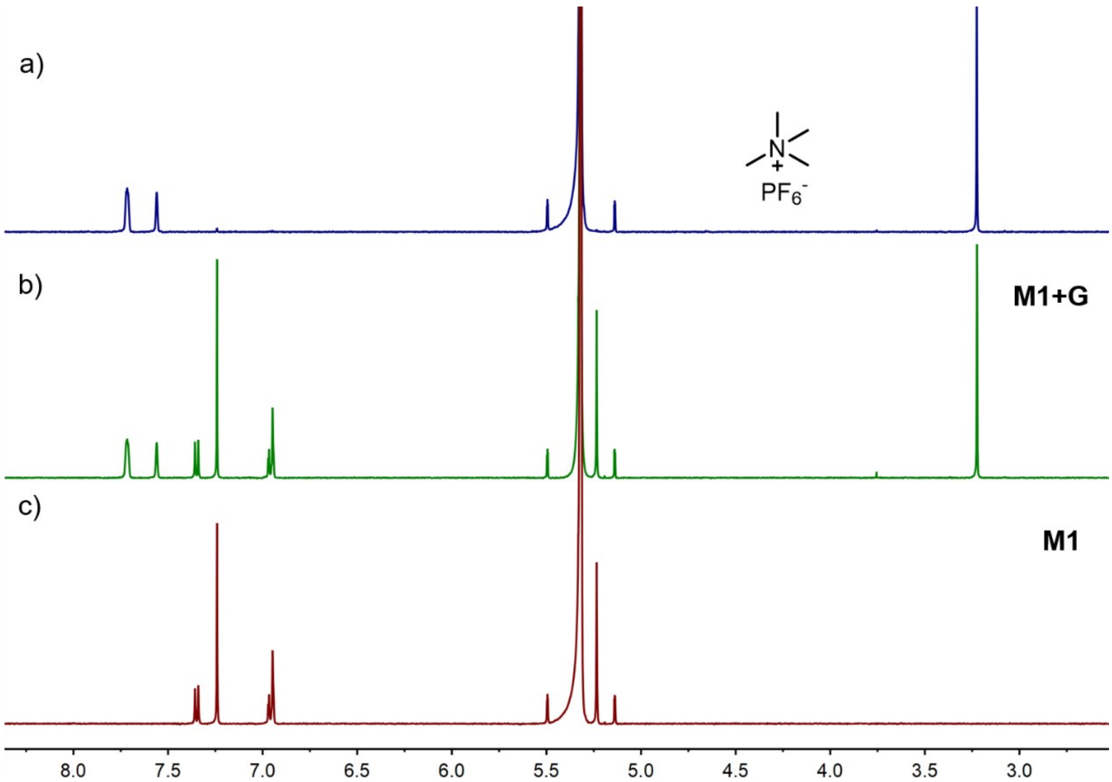


Figure S17. Partial [1]H NMR spectra (500 MHz, CD_2Cl_2, 0.2 mM, 298 K) of (a)tetramethylammonium, (c) **M1**, and (b) their equimolar mixture. No obvious chemical shift was observed for both the host and the guest, suggesting very weak interactions between **M1** and tetramethylammonium.

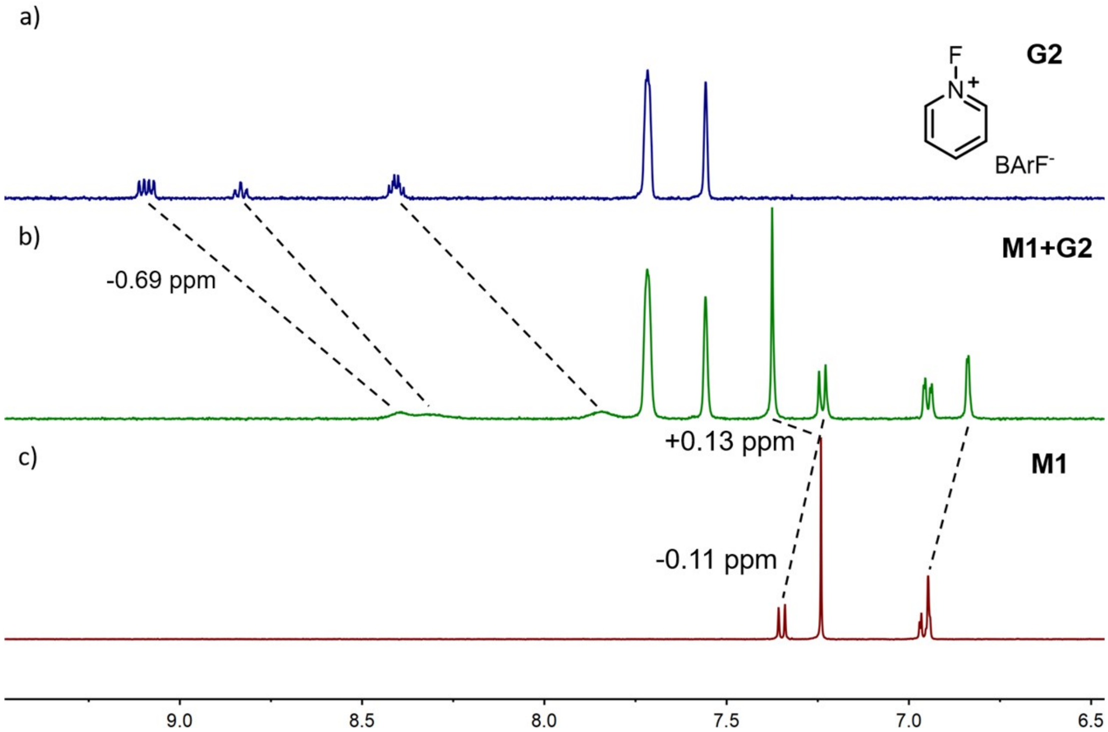


Figure S18. Partial ^{1}H NMR spectra (500 MHz, CD_2Cl_2, 0.2 mM, 298 K) of (a) **G2**, (c) **M1**, and (b) their equimolar mixture. The protons of the guest undergo significant shifts, suggesting that the complexation occurs between **M1** and **G2**.

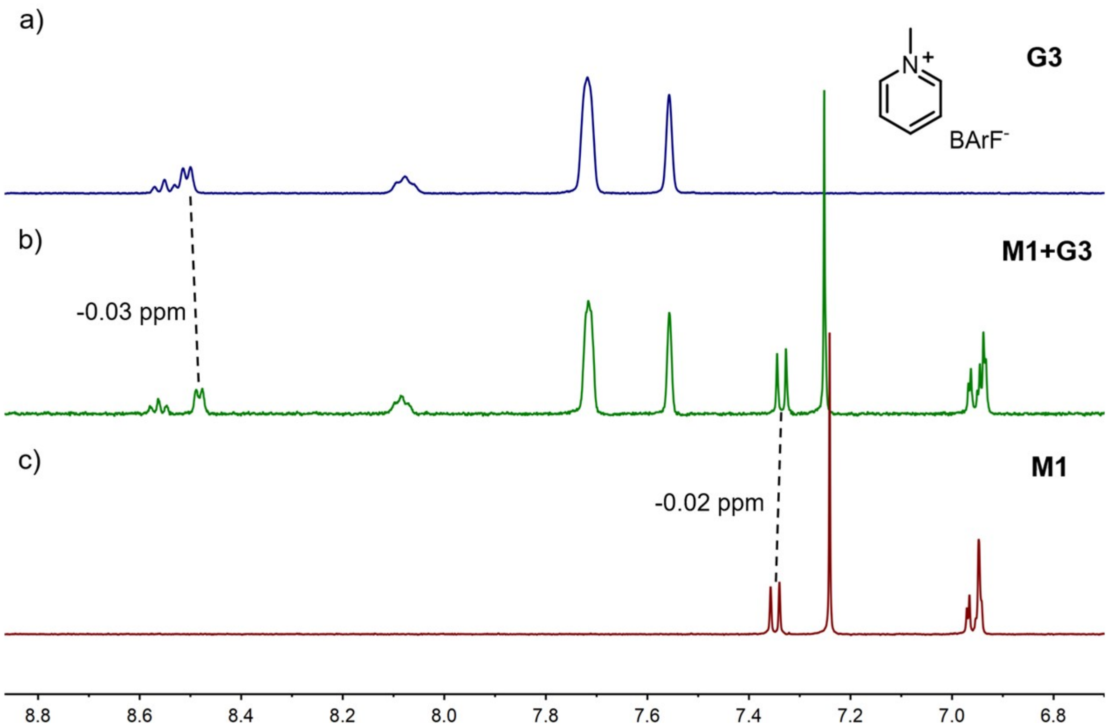


Figure S19. Partial ^{1}H NMR spectra (500 MHz, CD_2Cl_2, 0.2 mM, 298 K) of (a) **G3**, (c) **M1**, and (b) their equimolar mixture. The protons of the guest undergo minor shifts, suggesting that the complexation occurs between **M1** and **G3** although the interactions between them are weak.

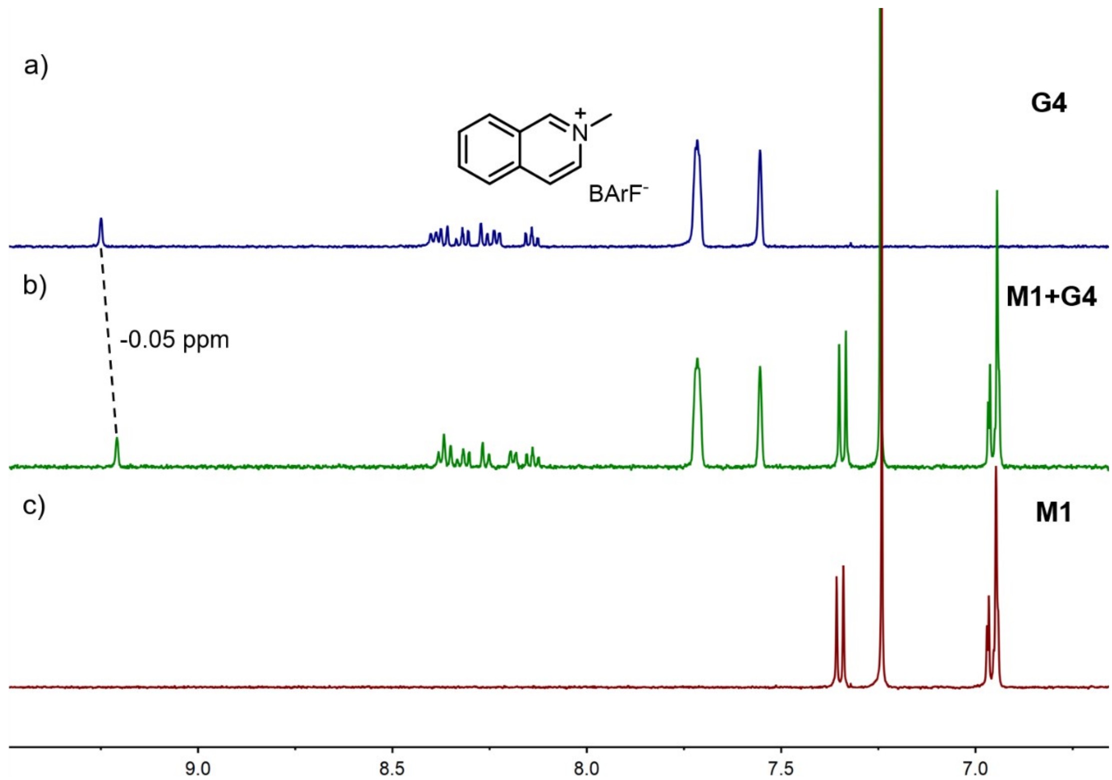


Figure S20. Partial ^{1}H NMR spectra (500 MHz, CD_2Cl_2, 0.2 mM, 298 K) of (a) **G4**, (c) **M1**, and (b) their equimolar mixture. The protons of the guest undergo minor shifts, suggesting that the complexation occurs between **M1** and **G4** although the interactions between them are weak.

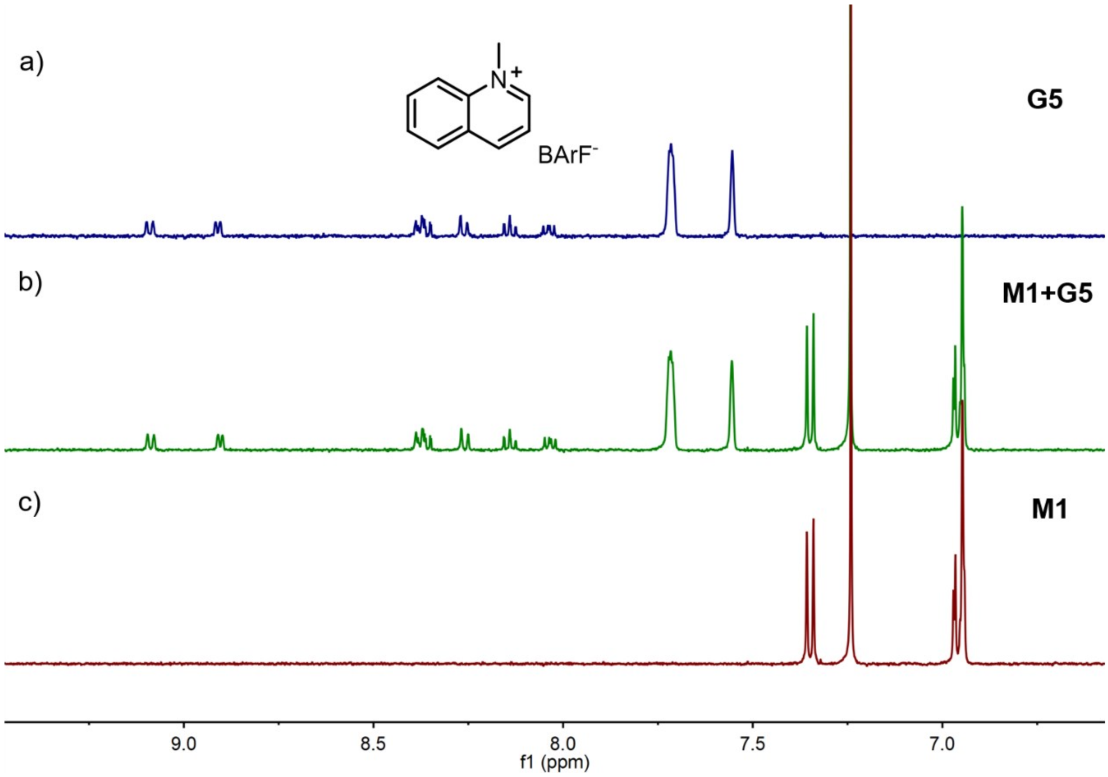


Figure S21. Partial ^{1}H NMR spectra (500 MHz, CD_2Cl_2, 0.2 mM, 298 K) of (a) **G5**, (c) **M1**, and (b) their equimolar mixture. No obvious chemical shift was observed for both the host and the guest, suggesting very weak interactions between **M1** and **G5**.

3. Determination of Association Constants by NMR Titrations

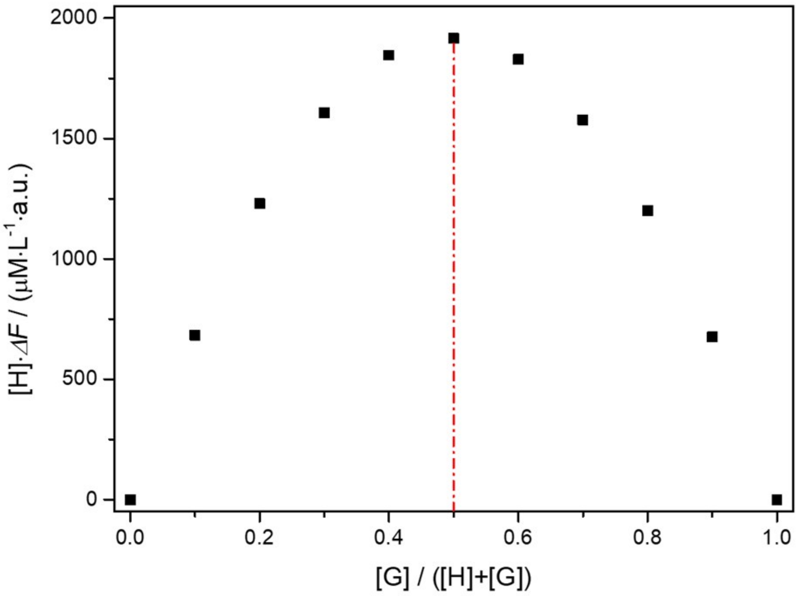


Figure S22. Job's plot constructed from the fluorescence strength change (ΔF) at 373 nm of **M1** in fluorescence emission spectra by varying the ratio of **M1** and **G1** with a fixed total concentration ([**M1**] + [**G1**] = 10 μM). This experiment supports the 1:1 binding stoichiometry between **M1** and **G1** in 1,2-dichloroethane.

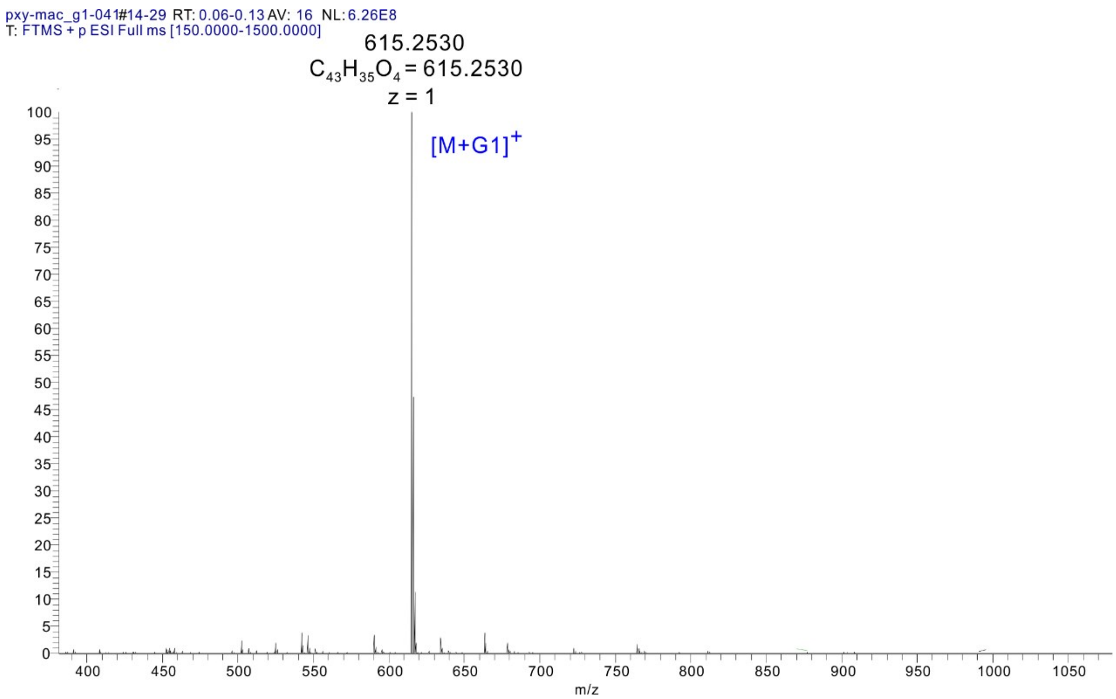
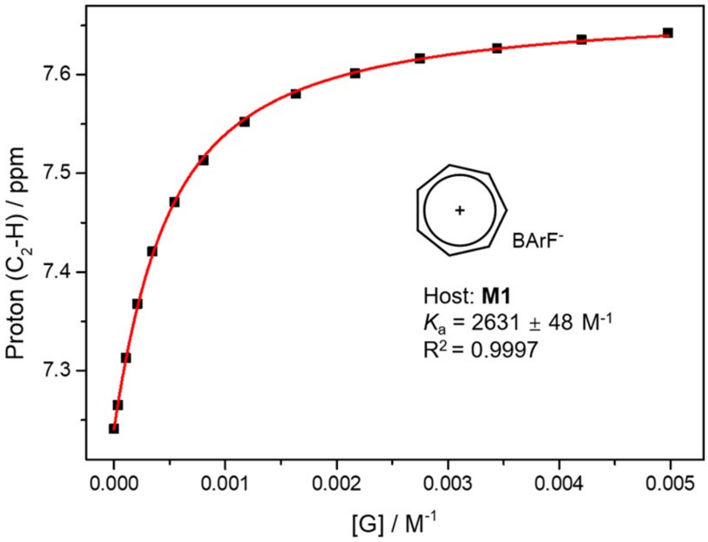
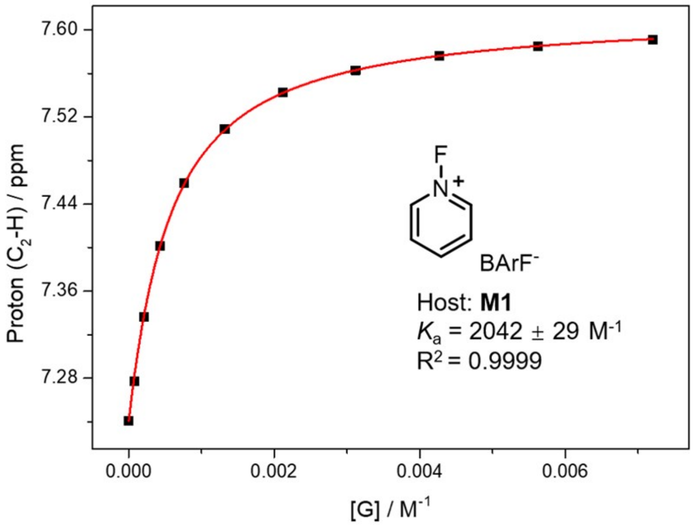


Figure S23. ESI mass spectrum of the complex [**G1@M1**]$^{+}$.



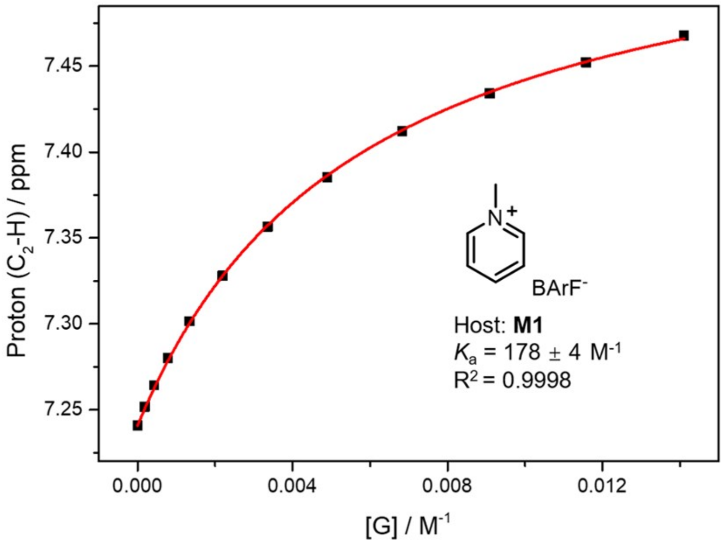
	K_a / M^{-1}	R^2
titration-1	2491	0.9998
titration-2	2593	0.9999
titration-3	2631	0.9997
average	2572 ± 59	

Figure S24. Non-linear curve-fitting for the complexation between **M1** and **G1** in CD_2Cl_2 at 298 K. The titration was repeated 3 times. Finally, K_a was given by averaging the values obtained from three independent titrations.



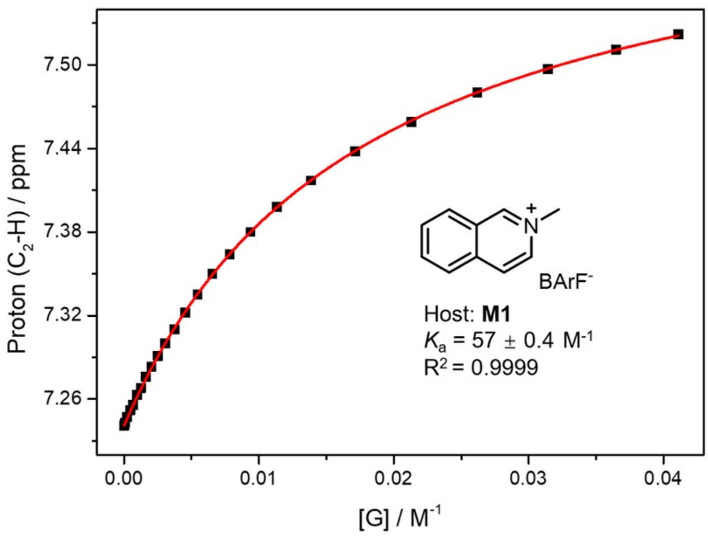
	K_a / M^{-1}	R^2
titration-1	2091	0.9997
titration-2	2042	0.9999
titration-3	1894	0.9996
average	2010 ± 84	

Figure S25. Non-linear curve-fitting for the complexation between **M1** and **G2** in CD_2Cl_2 at 298 K. The titration was repeated 3 times. Finally, K_a was given by averaging the values obtained from three independent titrations.



	K_a / M^{-1}	R^2
titration-1	180	0.9999
titration-2	178	0.9998
titration-3	171	0.9999
average	176 ± 4	

Figure S26. Non-linear curve-fitting for the complexation between **M1** and **G3** in CD_2Cl_2 at 298 K. The titration was repeated 3 times. Finally, K_a was given by averaging the values obtained from three independent titrations.



	K_a / M^{-1}	R^2
titration-1	57	0.9999
titration-2	66	0.9981
titration-3	54	0.9999
average	59 ± 5	

Figure S27. Non-linear curve-fitting for the complexation between **M1** and **G4** in CD_2Cl_2 at 298 K. The titration was repeated 3 times. Finally, K_a was given by averaging the values obtained from three independent titrations.

4. Control Experiments of Charge-Transfer System

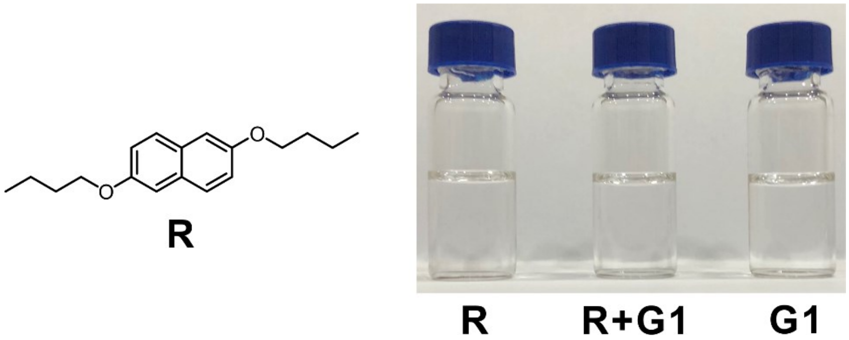


Figure S28. The color of the solution of **R**, **G1**, and **R+G1**. (0.5 mM, 1,2-dichloroethane, 298 K)

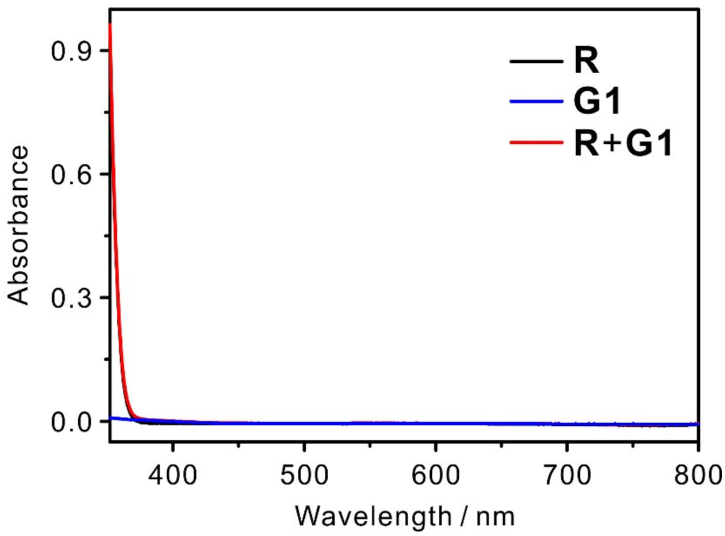


Figure S29. Partial UV-vis spectra of the solution of **R**, **G1**, and **R+G1**. (0.5 mM, 1,2-dichloroethane, 298 K)

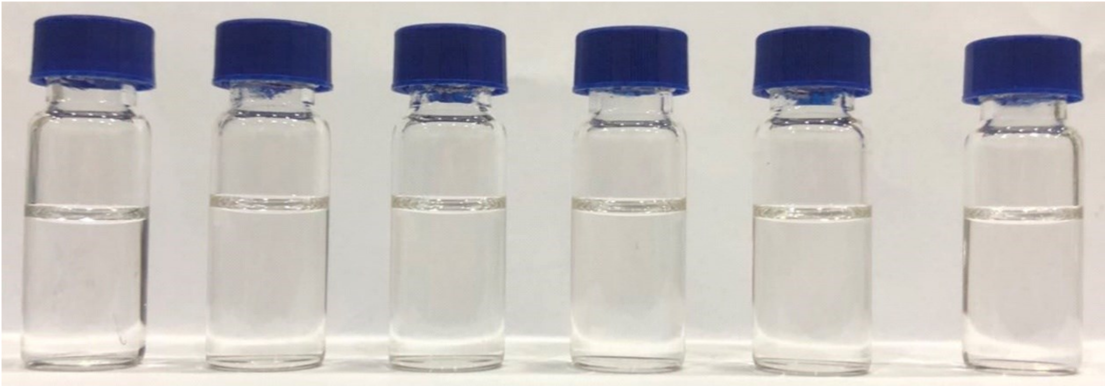


Figure S30. The color of **G1**'s solutions after adding different coordination anions (0.2 mM, DCM, 298 K).

5. X-Ray Crystallography

Suitable single crystals of **M2** for structural determination were obtained by slow diffusion of methanol into its saturated solution in CH_2Cl_2.

Single crystal X-ray data were collected on a Bruker D8 VENTURE with Cu Kα radiation (λ =1.54178 Å) at 200 K. The structures were solved by intrinsic phasing methods (SHELXT[2]) and refined by full-matrix least squares on F^2 using SHELXL[3] in the OLEX2 program package.[4] All non-hydrogen atoms were refined with anisotropic thermal parameters and the hydrogen atoms were fixed at calculated positions and refined by a riding mode. SQUEEZE routine implemented on PLATON[5] was used to remove electron densities corresponding to disordered solvent molecules in the crystal data.

Crystal data and structure refinement for **M2**

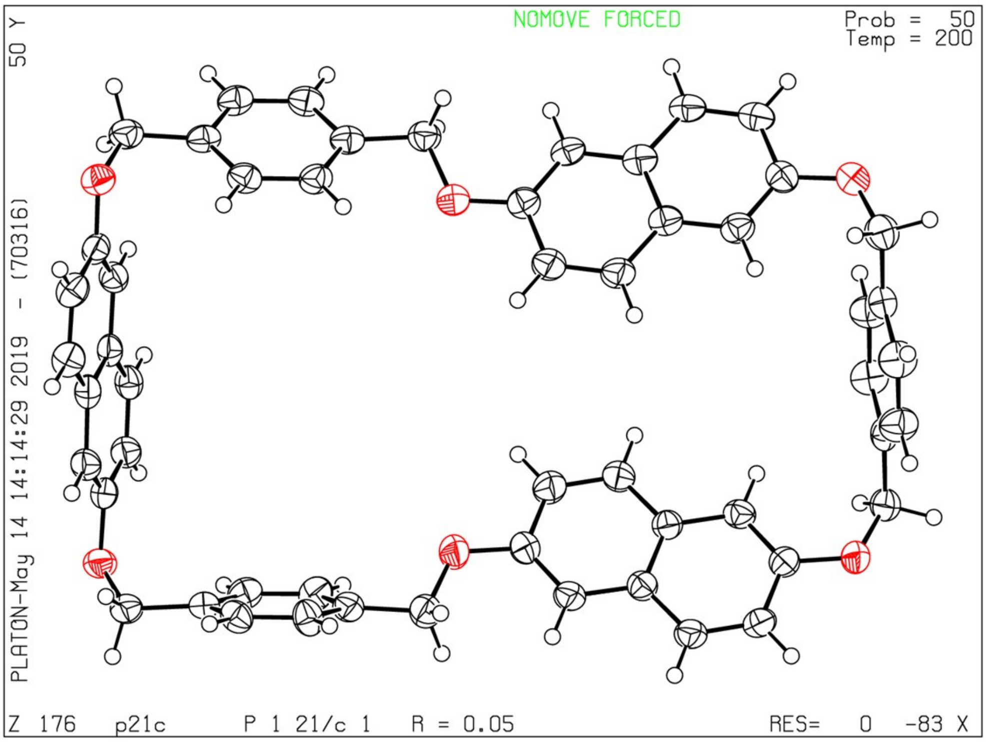
Entry	**M2**
Empirical formula	$C_{54}H_{42}O_6$
Formula weight	786.87
Temperature/K	200.0
Crystal system	monoclinic
Space group	$P2_1$/c
a/Å	11.6595(3)
b/Å	29.5566(7)
c/Å	13.7247(3)
α/°	90
β/°	112.5770(10)
γ/°	90
Volume/Å^3	4367.27(18)
Z	4
ρ_{calc}g/cm^3	1.197
μ/mm^{-1}	0.614
F(000)	1656.0
Reflections collected	24266
Independent reflections	6479 [R_{int} = 0.0510, R_{sigma} = 0.0450]
Data/restraints/parameters	6479/0/541
Goodness-of-fit on F^2	1.059
Final R indexes[I>=2σ(I)]	R_1 = 0.0454, wR_2 = 0.1048
Final R indexes	R_1 = 0.0690, wR_2 = 0.1162
CCDC number	2086311

M2

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575

Calculated sin(theta_max)/wavelength = 0.5631

Response: The crystal has too weak diffraction to obtain high resolution data.



6. Computational Data

Quantum chemistry calculations were performed using Gaussian 09 package.[6] The geometries of **M1** and complexes **G1@M1–G4@M1** have been optimized employing density functional theory (DFT) with dispersion corrected method (ωB97XD)[7] in combination with 6-311G(d,p) basis set. Single point energies of all structures are calculated at the ωB97XD/ma-def2-TZVP[8] level of theory and thermal correction to Gibbs free energy are calculated at the ωB97XD/6-311G(d,p) level of theory. Geometry optimizations were performed by considering the solvent effects (SMD, dichloromethane) without applying any geometry Constraints (C1 symmetry). Minima were characterized by the absence of imaginary frequencies. Independent gradient model (IGM) analysis[9] were carried out with Multiwfn 3.7 (dev)[10] program. Molecular plots were visualized by the VMD 1.9.3 program. [11]

Table S2. The theoretical values of single point energies $E^{sp}_{species}$, thermal corrections to the Gibbs free energies $E^{corr}_{species}$, and final Gibbs free energies $\Delta G°_{species}$ of **M1** and complexes **G1@M1–G4@M1**. All energies are reported in Hartrees.

Species	$E^{sp}_{species}$	$E^{corr}_{species}$	$\Delta G^{\circ}_{species}$
M1-I	-1689.6739882	0.491617	-1689.182371
M1-II	-1689.6742329	0.492183	-1689.182050
G1@M1-I	-1960.454315	0.607032	-1959.847283
G2@M1-I	-2037.613548	0.583361	-2037.030187
G3@M1-I	-1977.765432	0.617503	-1977.147929
G4@M1-I	-2131.412217	0.66373	-2130.748487
G1@M1-II	-1960.449524	0.608033	-1959.841491
G2@M1-II	-2037.610879	0.582469	-2037.02841
G3@M1-II	-1977.763903	0.620027	-1977.143876
G4@M1-II	-2131.411974	0.664466	-2130.747508

The calculation results show that **M1** adopts conformer I in all thermo-dynamically more stable complexes.

M1-I

There is no imaginary frequency after optimization and frequency analysis.

C	2.66051408	3.97061806	1.28222017
C	1.86313813	2.73237216	3.66765946
C	1.75629092	4.59684822	2.13620597
C	3.17326354	2.72613594	1.63917522
C	2.77848743	2.11295370	2.82033568
C	1.36157191	3.98356964	3.31839359
H	1.33608271	5.55989908	1.86228271
H	3.86907215	2.22231985	0.97747891
H	3.16810574	1.13369773	3.07497177
H	0.63556271	4.47166956	3.96166575
C	3.06743711	4.63622331	-0.01233695
H	3.97900132	5.21920128	0.13497019
H	2.28764987	5.32852078	-0.34905616
O	3.40559648	3.71817796	-1.04076195
C	2.43155145	2.94113159	-1.59212074
H	3.89685918	1.95986225	-2.78064685
C	2.84336870	2.02418303	-2.53031488
C	0.14709512	2.20954732	-1.86104394
C	1.91423034	1.17354182	-3.16660021
C	1.06022618	3.03428826	-1.25504460
C	0.53795799	1.25768462	-2.83076908
C	2.31052653	0.21728817	-4.14348126
H	0.71765781	3.74353349	-0.51370117
H	-1.44434860	0.47683064	-3.17033355
H	-0.90093887	2.28345126	-1.58938713
C	1.39311911	-0.59266666	-4.74232525
H	3.35976240	0.13940421	-4.40886968
H	1.68871809	-1.32085443	-5.48911280
C	0.01606403	-0.50156351	-4.40495077
C	-0.40451850	0.39916488	-3.46210423
O	-0.78301555	-1.36046974	-5.09208420
C	-3.28168238	-3.29676429	-1.12679881
C	-2.53658910	-2.01627726	-3.50843373
C	-4.07572826	-2.28822707	-1.66669933
C	-2.10529676	-3.65072521	-1.78284692
C	-1.73656291	-3.01671736	-2.96171526
C	-3.70695765	-1.65364225	-2.84655381
H	-4.98503190	-1.98767560	-1.15507258
H	-1.46934142	-4.42335568	-1.36511160
H	-0.81523956	-3.29791206	-3.45959550
H	-4.33187137	-0.86261168	-3.25012027

C	-3.72266381	-4.01529014	0.12825992
H	-4.31807207	-4.89106398	-0.13880983
O	1.45467709	0.64702562	4.89165791
C	-2.17463744	-1.35980180	-4.82140611
H	-2.61215915	-1.92469899	-5.64740477
H	-2.57681789	-0.34169550	-4.86960863
C	1.41089030	2.06433708	4.94616393
H	0.41029964	2.41168730	5.22747839
H	2.08709244	2.32139942	5.76426251
H	-4.35292521	-3.36445123	0.74510811
C	-1.87989068	-3.68300213	1.61396155
H	-2.79283378	-1.81114374	1.08762456
C	-2.03071469	-2.32211196	1.66245989
C	-0.00763006	-3.58184719	3.14193865
C	-1.16285733	-1.54050682	2.47476447
C	-0.85025669	-4.31497138	2.36163955
C	-0.13588610	-2.16693516	3.22739548
C	-1.28597870	-0.13439254	2.55893925
H	-0.75916719	-5.39323453	2.29481006
H	1.51375264	-1.85770817	4.59910740
H	0.77461372	-4.07502945	3.70952254
C	-0.44517176	0.61459404	3.34204999
H	-2.06199228	0.36079947	1.98436764
H	-0.56812319	1.68896299	3.37015902
C	0.57747070	-0.01781254	4.08836730
C	0.72458548	-1.38332296	4.02572951
O	-2.65005284	-4.54032241	0.89293931

M1-II

There is no imaginary frequency after optimization and frequency analysis.

C	4.78573138	-1.00664929	0.25519641
C	4.46716051	1.51575599	-0.92823270
C	4.96004776	-0.84236734	-1.11489155
C	4.45177869	0.10423354	1.02959135
C	4.29605835	1.35126012	0.44603465
C	4.79983304	0.40873621	-1.70243758
H	5.20222019	-1.70081265	-1.73391871
H	4.29938739	-0.01406383	2.09700930
H	4.02664830	2.20398014	1.05894851
H	4.91748618	0.51818318	-2.77623075
C	4.94640195	-2.35618124	0.91451026
H	5.86652572	-2.38542053	1.50119703
H	5.00675508	-3.15540618	0.16828518
O	3.91946358	-2.61566530	1.86502448
C	-4.69915267	0.71128351	-0.49912220
C	-4.35623181	-2.07091615	-0.46078981
C	-4.74315815	-0.02431164	-1.68313187
C	-4.48465467	0.04530728	0.70287777
C	-4.31172349	-1.33453147	0.71918439
C	-4.57772021	-1.40055339	-1.66387679
H	-4.89908401	0.48842984	-2.62756490
H	-4.43370951	0.60874208	1.62806686
H	-4.13239133	-1.84225547	1.66170509
H	-4.60548448	-1.96154602	-2.59245826
C	-4.90698802	2.20803797	-0.54012290
H	-5.95562104	2.44078101	-0.34175358
O	3.38346647	3.70894223	-0.87619351
C	-4.15093437	-3.56557882	-0.47559539
H	-5.00483715	-4.06164529	-0.93916941
C	4.31008838	2.87891267	-1.56196028
H	4.05162940	2.78694620	-2.62243206
H	5.25171630	3.42921127	-1.50578712
H	-4.66008027	2.59797214	-1.53421291
C	-2.85333568	3.09953852	0.29411178
H	-2.49653523	1.78915688	-1.36917677
C	-2.08006584	2.49487522	-0.66221863
C	-0.93428910	4.28811245	1.16302494
C	-0.68752347	2.77335268	-0.73108784
C	-2.26543527	4.00028225	1.22194594
C	-0.09877882	3.68745325	0.18016708
C	0.14960298	2.14969876	-1.68604518

H	-2.90647396	4.45754450	1.96726812
H	1.73896485	4.66324966	0.79117760
H	-0.49719346	4.98467724	1.87090305
C	1.49156582	2.42232407	-1.74828048
H	-0.28381439	1.43283969	-2.37574991
H	2.10043244	1.91594764	-2.48576756
C	2.06706290	3.35277072	-0.85102317
C	1.28378014	3.96341053	0.09857019
O	-4.19206433	2.92172780	0.45634144
H	-4.04707197	-3.96392568	0.53830811
O	-3.04508334	-3.94268217	-1.29417788
C	-1.78377798	-3.68224959	-0.85784804
H	-2.17414277	-3.26171179	1.21346429
C	-1.43458207	-3.36170268	0.42984862
C	0.53234119	-3.58786841	-1.54797403
C	-0.07105718	-3.16239616	0.76982432
C	-0.78196168	-3.79151476	-1.85536484
C	0.93315625	-3.27045457	-0.22308030
C	0.33062051	-2.86490892	2.09892189
H	-1.09076521	-4.03846609	-2.86474737
H	3.03603218	-3.13964802	-0.67002603
H	1.28882868	-3.67043880	-2.32158661
C	1.64760259	-2.69137887	2.41324901
H	-0.42700983	-2.77458716	2.87045917
H	1.95783499	-2.46527951	3.42705818
C	2.64786498	-2.79553349	1.41464351
C	2.29618256	-3.06932996	0.11717639

G1@M1-I

There is no imaginary frequency after optimization and frequency analysis.

C	2.54017054	4.11043731	1.31469021
C	1.80577780	2.83455818	3.70341892
C	1.29265080	4.34115644	1.88335110
C	3.42797943	3.24385321	1.95956165
C	3.06557232	2.61399806	3.13843338
C	0.92813169	3.70713533	3.06975112
H	0.59403319	5.01271120	1.39490024
H	4.40633926	3.06322686	1.52652915
H	3.76053307	1.94039116	3.62878569
H	-0.05265030	3.88673996	3.49811350
C	2.94777306	4.75565442	0.01387415
H	3.86698357	5.32740104	0.14718270
H	2.17916415	5.44602538	-0.34427053
O	3.28528504	3.78839781	-0.97987544
C	2.30746391	3.02616106	-1.54153550
H	3.76732949	1.60532438	-2.15293600
C	2.71620419	1.87218921	-2.17054994
C	0.02821308	2.58927773	-2.20862163
C	1.79404233	1.05425882	-2.85633260
C	0.93889981	3.38104191	-1.55435328
C	0.42070356	1.41060872	-2.88460644
C	2.19309856	-0.13451271	-3.52701343
H	0.59581243	4.27905802	-1.05771490
H	-1.55869641	0.88164143	-3.55495422
H	-1.01918998	2.87379413	-2.21446278
C	1.28272173	-0.90382596	-4.18857625
H	3.23937448	-0.42124743	-3.51191392
H	1.58257407	-1.80488658	-4.71122561
C	-0.09060094	-0.54259891	-4.21780863
C	-0.51683028	0.58604407	-3.56358671
O	-0.86770860	-1.37979989	-4.95124492
C	-3.57702878	-3.15510823	-1.15697542
C	-2.77124009	-1.93933727	-3.55420811
C	-3.93110408	-1.84076843	-1.43538844
C	-2.83045131	-3.86832467	-2.10002703
C	-2.43313280	-3.26871456	-3.28248339
C	-3.53039516	-1.23674456	-2.62674624
H	-4.51145392	-1.27543844	-0.71298104
H	-2.55598133	-4.89796928	-1.89616078
H	-1.84792184	-3.82951967	-4.00367635
H	-3.80093029	-0.20429236	-2.82508142

C	-3.95968846	-3.82904706	0.13763691
H	-4.56823955	-4.71245496	-0.06038786
O	1.47724389	0.69328640	4.81721844
C	-2.28750005	-1.30463916	-4.83488180
H	-2.65590272	-1.86224370	-5.69691150
H	-2.64014761	-0.27402741	-4.93099507
C	1.42213889	2.11152654	4.97034128
H	0.44205386	2.43755394	5.32873790
H	2.14618246	2.31955282	5.75891163
H	-4.54206268	-3.16380693	0.78080389
C	-1.98481170	-3.48499747	1.46872004
H	-3.25161643	-1.75640277	1.62033020
C	-2.29401369	-2.20507396	1.85427021
C	0.20820021	-3.30684643	2.47721240
C	-1.35445329	-1.43963349	2.59716693
C	-0.71314353	-4.03365653	1.78319102
C	-0.08257163	-1.98473142	2.91307054
C	-1.63765959	-0.12399827	3.03227209
H	-0.50111195	-5.04585367	1.45819847
H	1.82196750	-1.62889230	3.88205199
H	1.17676915	-3.73685179	2.70972708
C	-0.72380541	0.60976577	3.74655868
H	-2.60448309	0.31045897	2.79902265
H	-0.98648607	1.60819466	4.07016212
C	0.53941110	0.05851610	4.06196373
C	0.85077742	-1.21284325	3.63691960
O	-2.81314349	-4.34020560	0.81542173
H	-1.84398853	-0.12965675	-0.60644282
C	-0.79669795	-0.29556160	-0.37965446
C	1.15106629	0.76827194	0.76827185
C	-0.26864441	-1.48774066	-0.85253274
C	2.16520574	-0.16238047	0.58334172
H	1.21766562	-2.93669040	-1.17857515
C	1.02868659	-1.97132187	-0.72086100
H	3.03748766	-1.94790507	-0.10329553
C	2.11212459	-1.38190492	-0.08140484
H	-0.78319151	1.56605406	0.59986203
C	-0.16732518	0.71345504	0.33836536
H	1.42513511	1.65658293	1.32142950
H	-0.95816008	-2.12393134	-1.39374557
H	3.12521656	0.10208307	1.01522826

G1@M1-II

There is no imaginary frequency after optimization and frequency analysis.

C	4.83453749	-0.85816064	0.31136085
C	4.63935946	1.63666994	-0.96814887
C	4.79830350	-0.77521214	-1.07566550
C	4.82836493	0.32587232	1.05549057
C	4.73308423	1.55688796	0.42478295
C	4.70330821	0.46186095	-1.71006903
H	4.80786026	-1.68470972	-1.66821150
H	4.87285175	0.27722340	2.13846639
H	4.70060923	2.46653087	1.01422110
H	4.63989186	0.50593690	-2.79300979
C	4.84752202	-2.19123308	1.02092430
H	5.73725557	-2.27990101	1.64589128
H	4.85911413	-3.01978035	0.30695378
O	3.76424142	-2.31795344	1.94222562
C	-4.77946787	0.62362073	-0.55611242
C	-4.51027745	-2.17030443	-0.41380862
C	-4.63544755	-0.13534630	-1.71516255
C	-4.84676605	-0.03476311	0.67260970
C	-4.70709314	-1.41633610	0.74257682
C	-4.50926632	-1.51770005	-1.64567792
H	-4.59309131	0.36040565	-2.67964815
H	-4.96842678	0.54174384	1.58323297
H	-4.72283021	-1.91068404	1.70872041
H	-4.36806012	-2.09217066	-2.55505402
C	-4.85071211	2.13222904	-0.61564858
H	-5.86266644	2.47140512	-0.38690744
O	3.51147125	3.80581249	-0.96470394
C	-4.27809288	-3.66284745	-0.35247141
H	-5.11787678	-4.19582519	-0.80096283
C	4.44743141	2.97346240	-1.64723743
H	4.16763258	2.82983048	-2.69486616
H	5.37681212	3.54593857	-1.63225971
H	-4.59924373	2.49884503	-1.61437517
C	-2.70162947	2.88288812	0.21321126
H	-2.51158295	2.53126409	-1.89815855
C	-2.01238166	2.78431096	-0.97042782
C	-0.66438971	3.42074699	1.40643645
C	-0.60857940	3.02553011	-0.99908635
C	-2.00868733	3.19643091	1.41295498
C	0.08031306	3.35002353	0.19830656
C	0.14815082	2.95383596	-2.19648190

H	-2.58355437	3.25855104	2.32982422
H	2.00105706	3.81098760	1.09046665
H	-0.14778227	3.65973064	2.33010340
C	1.50160529	3.17897962	-2.20589842
H	-0.36290759	2.72223652	-3.12550924
H	2.04620808	3.13589526	-3.14183855
C	2.18065976	3.48610625	-1.00263297
C	1.47732501	3.56597516	0.17286362
O	-4.04269583	2.74257456	0.38571074
H	2.56991496	0.45639403	-0.06877900
C	1.55083284	0.19472173	-0.30938776
C	-0.69843518	-0.01190603	0.74421304
C	1.31546932	-0.14030081	-1.63414399
C	-1.48633179	-0.40335972	-0.33220833
H	0.17689025	-0.73901807	-3.29878261
C	0.12350970	-0.51250482	-2.23896322
H	-1.93276794	-0.93605638	-2.31020499
C	-1.12760159	-0.62655558	-1.65360344
H	1.08003922	0.56601591	1.70487019
C	0.65674039	0.26426946	0.75299017
H	-1.21600315	0.09463571	1.69140277
H	2.18353882	-0.10871973	-2.28302842
H	-2.52858662	-0.56039147	-0.10177507
H	-4.18416203	-4.00425219	0.68245303
O	-3.15500188	-4.06552624	-1.13475427
C	-1.89524083	-3.80513790	-0.69520045
H	-2.29518565	-3.28277183	1.35132140
C	-1.54942196	-3.42380263	0.57859734
C	0.42476414	-3.72543634	-1.38133075
C	-0.18871494	-3.18609336	0.90690217
C	-0.88626032	-3.97161797	-1.67664625
C	0.81925440	-3.31068298	-0.08209908
C	0.20431815	-2.77950949	2.20888166
H	-1.18707077	-4.28378136	-2.67027666
H	2.91015849	-3.09029319	-0.55890467
H	1.18231381	-3.84004334	-2.14984361
C	1.51091894	-2.50517328	2.49661446
H	-0.55101262	-2.68351858	2.98198008
H	1.81197860	-2.19738225	3.49142073
C	2.51424803	-2.61125158	1.50010742
C	2.17140301	-3.00499302	0.22854832

G2@M1-I

There is no imaginary frequency after optimization and frequency analysis.

C	0.48971750	-1.37985350	4.69457919
C	0.50112758	1.42403736	4.68119922
C	1.69070163	-0.67945733	4.67426590
C	-0.71052069	-0.66537722	4.69231765
C	-0.70487240	0.71936283	4.68558520
C	1.69641236	0.71385785	4.66757559
H	2.63041241	-1.22265816	4.66165710
H	-1.65242588	-1.20384281	4.70184511
H	-1.64230814	1.26569157	4.68994652
H	2.64046656	1.24928633	4.65013067
C	0.45935214	-2.88775220	4.74159307
H	0.07419722	-3.22558229	5.70502647
H	1.46333988	-3.30580612	4.62645443
O	-0.44733063	-3.44158091	3.79313957
C	-0.16459284	-3.32584592	2.46705595
H	-2.20092010	-3.71138298	1.99028037
C	-1.21023164	-3.51498902	1.59485169
C	1.35004021	-3.02953142	0.61078947
C	-1.00233389	-3.47846870	0.19955566
C	1.13301427	-3.06987927	1.96409674
C	0.29765467	-3.23025360	-0.31251371
C	-2.06165993	-3.68373069	-0.72736801
H	1.96534174	-2.91619375	2.63811611
H	1.51773904	-2.98716316	-2.07501120
H	2.34995569	-2.83955337	0.23548875
C	-1.83062228	-3.65931783	-2.07054637
H	-3.06214146	-3.86969430	-0.35113781
H	-2.63134614	-3.82770182	-2.78151981
C	-0.52653056	-3.41906179	-2.57822711
C	0.51486984	-3.18514481	-1.71705751
O	-0.43609811	-3.46843549	-3.93241384
C	0.74144953	1.38106099	-4.52775847
C	0.74125818	-1.42401487	-4.51447051
C	1.91576698	0.67654815	-4.28486813
C	-0.43922939	0.66998438	-4.75193626
C	-0.43932813	-0.71484290	-4.74514272
C	1.91577991	-0.71749467	-4.27833025
H	2.83807168	1.21599694	-4.09310580
H	-1.36176530	1.21036988	-4.93409494
H	-1.36200361	-1.25684315	-4.92168641
H	2.83811437	-1.25521046	-4.08198752

C	0.72273580	2.88954384	-4.58817720
H	0.64788391	3.22011768	-5.62550756
O	-0.42237527	3.48448081	3.76350265
C	0.72174339	-2.93299894	-4.56085359
H	0.64883854	-3.27310346	-5.59524919
H	1.63791219	-3.35768652	-4.14035835
C	0.48278378	2.93239772	4.71449195
H	1.48969150	3.34147488	4.59287562
H	0.10316879	3.28199535	5.67593217
H	1.64025972	3.31718811	-4.17366127
C	-0.52014363	3.39717252	-2.60738830
H	1.52271736	2.95737274	-2.10501791
C	0.52208890	3.16559266	-1.74659524
C	-2.04848193	3.69031084	-0.75502816
C	0.30901642	3.22656738	-0.34201109
C	-1.82134506	3.65054728	-2.09854124
C	-0.98786817	3.48835653	0.17115574
C	1.36275682	3.02833773	0.58025555
H	-2.62304631	3.81651315	-2.80899837
H	-2.17974836	3.74755903	1.96276257
H	-3.04673385	3.88660899	-0.37812203
C	1.14990017	3.08442184	1.93366356
H	2.36041301	2.82812579	0.20419440
H	1.98307018	2.93281811	2.60702181
C	-0.14451653	3.35372882	2.43772656
C	-1.19149113	3.54063612	1.56660582
O	-0.43320542	3.43205431	-3.96217641
H	-2.01965645	0.00276077	-2.20009098
C	-1.52201630	0.00481127	-1.24094004
C	-0.16408928	0.00813880	1.17473671
C	-2.22324106	0.01660326	-0.04194079
C	-0.14537103	-0.00437441	-1.21530617
N	0.44186020	-0.00188258	-0.01596133
C	-1.54061331	0.01797420	1.17030753
H	-3.30568010	0.02452772	-0.05031528
H	0.50812199	-0.01247878	-2.07584138
H	-2.05830997	0.02646159	2.11847385
H	0.47017121	0.00776164	2.05068329
F	1.78794590	-0.00931560	-0.01325919

G2@M1-II

There is no imaginary frequency after optimization and frequency analysis.

C	0.26209501	4.54866577	1.56074544
C	-1.65051936	4.52728745	-0.49766572
C	0.59839238	4.97067047	0.27858299
C	-1.04887156	4.14025499	1.81046889
C	-1.99435978	4.13172453	0.79573134
C	-0.34938645	4.96014489	-0.74151598
H	1.61399986	5.28894072	0.06502281
H	-1.32586521	3.81551023	2.80806560
H	-3.00638431	3.80287156	1.00197790
H	-0.06251909	5.26584686	-1.74310032
C	1.27675707	4.53769964	2.67960263
H	1.04321495	5.31762795	3.40605353
H	2.28493101	4.73029418	2.30103830
O	1.23192634	3.33200358	3.43641239
C	-0.35011288	-4.62976040	-1.26377775
C	2.26519675	-4.29875837	-0.29453125
C	0.67245904	-4.21208871	-2.11229716
C	-0.04756387	-4.90357557	0.07065174
C	1.24522438	-4.73170259	0.55136705
C	1.96864279	-4.05633467	-1.63477031
H	0.45224314	-3.99878022	-3.15366341
H	-0.83408926	-5.22946743	0.74283883
H	1.46135490	-4.92790616	1.59675344
H	2.75409333	-3.72020506	-2.30352490
C	-1.76522411	-4.79429793	-1.76513668
H	-2.04332734	-5.84952062	-1.76536881
O	-3.65865184	3.48298092	-1.43115351
C	3.67271408	-4.09212413	0.21459411
H	4.34399372	-4.83384793	-0.22093215
C	-2.66770369	4.48833696	-1.61578969
H	-2.16306252	4.38161378	-2.58080979
H	-3.23104649	5.42336078	-1.64613947
H	-1.86708358	-4.42544976	-2.78983680
C	-2.87945547	-2.83578667	-0.91151281
H	-1.80154330	-2.31629721	-2.69629784
C	-2.40352739	-1.97018574	-1.86529709
C	-3.93273383	-1.01444730	0.28283417
C	-2.70492625	-0.58137261	-1.77950982
C	-3.64874275	-2.34250575	0.17548515
C	-3.47179693	-0.08917619	-0.69218059
C	-2.25601365	0.34900202	-2.75058759

H	-4.00082017	-3.05364234	0.91366066
H	-4.32492418	1.67191022	0.24039802
H	-4.51702482	-0.64992922	1.12093910
C	-2.53880689	1.68675633	-2.64550735
H	-1.68298403	-0.01281730	-3.59815150
H	-2.19941131	2.37055160	-3.41469036
C	-3.28719132	2.17002509	-1.54686749
C	-3.73955121	1.29571461	-0.59148065
O	-2.71360730	-4.18323246	-0.89642247
H	3.71864767	-4.20294069	1.30197175
O	4.21792300	-2.84296429	-0.20026272
C	3.75796690	-1.69623601	0.36472506
H	2.66802592	-2.49699372	2.03663500
C	2.98536024	-1.61293414	1.49724881
C	3.75106239	0.71217960	0.13904917
C	2.57808775	-0.34410562	1.98902830
C	4.14929261	-0.51361877	-0.31148269
C	2.94436203	0.83897735	1.30061103
C	1.77357707	-0.21821465	3.15182032
H	4.76454775	-0.61256883	-1.19852125
H	2.76951823	2.98443950	1.19428562
H	4.04884694	1.60823709	-0.39565163
C	1.35296380	1.00618986	3.58632628
H	1.48686109	-1.11294119	3.69428503
H	0.73842027	1.10532876	4.47383382
C	1.70908759	2.18581012	2.88477345
C	2.48989148	2.10302611	1.75834030
H	-0.11196053	2.46556160	-0.48124170
C	-0.00744691	1.39792696	-0.36920103
C	0.21203858	-1.33426863	-0.06461651
C	0.70625848	0.64586418	-1.29577049
C	-0.60628005	0.77423325	0.69749368
N	-0.45440125	-0.55174817	0.78441823
C	0.81225566	-0.72718237	-1.14546919
H	1.17843758	1.13673704	-2.13692002
H	-1.18150815	1.25588518	1.47441363
H	1.35931222	-1.34188998	-1.84467474
H	0.23003388	-2.38957043	0.16487204
F	-1.01958826	-1.15880197	1.84497572

G3@M1-I

There is no imaginary frequency after optimization and frequency analysis.

C	2.93574441	13.79265485	11.64250429
C	0.59989846	12.74398340	12.78695500
C	2.15872300	12.87551243	10.94425555
C	2.54947723	14.16258617	12.93274446
C	1.39684432	13.64429282	13.49769055
C	0.99759257	12.35461794	11.51295232
H	2.45606827	12.56809636	9.94644289
H	3.15503049	14.87123475	13.48828588
H	1.09932496	13.94601449	14.49655088
H	0.39590351	11.64378002	10.95515681
C	4.16497465	14.41654809	11.02910025
H	4.00953892	15.48697107	10.88572903
H	4.38044528	13.98400546	10.04774351
O	5.29704382	14.34281296	11.89055572
C	5.84681950	13.12352651	12.14517737
H	6.74715490	13.88138228	13.91633700
C	6.62982034	13.01887650	13.26955540
C	6.32879701	10.82805358	11.57737597
C	7.29542537	11.81237480	13.57643354
C	5.68851200	12.00584411	11.29202197
C	7.14334547	10.68831781	12.72484804
C	8.12579178	11.67896678	14.72300617
H	5.07727359	12.07361801	10.40164991
H	7.65455275	8.62415534	12.36705027
H	6.21374252	9.98320664	10.90655409
C	8.76366653	10.50446999	14.99239769
H	8.25100362	12.52991174	15.38427878
H	9.40470158	10.39952274	15.86016070
C	8.60550950	9.38113691	14.13895095
C	7.79681743	9.46493300	13.03475987
O	9.32613408	8.28937615	14.50723124
C	5.34711020	5.48487121	15.77022473
C	7.67583344	6.50644076	14.58392354
C	5.54264441	5.38216677	14.39728320
C	6.32024520	6.12025519	16.54537423
C	7.46926773	6.62427303	15.96054843
C	6.70000713	5.89091159	13.80781388
H	4.78810939	4.90525667	13.77937550
H	6.17145704	6.21432611	17.61556499
H	8.21891759	7.11208712	16.57396823
H	6.84055774	5.80527102	12.73472765

C	4.13117598	4.90075147	16.44880515
H	4.41386308	4.01221840	17.01599461
O	-0.49760223	11.76004485	14.72948637
C	8.96224647	7.01865546	13.98147416
H	9.79018620	6.36487250	14.26104191
H	8.91281453	7.03315747	12.88878467
C	-0.68435450	12.24438373	13.40256183
H	-1.16352229	11.49427304	12.76644987
H	-1.38897916	13.06960257	13.51804400
H	3.37287910	4.59584167	15.72140588
C	2.92885830	6.89340124	17.01191269
H	2.55817261	6.36557657	14.96281918
C	2.42763787	7.09573920	15.75187614
C	2.05894865	9.02592490	17.75125697
C	1.68697919	8.27401104	15.46321547
C	2.74506374	7.87827512	18.01784318
C	1.49987784	9.26071333	16.46474145
C	1.11713436	8.50200302	14.18911341
H	3.16448924	7.68953861	18.99947201
H	0.63101946	11.19262575	16.92603004
H	1.92780792	9.77374216	18.52633497
C	0.41643468	9.64647490	13.91130778
H	1.23578651	7.74816388	13.41775582
H	-0.00767496	9.77915044	12.92464435
C	0.23644161	10.62797065	14.91453015
C	0.77642742	10.43527555	16.16341215
O	3.59457266	5.78411115	17.42633655
H	3.17376699	11.13580111	13.14952769
C	3.75251499	10.81560943	14.00554545
C	5.24897012	9.85923311	16.09944348
N	4.29537813	9.58778298	13.95192166
C	3.94095313	11.61000996	15.11611423
C	4.69645931	11.13135698	16.17615060
C	5.03116002	9.10486263	14.97154319
H	3.49132630	12.59205635	15.13530080
H	4.85413765	11.74308883	17.05569131
H	5.42788305	8.10852359	14.84424597
H	5.84384003	9.44482759	16.90140100
H	3.51205888	9.25642558	12.03561063
C	4.09474622	8.72332266	12.78256471
H	5.06774326	8.45360040	12.37575171
H	3.56586198	7.82514778	13.09822236

G3@M1-II

There is no imaginary frequency after optimization and frequency analysis.

C	2.73262678	1.05383890	-4.66694458
C	0.57827215	2.85290326	-4.74372932
C	1.60073132	0.76965762	-5.42304953
C	2.78156086	2.25436209	-3.95450660
C	1.71921342	3.14276680	-3.99192980
C	0.53004561	1.66123527	-5.45930846
H	1.54551647	-0.16203736	-5.97715368
H	3.66162278	2.48916851	-3.36453435
H	1.76757382	4.07113147	-3.43307288
H	-0.35332484	1.41875645	-6.04183867
C	3.89980631	0.09918624	-4.59098112
H	4.80665979	0.58124663	-4.95854935
H	3.72598088	-0.79053896	-5.20264162
O	4.21437638	-0.25404582	-3.24470038
C	-3.27759641	-1.29304659	2.48045390
C	-1.84840071	-3.60809169	1.78158087
C	-3.73056222	-2.12530257	1.45868499
C	-2.10106422	-1.62956928	3.14812085
C	-1.39062189	-2.77189613	2.79740382
C	-3.02692423	-3.27322458	1.11575864
H	-4.64184598	-1.87295186	0.92550567
H	-1.73565987	-0.98872699	3.94367118
H	-0.47259120	-3.01713377	3.32216234
H	-3.38880562	-3.91036519	0.31602134
C	-4.05882223	-0.06494759	2.88844904
H	-4.49359488	-0.21335045	3.87836915
O	-0.84353540	4.41712514	-3.52177368
C	-1.10763337	-4.87247367	1.41267038
H	-1.68200562	-5.74634457	1.72480797
C	-0.56263243	3.84061159	-4.79399147
H	-1.45137779	3.38357343	-5.23755435
H	-0.29182386	4.69400698	-5.41857664
H	-4.88116508	0.12641239	2.19238856
C	-2.78530451	1.72729586	1.92851989
H	-3.83945713	0.65068968	0.39695670
C	-3.14757026	1.44854910	0.63548423
C	-1.31201587	3.49574819	1.18166223
C	-2.58394904	2.19198134	-0.43653240
C	-1.85907600	2.76962530	2.19792987
C	-1.64938766	3.22557179	-0.17261390
C	-2.90022889	1.90935046	-1.78726498

H	-1.60336458	2.97019419	3.23232736
H	-0.35096049	4.72574531	-1.04999711
H	-0.60536111	4.28950250	1.40080280
C	-2.32532681	2.60540478	-2.81886647
H	-3.61358854	1.12094450	-2.00468630
H	-2.59744335	2.36626828	-3.83924918
C	-1.39530233	3.63589454	-2.54763633
C	-1.06245026	3.93094776	-1.24767562
O	-3.23869821	1.08884029	3.03785985
H	-0.13670121	-4.92197095	1.91452729
O	-0.97128970	-5.02847172	0.00486908
C	-0.09671069	-4.23230820	-0.66551023
H	1.05589357	-3.45534225	0.97424308
C	0.90441561	-3.48487479	-0.09787523
C	0.53934058	-3.47904126	-2.87408038
C	1.76177417	-2.70553562	-0.91841963
C	-0.27395383	-4.22657983	-2.07286136
C	1.58138549	-2.68692068	-2.32243350
C	2.78700166	-1.89266894	-0.36735954
H	-1.07230517	-4.83006855	-2.48949582
H	2.22428274	-1.86766972	-4.20676431
H	0.38838997	-3.47715664	-3.94866077
C	3.56664333	-1.10551495	-1.16615167
H	2.94380812	-1.89732071	0.70660654
H	4.34729725	-0.48010257	-0.74762882
C	3.37208083	-1.08131210	-2.57061792
C	2.40077650	-1.86558509	-3.13873973
H	0.01001450	0.08906869	1.92070293
C	0.07521827	0.18530753	0.84640996
C	0.35460801	0.56176252	-1.85265252
N	0.94151410	1.09833273	0.37372937
C	-0.68540691	-0.56761443	-0.01667125
C	-0.54867388	-0.38019765	-1.38377400
C	1.08929332	1.29231626	-0.94956427
H	-1.37761769	-1.29066491	0.38629426
H	-1.13810496	-0.96648657	-2.07709275
H	1.80757644	2.04232570	-1.24834837
H	0.49309217	0.73908029	-2.90875671
H	1.31200478	1.87679076	2.28429219
C	1.77880487	1.87053986	1.30239447
H	2.76407847	1.40673514	1.35909845
H	1.86790331	2.88959339	0.93127860

G4@M1-I

There is no imaginary frequency after optimization and frequency analysis.

C	-3.80995271	3.34083131	4.21209727
C	-4.48049603	0.68461568	4.82530926
C	-4.90000117	2.72813967	3.60201128
C	-3.06018778	2.61384757	5.13948026
C	-3.39146461	1.30418169	5.44234571
C	-5.23321406	1.40927306	3.90656020
H	-5.49765571	3.28399300	2.88675146
H	-2.21360998	3.08484344	5.62876151
H	-2.80381747	0.75119914	6.16829713
H	-6.08853075	0.94430959	3.42666469
C	-3.40302673	4.75613230	3.88908398
H	-3.22377988	5.31523678	4.80777663
H	-4.18404493	5.27981982	3.33217392
O	-2.14923627	4.80334169	3.20544316
C	-2.07648733	4.40095187	1.90655498
H	0.01177531	4.05768666	2.11529811
C	-0.83359855	4.04908322	1.43590705
C	-3.02007124	4.04683653	-0.28752917
C	-0.64491387	3.69816520	0.08089155
C	-3.18625891	4.39412113	1.02750109
C	-1.75481823	3.68112202	-0.80217252
C	0.63296320	3.35958996	-0.44245079
H	-4.16995022	4.68067657	1.37490049
H	-2.45043505	3.29565900	-2.80697347
H	-3.87570789	4.05931264	-0.95474749
C	0.78714736	3.03403890	-1.75775979
H	1.49072767	3.36380884	0.22188300
H	1.76071351	2.78347973	-2.16346902
C	-0.32893688	3.00881040	-2.63464545
C	-1.57977835	3.31002123	-2.16260165
O	-0.02891861	2.69646718	-3.92408644
C	-2.14177278	-1.85613417	-3.78993262
C	-1.46559612	0.79795947	-4.40666161
C	-3.13287530	-0.92075905	-4.06665308
C	-0.80593001	-1.44969692	-3.81526942
C	-0.47267590	-0.14099047	-4.11895930
C	-2.79700861	0.39802311	-4.37366560
H	-4.17679616	-1.21752978	-4.03905568
H	-0.02534418	-2.16921739	-3.59319822
H	0.56841074	0.16270695	-4.13374373
H	-3.58161104	1.11894735	-4.58195354

C	-2.46813939	-3.30053328	-3.49315349
H	-2.20233962	-3.92597981	-4.34732758
O	-3.77050424	-1.63617940	4.69376884
C	-1.06451212	2.20801755	-4.76983016
H	-0.62593158	2.22553848	-5.76904149
H	-1.92781016	2.87952864	-4.78179576
C	-4.79113231	-0.75200030	5.16111286
H	-5.77615585	-1.04756574	4.79153954
H	-4.78998988	-0.89460838	6.24194676
H	-3.53693527	-3.43946013	-3.30755094
C	-1.95328465	-3.40593997	-1.15598027
H	-3.97448062	-2.72669667	-1.41327284
C	-3.14669114	-2.88221141	-0.73194629
C	-1.03779461	-3.25056595	1.07828381
C	-3.32944007	-2.55165164	0.63799804
C	-0.88876843	-3.58813780	-0.23450557
C	-2.26703550	-2.72433620	1.56190568
C	-4.55831310	-2.05004958	1.12494740
H	0.04378504	-3.99671158	-0.60686969
H	-1.63984848	-2.49626664	3.62421282
H	-0.21377455	-3.38206785	1.77165754
C	-4.72554630	-1.71756789	2.44348627
H	-5.38898191	-1.93347763	0.43662440
H	-5.68633218	-1.34681783	2.77421254
C	-3.65883421	-1.88258572	3.35924806
C	-2.45250320	-2.37187331	2.91687695
O	-1.67841077	-3.81099385	-2.42480494
H	1.08145759	0.64138656	4.57311253
C	0.75829411	0.50449062	3.54809983
H	-1.26344894	1.08630836	3.93140906
C	-0.53952919	0.75208395	3.19982840
C	1.31441658	-0.11741887	1.27210321
C	-0.95131691	0.57026242	1.85744059
C	1.68964535	0.06709017	2.57625922
C	-0.02087887	0.13151930	0.88420510
C	-2.27520380	0.81623162	1.46276334
H	2.71442812	-0.12356160	2.87393067
H	0.19457422	-0.37432786	-1.22019558
H	2.02560073	-0.45374347	0.52674531
N	-2.65263947	0.64556429	0.20762742
H	-3.02719132	1.15087185	2.16790685
C	-1.77065292	0.21911629	-0.75310345
H	-2.18218925	0.10740380	-1.74486795
C	-0.47891663	-0.03817522	-0.44345108

H	-4.01621100	1.65378144	-1.00902591
C	-4.03192864	0.90308391	-0.22044716
H	-4.45635996	-0.02302532	-0.60561520
H	-4.61364046	1.26162483	0.62550866

G4@M1-II

There is no imaginary frequency after optimization and frequency analysis.

C	5.75383151	-1.27621990	-0.05321226
C	5.21793402	1.39237078	-0.75557901
C	5.69703206	-0.89248871	-1.39015944
C	5.53292327	-0.31211037	0.93018023
C	5.27138725	1.00711719	0.58403799
C	5.43185622	0.42822629	-1.73750034
H	5.85284461	-1.63290694	-2.16884877
H	5.56827643	-0.59680267	1.97633155
H	5.10958154	1.74488778	1.36128915
H	5.38272218	0.70787274	-2.78564314
C	6.09282161	-2.69805896	0.33304350
H	7.12353700	-2.75013515	0.68833977
H	6.00756369	-3.36925902	-0.52744020
O	5.32266441	-3.17350400	1.42982738
C	-3.43716454	0.17171939	1.67323051
C	-3.17921079	-2.57607991	1.14173847
C	-3.99552443	-0.38324576	0.52245974
C	-2.74810700	-0.65717800	2.55415088
C	-2.61843506	-2.01669651	2.28778077
C	-3.87206257	-1.74114511	0.26427559
H	-4.53788584	0.25097216	-0.17233136
H	-2.31287247	-0.24033096	3.45539757
H	-2.08305072	-2.64833456	2.98880471
H	-4.31785104	-2.16145783	-0.63182899
C	-3.66051447	1.63424603	1.98406764
H	-4.60943841	1.74990735	2.51199104
O	4.27535544	3.57861810	-0.16639367
C	-3.03711153	-4.04140291	0.81023599
H	-3.99167827	-4.44585296	0.47328397
C	4.97699473	2.83195314	-1.15062399
H	4.48075400	2.88129786	-2.12490619
H	5.93209364	3.35180890	-1.25199481
H	-3.72539970	2.22454239	1.06383117
C	-1.45199565	2.45381467	2.39972125
H	-1.72454483	2.04124751	0.30862196
C	-1.05076599	2.36801450	1.09119599
C	0.74473614	3.19844451	3.08133493
C	0.28385062	2.70886582	0.73593916
C	-0.53858877	2.87478664	3.40301012
C	1.20150482	3.11941524	1.73677062
C	0.74884189	2.62023349	-0.59831188

H	-0.89445670	2.93213606	4.42529076
H	3.25034617	3.68950590	2.15450566
H	1.43673444	3.51602180	3.85413267
C	2.05500056	2.88554628	-0.91893954
H	0.05466754	2.32316884	-1.37788631
H	2.37781583	2.80307532	-1.94937459
C	2.96969601	3.26677448	0.09004823
C	2.54352109	3.38845935	1.38892764
O	-2.69457676	2.17319681	2.86906304
H	-2.71820445	-4.62197097	1.67983921
O	-2.15922231	-4.24970516	-0.29964798
C	-0.82056686	-4.10427434	-0.11883334
H	-0.70296462	-4.26412597	2.02243422
C	-0.17113554	-4.12274064	1.09059610
C	1.27684230	-3.77341060	-1.27668578
C	1.23575759	-3.95083503	1.14773894
C	-0.07639267	-3.94578449	-1.31562380
C	1.97512217	-3.74465746	-0.04103911
C	1.93568775	-3.93909166	2.38417625
H	-0.61467375	-3.94600168	-2.25660593
H	3.89505897	-3.28547870	-0.90332528
H	1.83137166	-3.63439837	-2.19863697
C	3.27616398	-3.68833063	2.42948358
H	1.38583861	-4.11555210	3.30284551
H	3.81273369	-3.66807849	3.37109063
C	4.00391714	-3.43402534	1.23806912
C	3.36678071	-3.47277210	0.02317482
H	-0.85035781	-0.62806728	-5.73894230
C	-0.71423266	-0.62412507	-4.66376213
H	1.41938726	-0.49624946	-4.78152718
C	0.54916985	-0.55063219	-4.13776622
C	-1.70876705	-0.69551307	-2.46555637
C	0.72673231	-0.54825299	-2.73681019
C	-1.85103515	-0.69535646	-3.82528301
C	-0.41383383	-0.62314407	-1.89851329
C	1.99829509	-0.48220893	-2.11960263
H	-2.83750050	-0.75228484	-4.26913941
H	-1.06295694	-0.71870901	0.17844513
H	-2.56713957	-0.75511456	-1.80890048
C	2.10058895	-0.49196222	-0.76922406
H	2.89775792	-0.42082740	-2.71771760
H	3.03970056	-0.43670345	-0.23836778
N	0.98284606	-0.57862915	0.01876229
C	-0.22747137	-0.64583866	-0.50790358

H	0.23192639	-0.80395428	1.96113761
C	1.17090585	-0.54945066	1.47505817
H	1.94163785	-1.27054557	1.74185119
H	1.48235838	0.45438606	1.76408510

7. References

[1] (a) E. T. Jarvi and H. W. Whitlock, *J. Am. Chem. Soc.* 1982, **104**, 7196-7204; (b) B. J. Whitlock, E. T. Jarvi, H. W. Whitlock, *J. Org. Chem.* 1981, **46**, 1832-1835. (c) B. J. Whitlock and H. W. Whitlock, *J. Am. Chem. Soc.* 1994, **116**, 2301-2311.

[2] G. M. Sheldrick, *Acta Cryst.* 2015, **A71**, 3–8.

[3] G. M. Sheldrick, *Acta Cryst.* 2015, **C71**, 3–8.

[4] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Cryst.* 2009, **42**, 339–341.

[5] A. L. Spek, *Acta Crystallorgr.* 2015, **C71**, 9-18.

[6] *Gaussian 09, Revision D.01,* M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. 10 Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc.: Wallingford CT, USA, 2013.

[7] (a) J.-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615–6620; (b) A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B.*, 2009, **113**, 6378–6396;

[8] (a) E. Papajak, J. Zheng, X. Xu, H. R. Leverentz and D. G. Truhlar, *J. Chem. Theory Comput.*, 2011, **7**, 3027-3034; (b) J. Zheng, X. Xu and D. G. Truhlar, *Theor. Chem. Acc.*, 2011, **128**, 295-305.

[9] C. Lefebvre, G. Rubez, H. Khartabil, J.-C. Boisson, J. Contreras-García, E. Hénon, *Phys. Chem. Chem. Phys.* 2017, **19**, 17928−17936.

[10] T. Lu, F. Chen, *J. Comput. Chem.* 2012, **33***,* 580−592.

[11] W. Humphrey, A. Dalke, K. Schulten, *J. Mol. Graph. Model.* 1996, **14***,* 33−38.