

Electronic Supplementary Information

Synthesis and property of an *O*-doped aromatic belt

Ying Han,^{a,*} Wei-Chen Guo,^{a,b} Xu-Sheng Du^a and Chuan-Feng Chen^{a,b,*}

^a *Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Molecular Recognition and Function, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.*

^b *University of Chinese Academy of Sciences, Beijing 100049, China.*

Email: hanying463@iccas.ac.cn; cchen@iccas.ac.cn

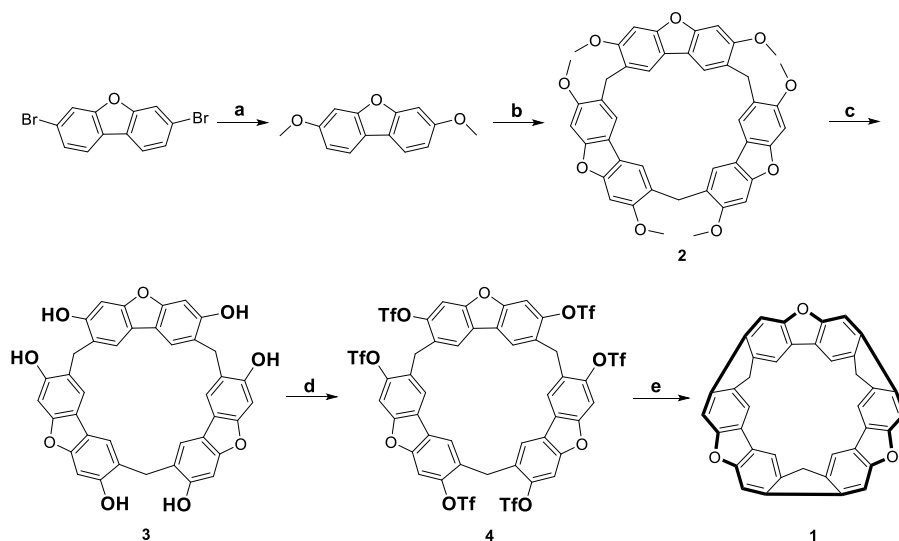
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1. General information

The commercially available reagents were used without further purification. Solvents were employed as purchased or dried with Molecular Sieves. ^1H NMR spectra and ^{13}C NMR spectra were recorded on the Bruker NMR spectrometer. Atmospheric pressure chemical ionization mass spectra (APCI-MS) were recorded on the Thermo Fisher® Exactive high-resolution LC-MS spectrometer. Circular dichroism spectroscopy was recorded on a J-815 spectrometer. UV-vis absorption spectroscopy was recorded on a UV/VIS/NIR spectrometer. Fluorescence emission spectroscopy was recorded on a Lambda 950 spectrometer. Preparative silica gel plates separation and normal TLC analysis were performed on pre-coated, glass-backed silica gel plates. The energy-minimized structures of aromatic belts were optimized using the Gaussian 09 program,^{S1} based on the density functional theory (DFT) using the B3LYP functional and 6-31G(d) basis set.

2. Synthesis and optimization of the reaction conditions



Scheme S1. Synthesis route of *O*-doped aromatic belt **1**. Reagents and conditions: (a) NaOMe, MeOAc, CuBr, Toluene, 110 °C, 72 h, 98%; (b) $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$, $(\text{CH}_2\text{O})_n$, CH_2Cl_2 , 0 °C, 2 h, 33%; (c) BBr_3 , CH_2Cl_2 , 0 °C, 12 h, 86%; (d) Tf_2O , pyridine, CH_2Cl_2 , 0 °C, 6 h, 61%; (e) $\text{Ni}(\text{cod})_2$, bpy, NMP, 95 °C, 6 h, 10%.

2.1 Synthesis of 3,7-dimethoxydibenzofuran

To a solution of 3,7-dibromodibenzofuran (3.25 g, 10 mmol) and copper(I) bromide (0.75 g, 0.5 mmol) in anhydrous toluene (300 mL) was added methyl acetate (100 mL) at room temperature under argon atmosphere. The mixture was stirred 5 minutes, and then added sodium methoxide (30% ww, methanol solution) (50 mL). The mixture was heated to 110 °C in an oil bath for 72 hours. Then the mixture was cooled down to room temperature, and quenched with water, and extracted with dichloromethane (200 mL×3). The combined organic layer was dried with anhydrous MgSO₄, and concentrated under a reduced pressure to give a crude solid. The crude solid was purified by silica gel column chromatography (eluent: dichloromethane/petroleum ether=1/3, v/v) to obtain the target compound. Yield: 98% (2.24 g), white solid. M.p.: 161-163 °C. ¹H NMR (400 MHz, CDCl₃, 298 K): δ 7.62 (d, *J*=12.0 Hz, 2H), 6.99 (s, 2H), 6.82 (dd, *J*=12.0, 2H), 3.82 (s, 6 H). ¹³C NMR (100 MHz, CDCl₃, 298 K): δ 157.9, 156.5, 119.0, 116.5, 109.6, 95.6, 54.7. HRMS (APCI): *m/z* calcd for [M+H]⁺: C₁₄H₁₃O₃⁺: 229.0859, found 229.0862.

2.2 Synthesis of dibenzofuran[3]arene (2)

To a solution of 3,7-dimethoxydibenzofuran (1.14 g, 5 mmol) and paraformaldehyde (465 mg, 15 mmol) in anhydrous dichloromethane (500 mL) was added FeCl₃·6H₂O (270 mg, 1 mmol) at 0 °C. The mixture was stirred for 2 h at 0 °C. Then the reaction was quenched by the addition of water (200 mL), and extracted with dichloromethane (3×200 mL). The combined organic layer was dried with anhydrous MgSO₄, and concentrated under a reduced pressure to give a crude solid. The crude solid was purified by silica gel column chromatography (eluent: dichloromethane/petroleum ether=2/3, v/v) to obtain macrocycle **2**. Yield: 33% (1.11 g), white solid, M.p.: >280 °C. ¹H NMR (400 MHz, CDCl₃, 298 K): δ 7.46 (s, 6H), 7.09 (s, 6H), 4.14 (s, 6H), 3.92 (s, 18 H). ¹³C NMR (100 MHz, CDCl₃, 298 K): δ 156.6, 155.3, 124.6, 120.6, 116.7, 93.4, 55.9, 27.2. HRMS (APCI): *m/z* calcd for [M+H]⁺: C₄₅H₃₇O₉⁺: 721.2432, found 721.2440.

2.3 Synthesis of dihydroxydibenzofuran[3]arene (3)

To a solution of **2** (0.72 g, 1.0 mmol) in anhydrous dichloromethane (200 mL) was added BBr₃ (473 μL, 5 mmol) at 0 °C. The mixture was warmed slowly to room temperature and stirred for 12 h. Then the reaction was quenched by the addition of water (100 mL), and extracted with dichloromethane (3×200 mL). The combined organic layer was dried with anhydrous MgSO₄, then concentrated under a reduced pressure to give a crude solid. The crude solid was purified by silica gel column chromatography (eluent: dichloromethane/methanol=10/1, v/v), to obtain compound **3**. Yield: 86% (0.55 g), white solid, M.p.: >280 °C. ¹H NMR (400 MHz, CDCl₃, 298 K): δ 8.84 (s, 6 H), 7.88 (s, 6 H), 7.31 (s, 6 H), 3.79 (s, 6 H). ¹³C NMR (100 MHz, CDCl₃, 298 K): δ 155.9, 153.2, 123.9, 120.6, 117.3, 98.2. HRMS (APCI): *m/z* calcd for [M+H]⁺: C₃₉H₂₅O₉⁺: 637.1499, found 637.1496.

2.4 Synthesis of dimethoxydibenzofuran[3]arene triflate (4)

To a solution of **3** (0.55 g, 0.86 mmol) and pyridine (2 mL) in anhydrous CH₂Cl₂ (200 mL) was added trifluoromethanesulfonic anhydride (1.1 ml, 3 mmol) at 0 °C for 6 hours. After the reaction was completed, the mixture was quenched by the addition of water (150 mL), and extracted with dichloromethane (3×200 mL). The organic phase was combined and the solvent was removed by rotary evaporation. The residue was purified by silica gel column chromatography (eluent: dichloromethane/petroleum ether=1/3, v/v) to obtain compound **4**. Yield: 61% (0.74 g), white solid, M.p.: 232-234 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.37 (s, 6 H), 7.05 (s, 6 H), 4.06 (s, 6 H). ¹³C NMR (100 MHz, CDCl₃, 298 K): δ 155.9, 146.8, 127.6, 123.1, 122.8, 118.6 (q, *J*_(C,F)=320 Hz), 106.6, 28.7. HRMS (APCI): *m/z* calcd for [M]⁻: C₄₅H₁₈F₁₈O₂₁S₆⁻: 1427.8377, found 1427.8364.

2.5 Synthesis of O-doped aromatic belt 1

In the glovebox, to a dry Schlenk tube was added Ni(cod)₂ (444 mg, 1.62 mmol), and then added a fresh solution of 2,2'-bipyridyl (bpy, 252.9 mg, 1.62 mmol) in *N*-methyl-2-pyrrolidone (NMP) (18.0 mL). The mixture was stirred for 40 minutes at

room temperature and a dark purple solution was obtained. Then the mixture was heated to 80 °C in an oil bath for 5 minutes, and the solution of **4** (385.2 mg, 0.27 mmol) in anhydrous NMP (27.0 mL) was added and kept stirring at 95 °C for 6 h. The mixture was cooled down to room temperature, and then poured into a mixture of CH₂Cl₂ (50 mL) and NH₄Cl (saturated solution, 50 mL), and vigorously stirred for 10 minutes. The red organic layer was separated and washed with water (3×20 mL), and then concentrated to a minimum by a rotary evaporator. The concentrated dark red mixture was washed twice with water (50 mL), dichloromethane (5 mL) and toluene (20 mL) to completely remove NMP. Finally, the red product **1** were obtained by rapid separation using silica gel plate (eluent: dichloromethane/*n*-hexane/carbon disulfide=25/50/2, v/v/v). Yield: 10% (8 mg), red solid, M.p.: 150-152 °C. ¹H NMR (400 MHz, CDCl₃, 298 K): δ 8.08 (s, 6H), 7.92 (s, 6H), 4.39 (d, *J*=16.0, 3H), 3.94 (d, *J*=16.0, 3H). ¹³C NMR (126 MHz, CDCl₃, 298 K): δ 163.1, 145.1, 140.6, 121.3, 120.9, 111.8, 41.0. HRMS (APCI): *m/z* calcd for [M+H]⁺: C₃₉H₁₉O₃⁺: 535.1334, found 535.1332.

Table S1. Optimization of the reaction conditions for **2**

Entry	Catalyst	Solvent	T	Time	Yield
1	AlCl ₃	DCM ^a	0 °C	2 h	- ^c
2	AlCl ₃	DCM	25 °C	2 h	-
3	FeCl ₃ ·6H ₂ O	DCM	0 °C	2 h	33%
4	FeCl ₃ ·6H ₂ O	DCM	25 °C	4 h	11%
5	BF ₃ ·Et ₂ O	DCM	0 °C	2 h	29%
6	BF ₃ ·Et ₂ O	DCE ^b	0 °C	2 h	13%
7	BF ₃ ·Et ₂ O	DCM	25 °C	1 h	27%
8	CF ₃ CO ₂ H	DCM	0 °C	1 h	-

^aDCM=dichloromethane; ^bDCE=1,2-dichloroethane; ^c-=No product.

Table S2. Optimization of the reaction conditions for **1**

Entry	Catalyst	Solvent	T	Time	Yield
1	Ni(cod) ₂ , bpy ^a	NMP ^b	80 °C	2 h	1%
2	Ni(cod) ₂ , bpy	NMP	85 °C	2 h	1%
3	Ni(cod) ₂ , bpy	NMP	90 °C	2 h	3%
4	Ni(cod) ₂ , bpy	NMP	95 °C	4 h	4%
5	Ni(cod) ₂ , bpy	NMP	95 °C	6 h	10%
6	Ni(cod) ₂ , bpy	NMP	95 °C	8 h	8%
7	Ni(cod) ₂ , bpy	NMP	100 °C	2 h	- ^c

^abpy=2,2'-bipyridyl; ^bNMP= *N*-methyl-2-pyrrolidone; ^c-=No product.

3. ^1H , ^{13}C NMR and HRMS spectra for new compounds

ysl-1 #13 RT: 0.16 AV: 1 NL: 8.13E5
T: FTMS (1,1) + p APCI corona Full ms [100.00-1000.00]

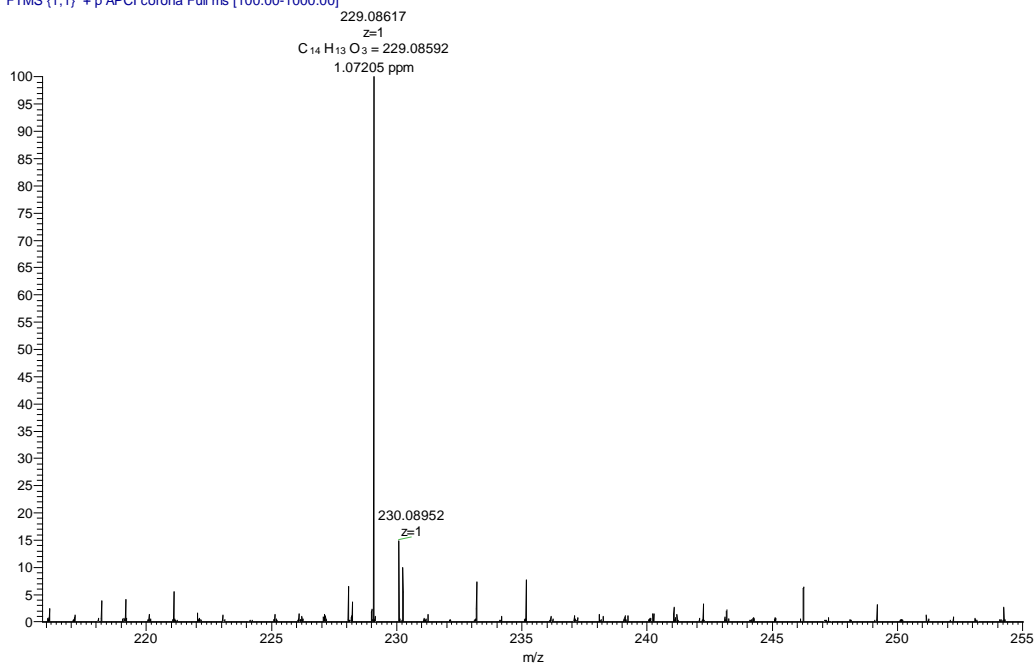


Fig. S1. HRMS (APCI, positive ion mode) spectrum of 3,7-dimethoxydibenzofuran.

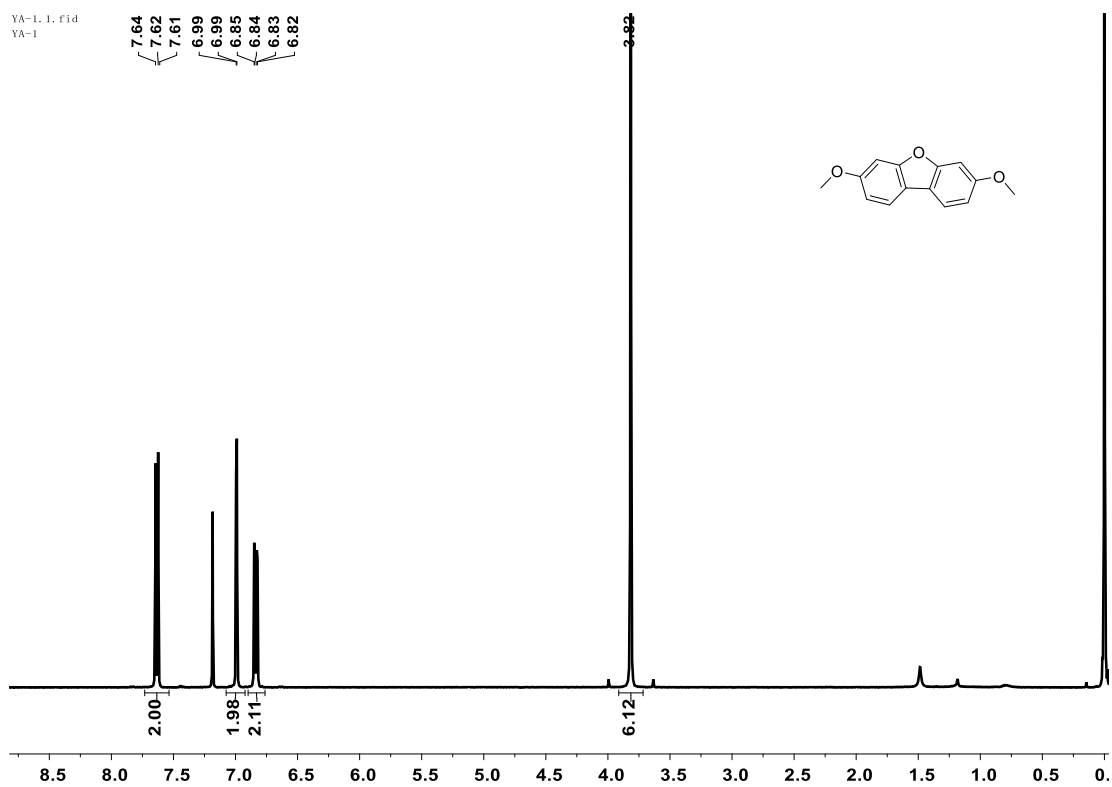


Fig. S2. ^1H NMR spectrum (400 MHz, CDCl_3 , 298K) of 3,7-dimethoxydibenzofuran.

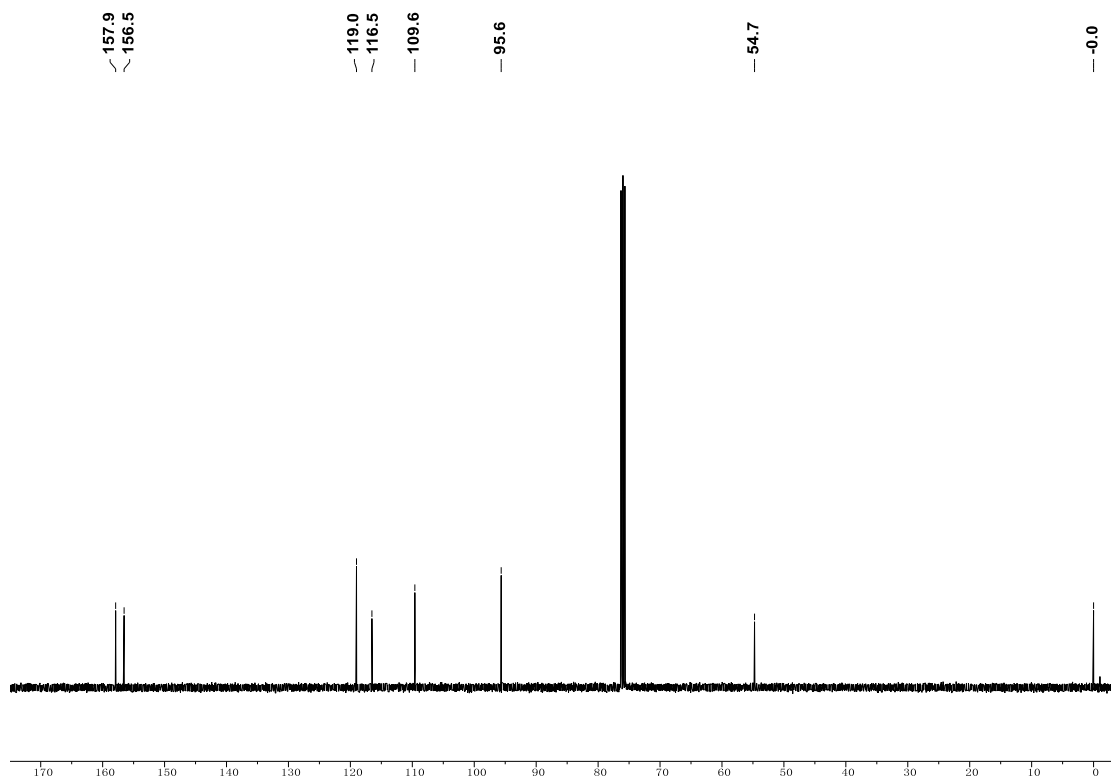


Fig. S3. ^{13}C NMR spectrum (100 MHz, CDCl_3 , 298K) of 3,7-dimethoxydibenzofuran.

ysl-2 #13 RT: 0.16 AV: 1 NL: 3.94E5
T: FTMS (1,1) + p APCI corona Full ms [100.00-1000.00]

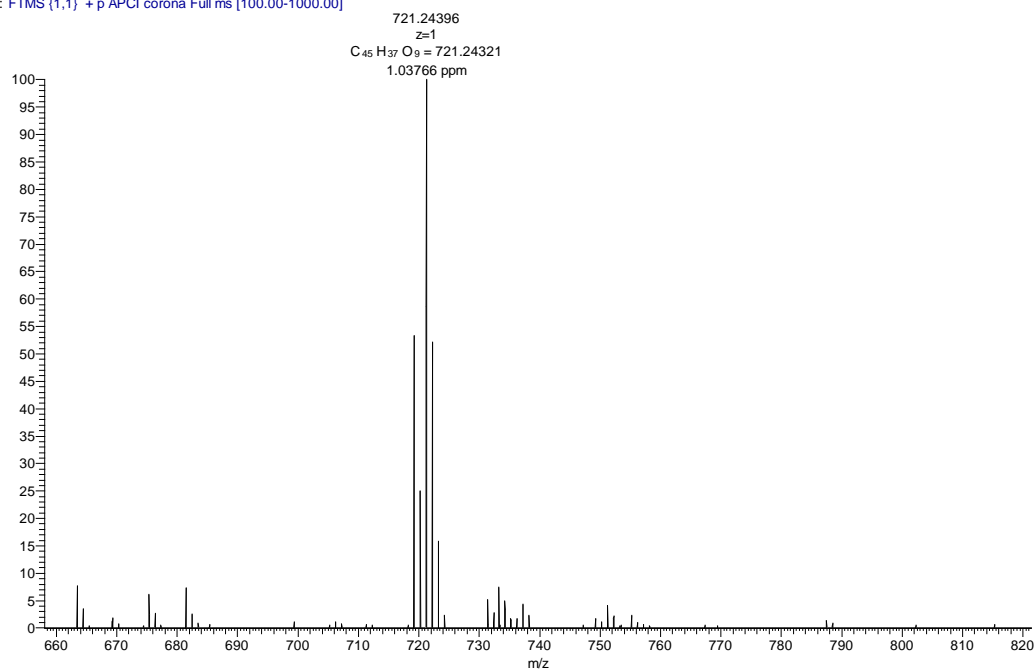


Fig. S4. HRMS (APCI, positive ion mode) spectrum of **2**.

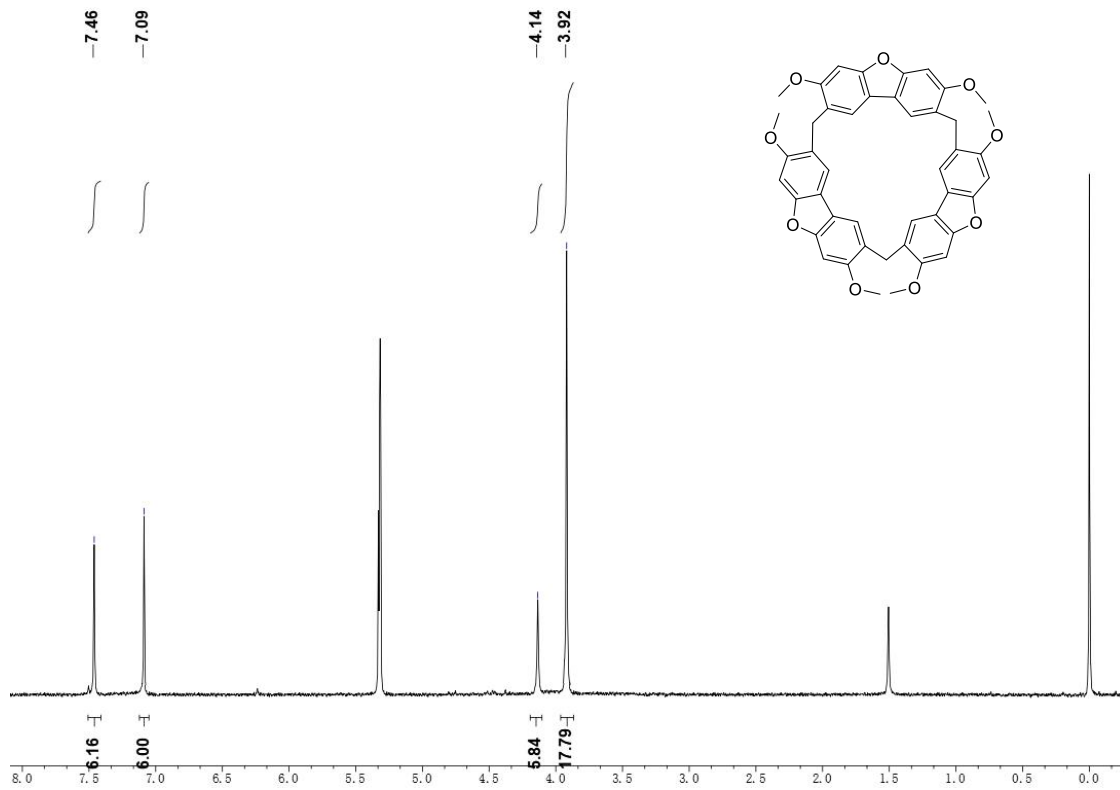


Fig. S5. ^1H NMR spectrum (400 MHz, CD_2Cl_2 , 298 K) of **2**.

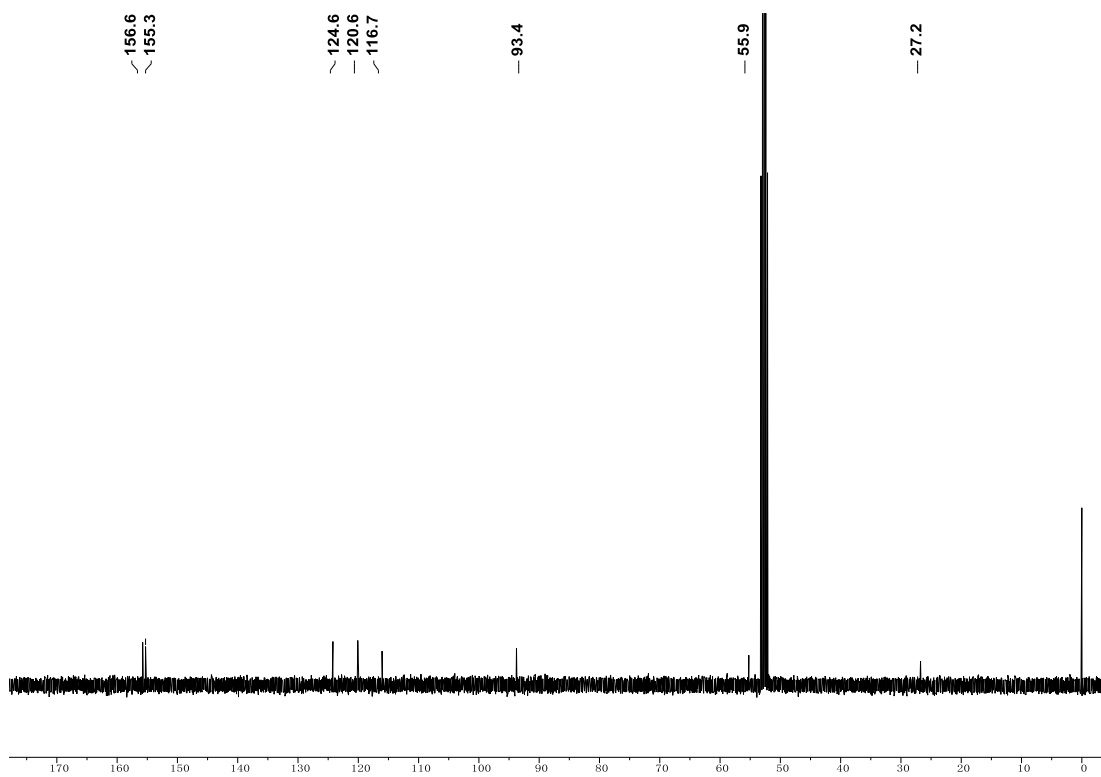


Fig. S6. ^{13}C NMR (100 MHz, CD_2Cl_2 , 298 K) spectrum of **2**.

ysl-3 #11 RT: 0.14 AV: 1 NL: 4.60E6
T: FTMS (1,1) + p APCI corona Full ms [100.00-1000.00]

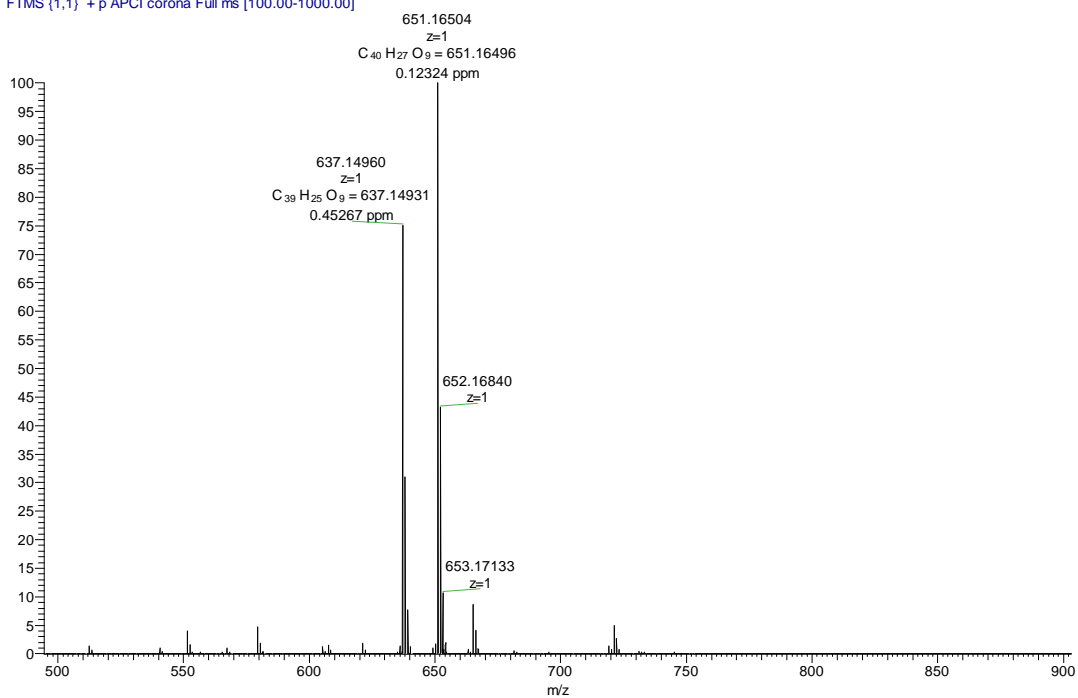


Fig. S7. HRMS (APCI, positive ion mode) spectrum of **3**.

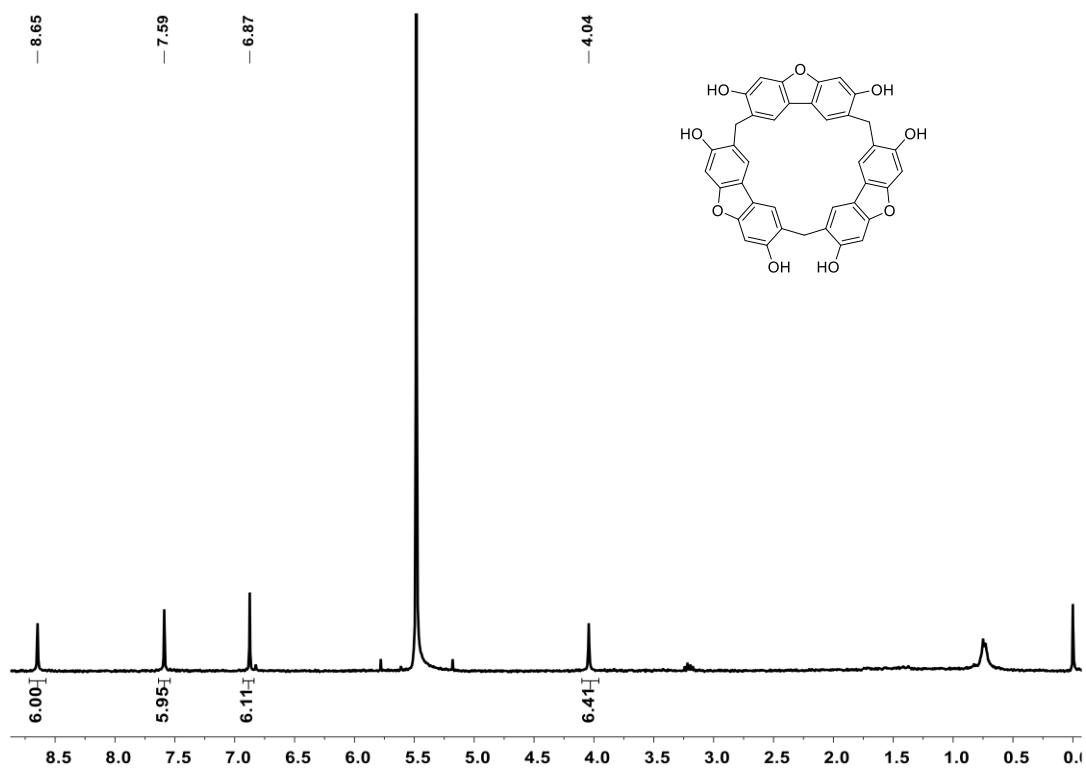


Fig. S8. ¹H NMR spectrum (400 MHz, acetone-*d*₆, 298K) of **3**.

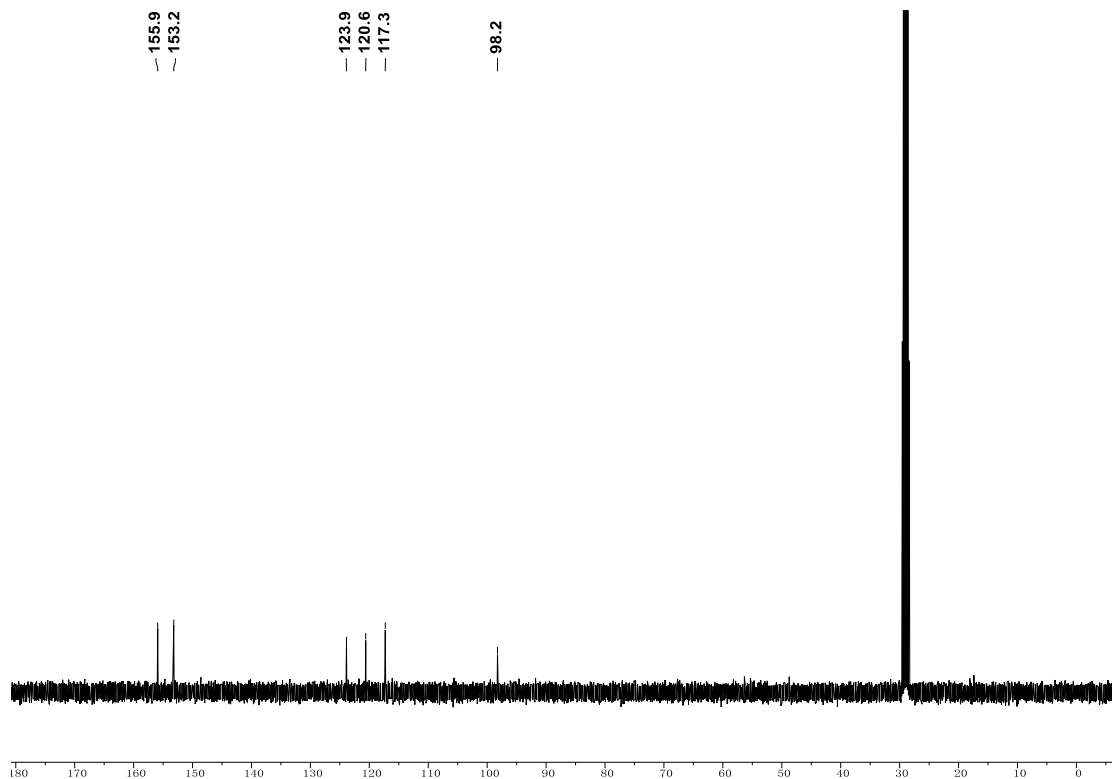


Fig. S9. ^{13}C NMR (100 MHz, acetone- d_6 , 298 K) spectrum of **3**.

ysl-4 #10 RT: 0.12 AV: 1 NL: 1.59E7
 T: FTMS (1,2) - p APCI corona Full ms [200.00-2000.00]

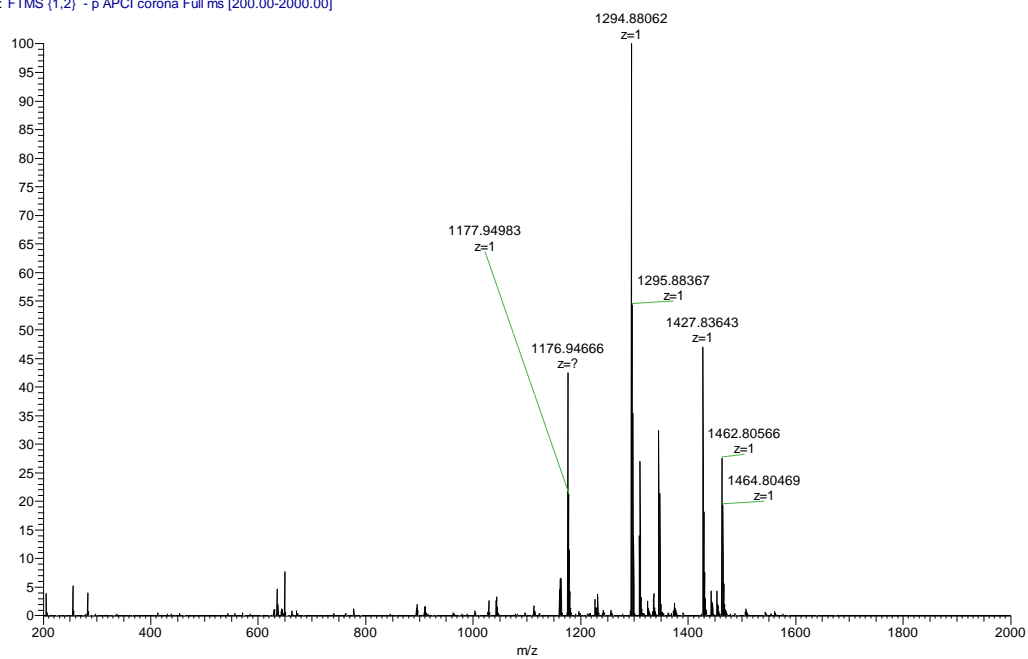


Fig. S10. HRMS (APCI, negative ion mode) spectrum of **4**.

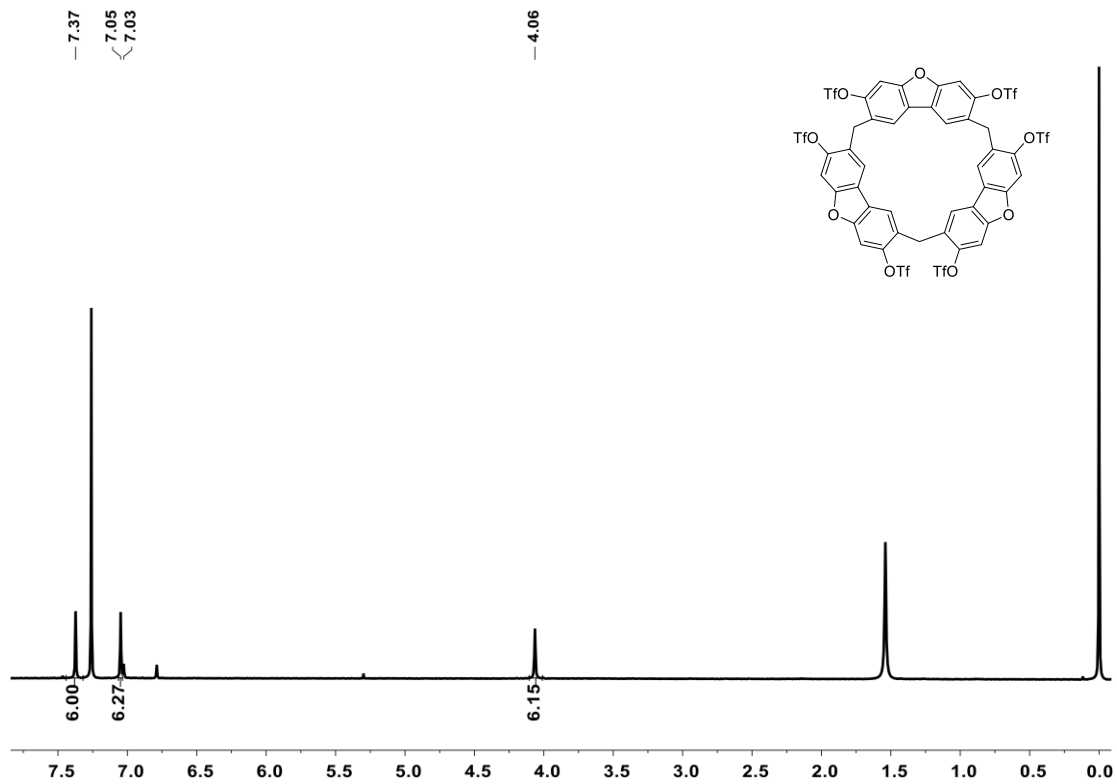


Fig. S11. ¹H NMR spectrum (400 MHz, CDCl₃, 298K) of 4.

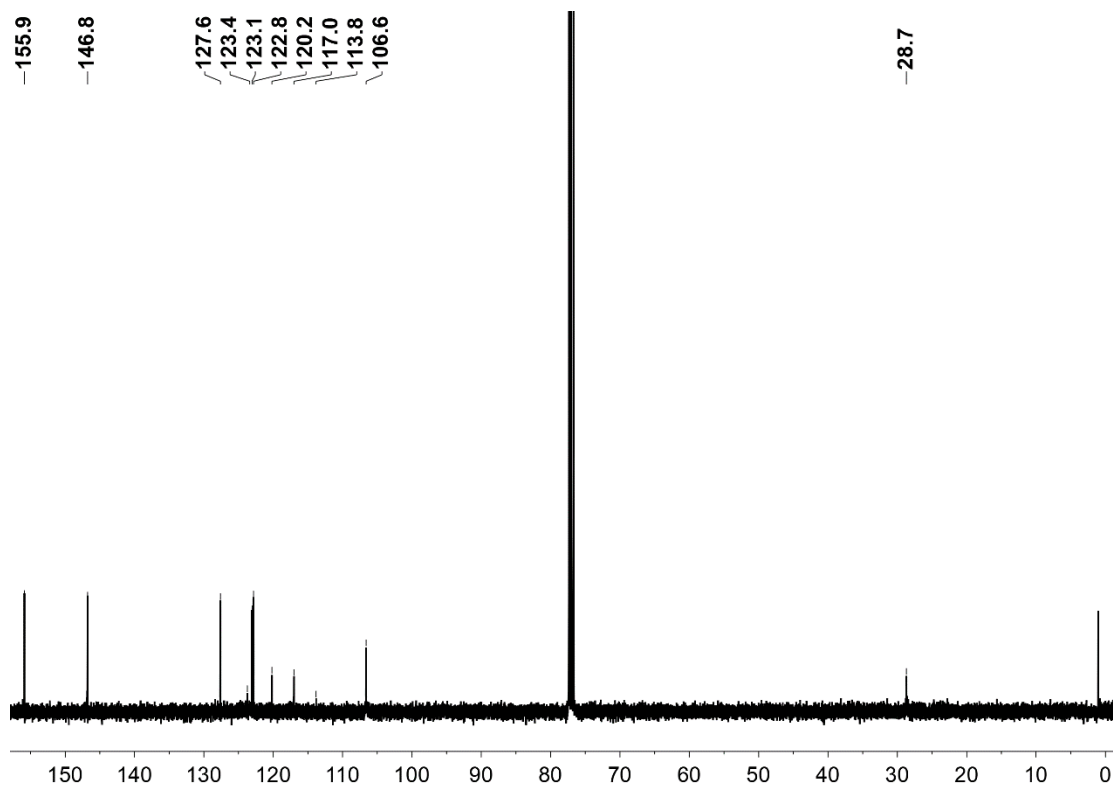


Fig. S12. ¹³C NMR (100 MHz, CDCl₃, 298 K) spectrum of 4.

ysl-5 #23 RT: 0.28 AV: 1 NL: 1.68E6
T: FTMS (1,1) + p APCI corona Full ms [100.00-1000.00]

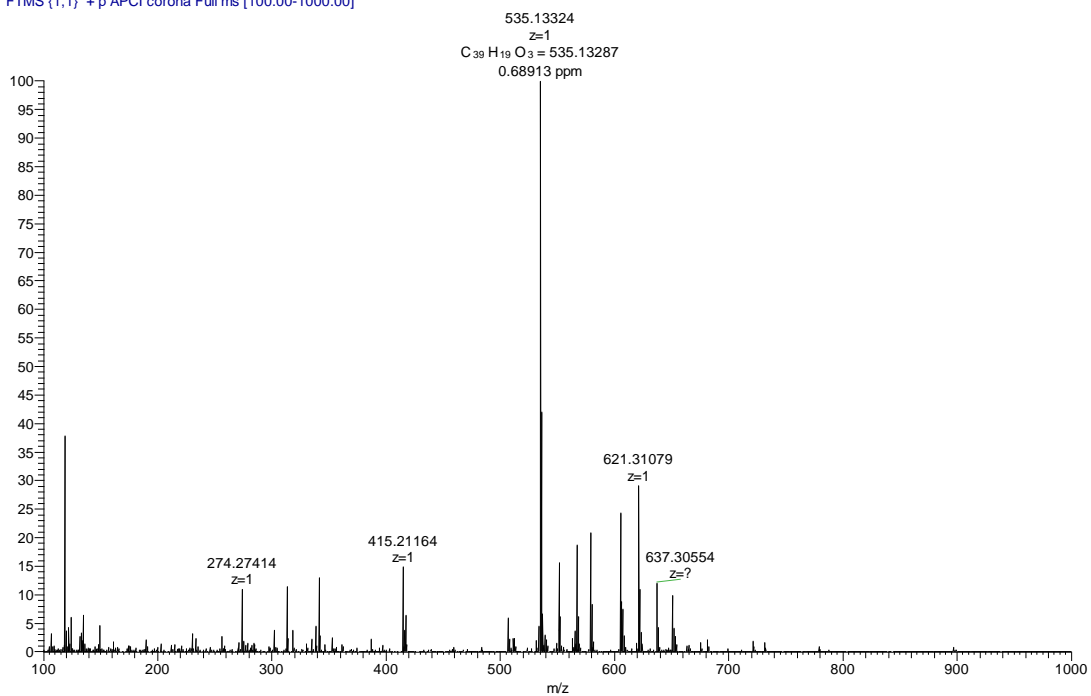


Fig. S13. HRMS (APCI, positive ion mode) spectrum of **1**.

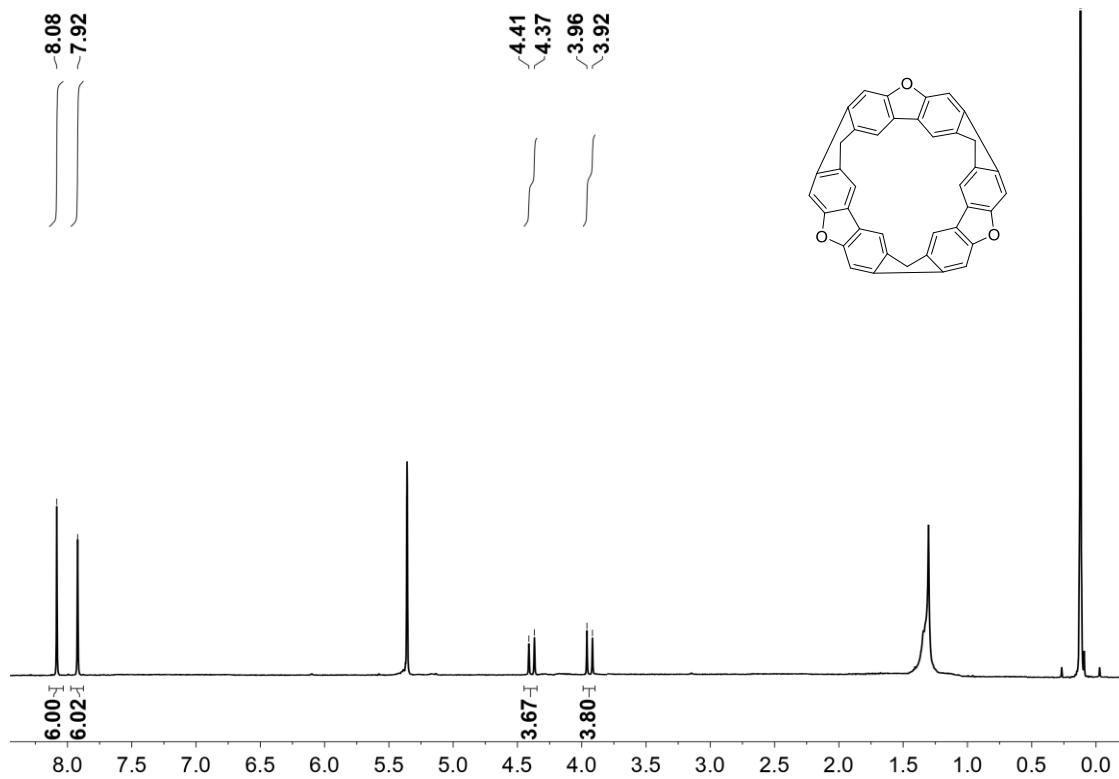


Fig. S14. ¹H NMR spectrum (400 MHz, CD₂Cl₂, 298K) of **1**.

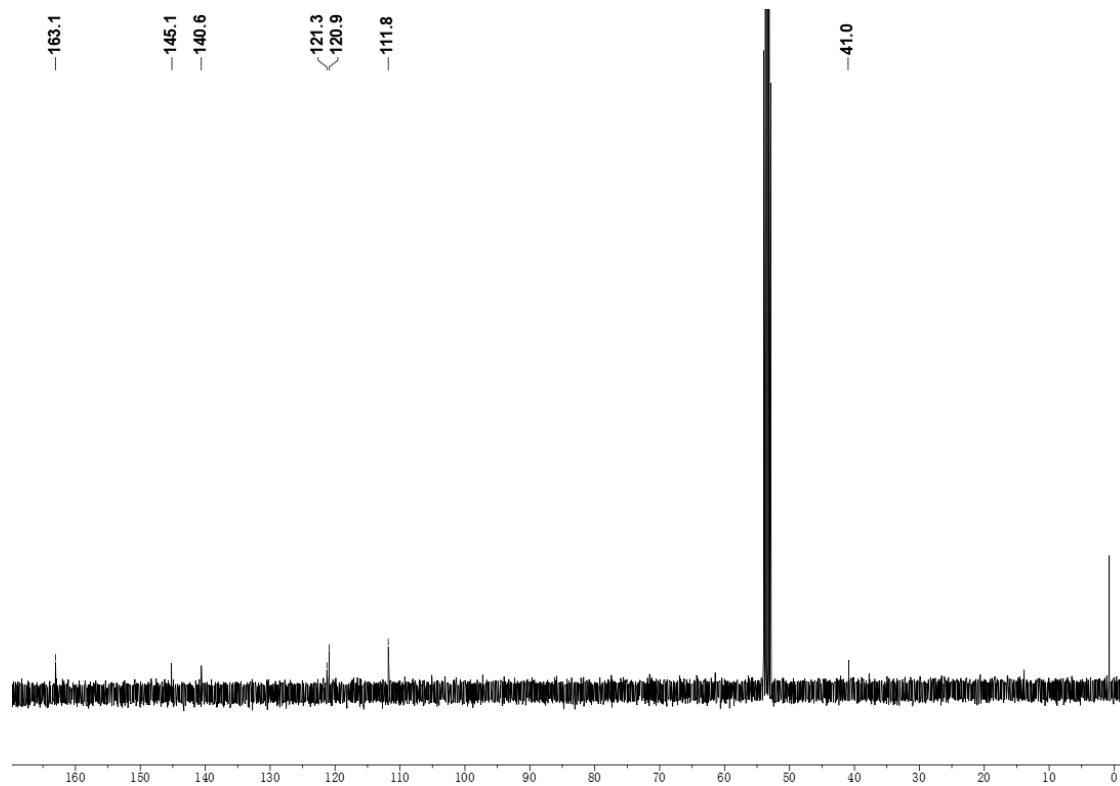


Fig. S15. ^{13}C NMR (126 MHz, CD_2Cl_2 , 298 K) spectrum of **1**.

4. X-Ray crystallographic analysis

Crystallographic data are summarized in Table S3-S4. A single crystal of belt **1** was obtained by vapor diffusion of CH₃CN into a solution of **1** in CH₂Cl₂. The crystal of **2** were cultivated by vapor diffusion of CH₃CN into a solution of **2** in CH₂Cl₂. The data of **1** and **2** were collected at 170 K on a Rigaku Synergy-R diffractometers with MoK α radiation ($\lambda = 1.54184 \text{ \AA}$) focused by multilayer confocal mirror.

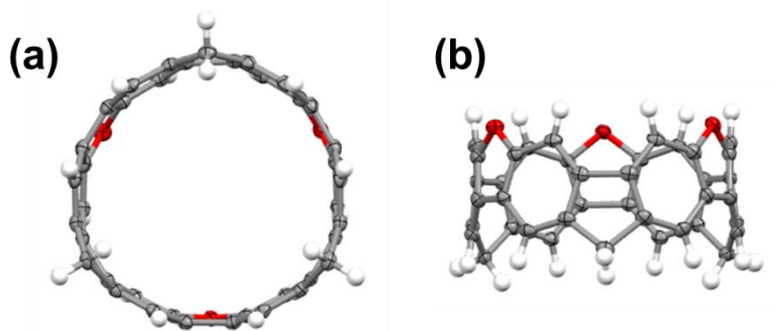


Fig. S16. ORTEP drawing of belt **1** from (a) top view and (b) side view (the thermal ellipsoids are displayed at a 30 % probability).

Table S3. X-ray crystallographic and the refinement data of **1**
(CCDC 2279354)

Empirical formula	C ₃₉ H ₁₈ O ₃
Formula weight	534.53
Temperature/K	169.99(10)
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	11.4275(4)
b/Å	15.9886(6)
c/Å	16.0325(4)
α /°	90
β /°	97.391(3)

$\gamma/^\circ$	90
Volume/ \AA^3	2904.96(17)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.222
μ/mm^{-1}	0.610
F(000)	1104.0
Crystal size/ mm^3	$0.18 \times 0.02 \times 0.02$
Radiation	CuK α ($\lambda = 1.54184$)
2 Θ range for data collection/	7.842 to 152.678
Index ranges	$-14 \leq h \leq 14, -20 \leq k \leq 19, -15 \leq l \leq 20$
Reflections collected	40878
Independent reflections	5953 [$R_{\text{int}} = 0.0715, R_{\text{sigma}} = 0.0430$]
Data/restraints/parameter s	5953/0/379
Goodness-of-fit on F^2	1.056
Final R indexes [$I \geq 2\sigma$ (I)]	$R_1 = 0.0634, wR_2 = 0.1471$
Final R indexes [all data]	$R_1 = 0.0845, wR_2 = 0.1585$
Largest diff. peak/hole / e \AA^{-3}	0.25/-0.22

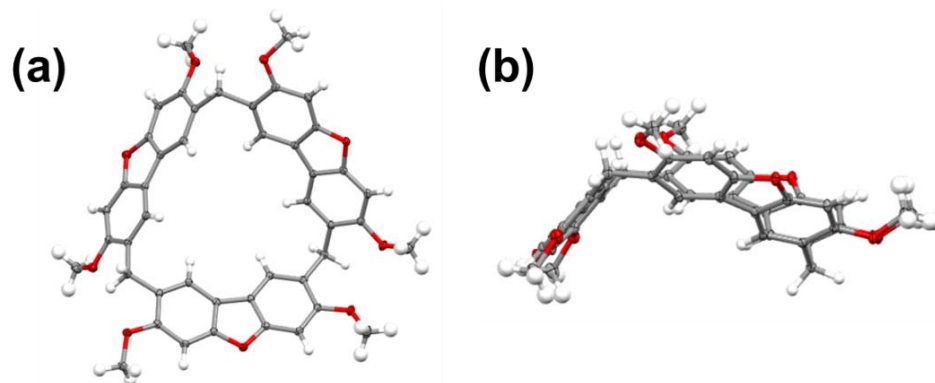


Fig. S17. ORTEP drawing of **2** from (a) top view and (b) side view (the thermal ellipsoids are displayed at a 30 % probability).

Table S4. X-ray crystallographic and the refinement data of **2**
(CCDC 2279353)

Empirical formula	C ₄₅ H ₃₆ O ₉
Formula weight	720.74
Temperature/K	169.99(10)
Crystal system	orthorhombic
Space group	Pbcm
a/Å	16.1779(3)
b/Å	7.77835(17)
c/Å	27.1947(7)
α /°	90
β /°	90
γ /°	90
Volume/Å ³	3422.12(13)
Z	4
ρ_{calc} /cm ³	1.399
μ /mm ⁻¹	0.795

F(000)	1512.0
Crystal size/mm ³	0.5 × 0.5 × 0.05
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/	5.462 to 150.634
Index ranges	-20 ≤ h ≤ 12, -7 ≤ k ≤ 9, -33 ≤ l ≤ 33
Reflections collected	13451
Independent reflections	3546 [R _{int} = 0.0636, R _{sigma} = 0.0584]
Data/restraints/parameters	3546/0/251
Goodness-of-fit on F ²	1.072
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0471, wR ₂ = 0.1158
Final R indexes [all data]	R ₁ = 0.0526, wR ₂ = 0.1194
Largest diff. peak/hole / e Å ⁻³	0.29/-0.22

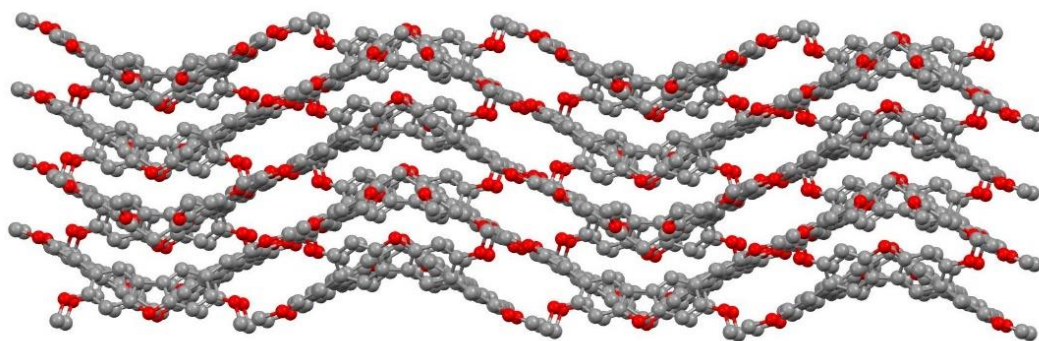


Fig. S18. Packing of the crystal structure of **2** viewed along the *a*-axis.

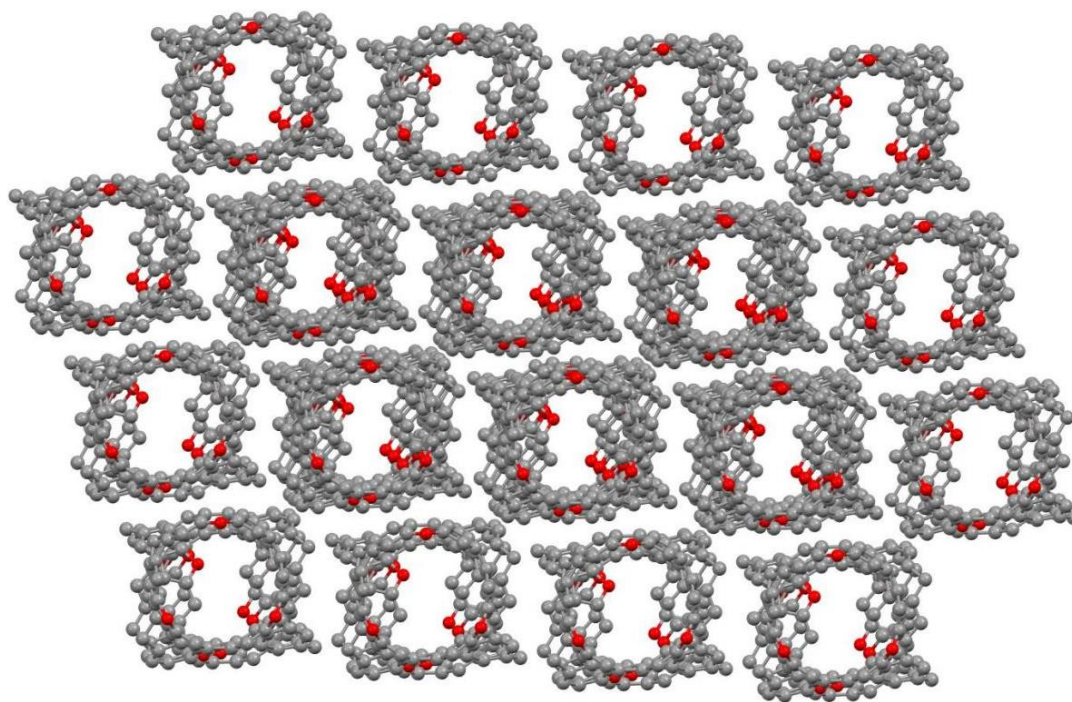


Fig. S19. Packing of the crystal structure of belt **1** viewed along the *a*-axis.

5. Theoretical calculations

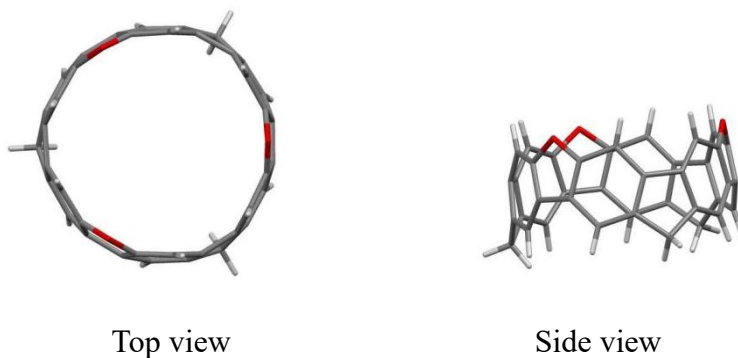


Fig. S20. Energy minimized structures of **1** depicting (a) top and (b) side views.

Excitation energies and oscillator strengths:

Excited State 1:	Singlet-A	2.6358 eV	470.38 nm	f=0.0009	$\langle S^{*2} \rangle = 0.000$
	136 ->141	-0.11387			
	137 ->140	-0.13460			
	138 ->139	0.68004			

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -1721.59825989

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2:	Singlet-A	3.8351 eV	323.29 nm	f=0.9671	$\langle S^{*2} \rangle = 0.000$
	137 ->139	-0.46368			
	138 ->140	0.48898			

Excited State 3:	Singlet-A	3.9432 eV	314.42 nm	f=0.7726	$\langle S^{*2} \rangle = 0.000$
	136 ->139	-0.43042			
	138 ->141	0.48774			
	138 ->143	-0.10835			

Excited State 4:	Singlet-A	4.1685 eV	297.43 nm	f=0.1152	<S**2>=0.000
133 ->139	0.11739				
134 ->139	0.33092				
135 ->139	0.28906				
135 ->141	0.13663				
137 ->144	0.10066				
138 ->140	-0.12885				
138 ->141	0.12727				
138 ->142	0.28623				
138 ->143	0.10984				
138 ->144	-0.21467				

Excited State 5:	Singlet-A	4.2001 eV	295.20 nm	f=0.1769	<S**2>=0.000
133 ->139	0.43903				
134 ->139	-0.12826				
134 ->140	0.11636				
138 ->140	-0.10981				
138 ->141	-0.15315				
138 ->143	-0.33610				
138 ->144	-0.14230				

Cartesian coordinates of the optimized structures

All compounds mentioned in this article were optimized to the minimum with no imaginary frequency.

Atom	X	Y	Z
C	-0.02292600	-3.84985300	-1.02188500
C	-1.31947600	-3.57025500	-1.40612000
C	0.39386400	-3.97164700	0.31978300

C	-2.21147700	-3.36143200	-0.35259300
H	-1.54329800	-3.29218700	-2.42890800
O	1.07009500	-3.60229000	-1.86549900
C	-0.57085800	-3.94965200	1.33370100
C	1.79448300	-3.54685700	0.32153300
C	-1.87404600	-3.60329100	0.97839500
C	-3.27226200	-2.33592400	-0.37327400
C	2.09705200	-3.24064000	-1.01456300
H	-0.27744100	-3.98381700	2.37884200
C	2.59122500	-3.00454900	1.33438500
C	-2.94907800	-3.03298400	1.88686900
C	-3.55568400	-1.46626300	-1.39439100
C	-3.56395000	-2.00741700	0.99944900
C	3.07162100	-2.33420500	-1.38302200
C	3.51331500	-2.06115600	1.01492800
H	2.33649500	-3.18681000	2.37581000
H	-2.53546200	-2.60784400	2.80598700
H	-3.66805000	-3.80705100	2.18860900
C	-3.88515600	-0.17097600	-1.01834700
H	-3.27562400	-1.66487900	-2.42339500
C	-3.94950800	-0.73096500	1.32370600
C	3.71280300	-1.65202900	-0.34580300
H	3.12572900	-1.99809900	-2.41281800
C	4.08147300	-0.97243100	1.91188400
C	-4.02160600	0.23664300	0.32028600
O	-3.71193800	0.91457500	-1.86594100
H	-4.00851000	-0.43206100	2.36769000

C	4.07830900	-0.24769700	-0.32952700
C	4.09336400	0.20992300	0.99545700
H	5.09041200	-1.22827600	2.26455700
H	3.46856600	-0.80961300	2.80331900
C	-3.69601000	1.62909600	0.33932800
C	-3.40110800	1.98288100	-1.02118100
C	3.85108300	0.66208700	-1.40421100
C	3.73606100	1.48888700	1.33535100
C	-3.16435100	2.46566900	1.34767400
C	-2.48867900	2.95697000	-1.40210500
C	3.41261000	1.93065300	-1.01665600
H	3.72959100	0.33379100	-2.42927500
C	3.30648000	2.34895600	0.30103400
H	3.59176500	1.76376000	2.37591300
C	-2.23700800	3.42123200	0.99805000
H	-3.32049200	2.22117400	2.39523300
C	-1.83902000	3.59799500	-0.36129700
H	-2.14123600	2.99862900	-2.42792500
O	2.63973500	2.69847100	-1.85465200
C	2.21685700	3.33332600	0.29856900
C	-1.17899900	4.01932700	1.90860600
C	-0.40124900	3.95301200	-0.36184100
C	1.79459200	3.40540200	-1.02533000
C	1.35471400	3.71566300	1.33364700
C	0.01967700	4.00933100	0.99373300
H	-1.02449200	3.42691400	2.81455100
H	-1.44002700	5.03750300	2.22665900

C	0.49707600	3.73388600	-1.38840200
H	1.64685900	3.60822000	2.37370800
H	0.17681400	3.59029100	-2.41472800

Table S5. Major electronic transitions of aromatic belt **1**

Excited State	Energy (eV)	Excitation (nm)	Oscillator strength (f)	Transition type		
s ₀ -s ₁	2.6191	473.38	0.0005	H->L 92.6%		
s ₀ -s ₂	3.9259	315.81	0.63470	H->L+1 44.6%	H-1->L 39.2%	
s ₀ -s ₃	3.9994	310.01	0.41080	H->L+2 40.6%	H-2->L 30.3%	

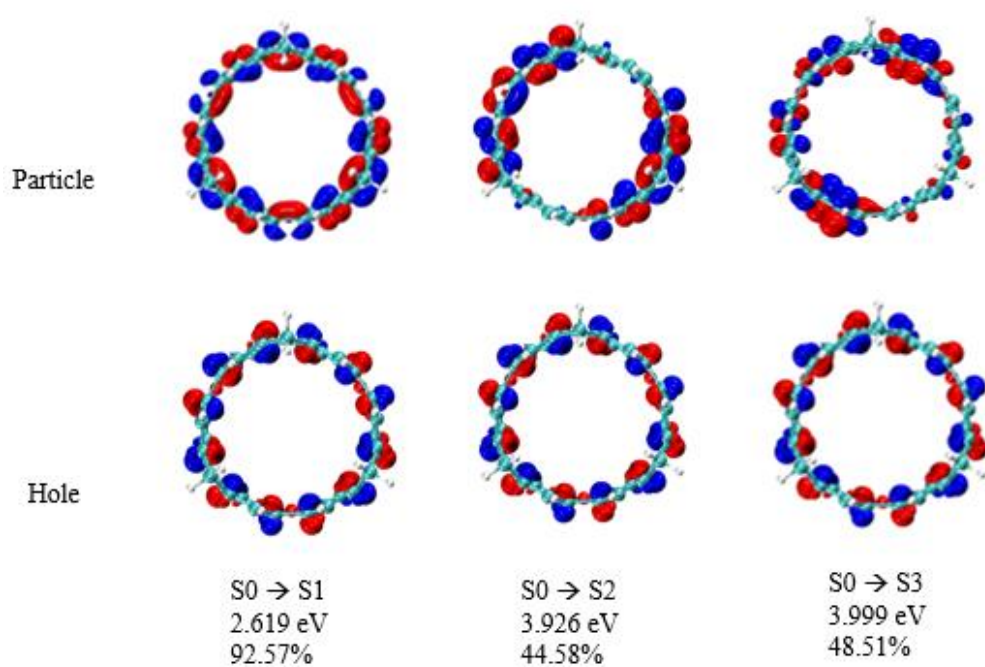


Fig. S21. Frontier molecular orbitals of **1** calculated at the B3LYP/6-31G(d) level of theory.

6. Reference:

- S1. Gaussian 09, Revision A.02, 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. Montgomery, Jr., 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, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.