Selective Syntheses of [7]-[12]Cycloparaphenylenes Using Orthogonal Suzuki-Miyaura Cross-Coupling Reactions

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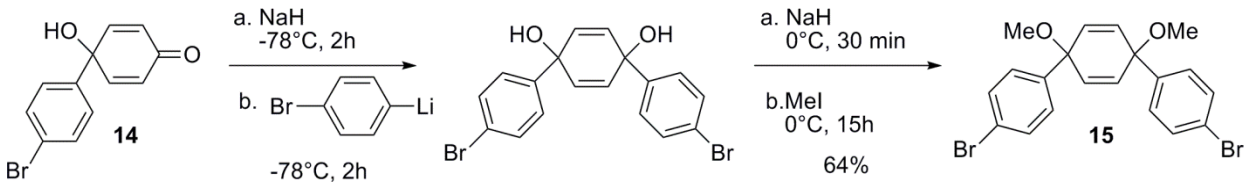
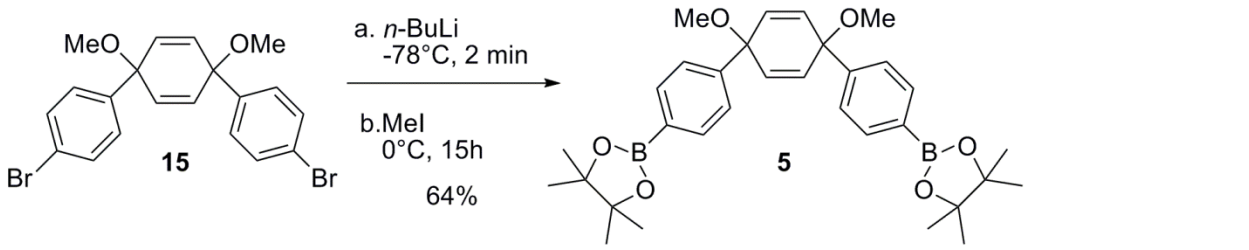
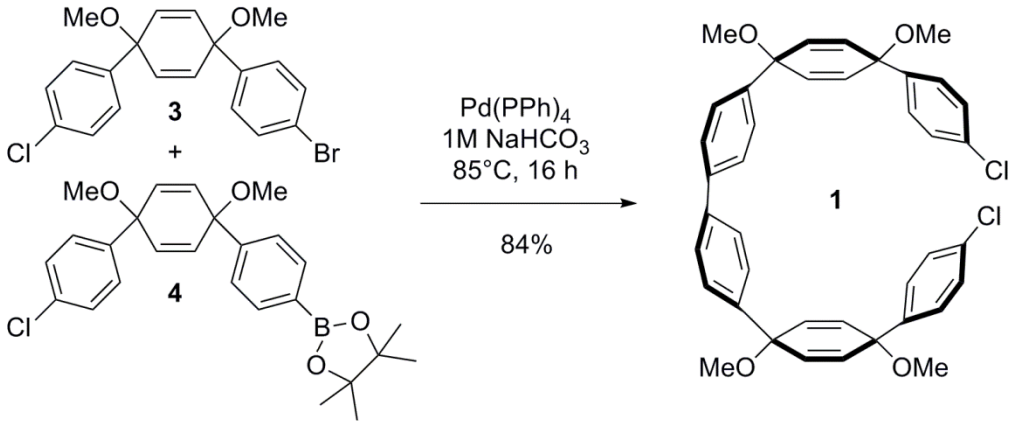
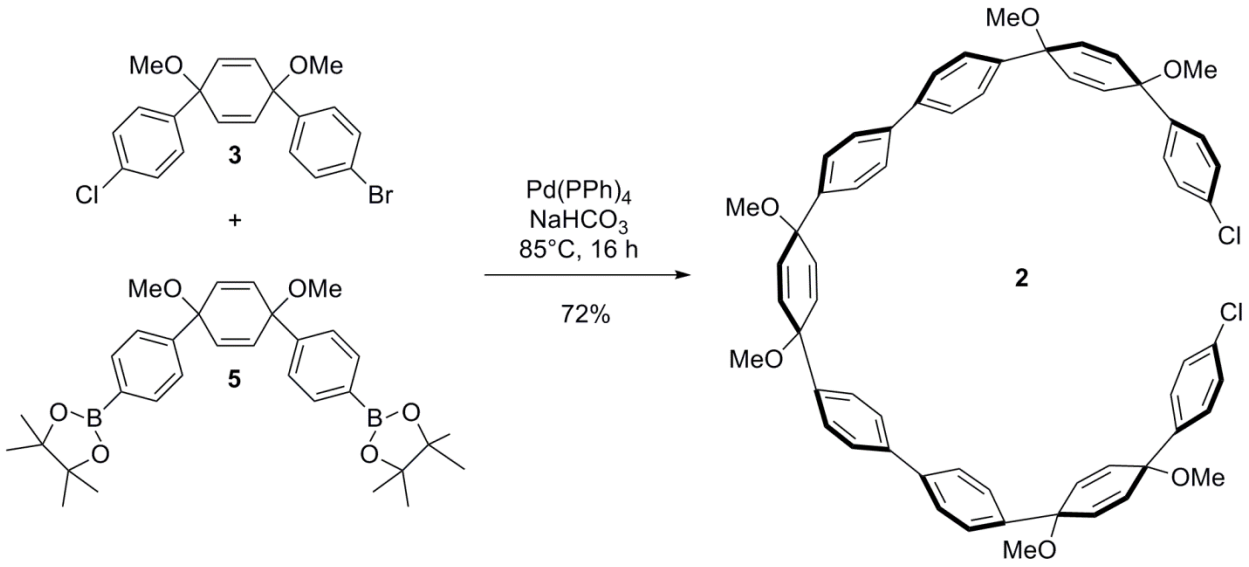
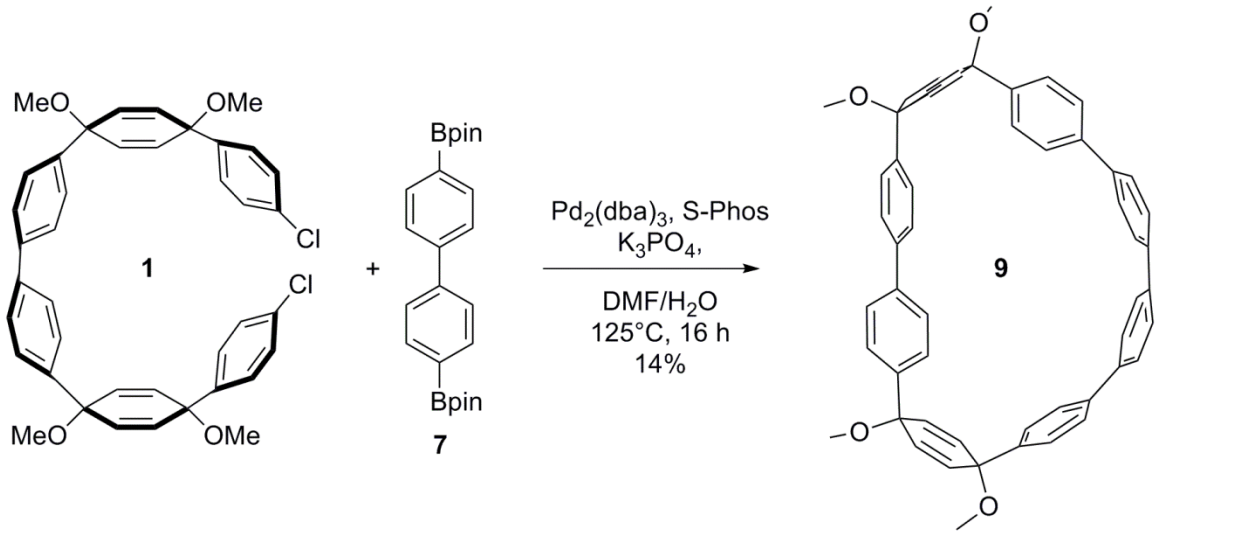
Supplementary Schemes

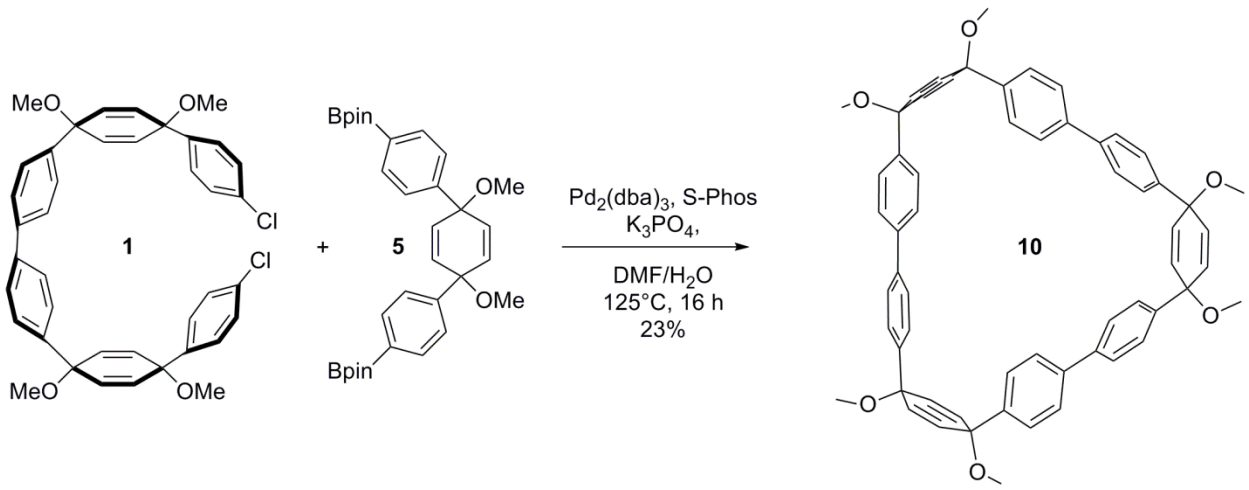


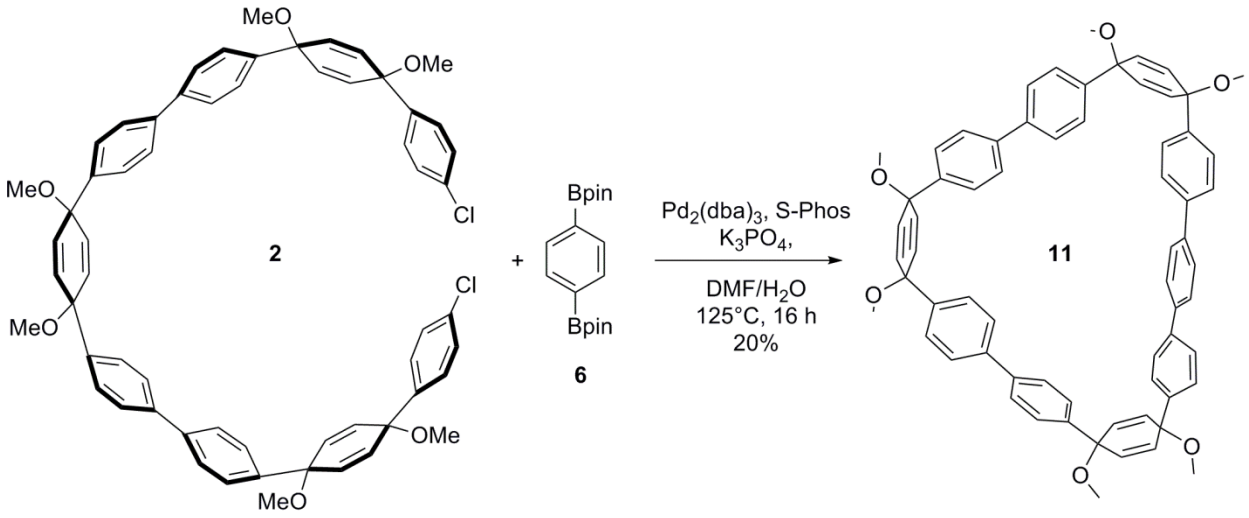


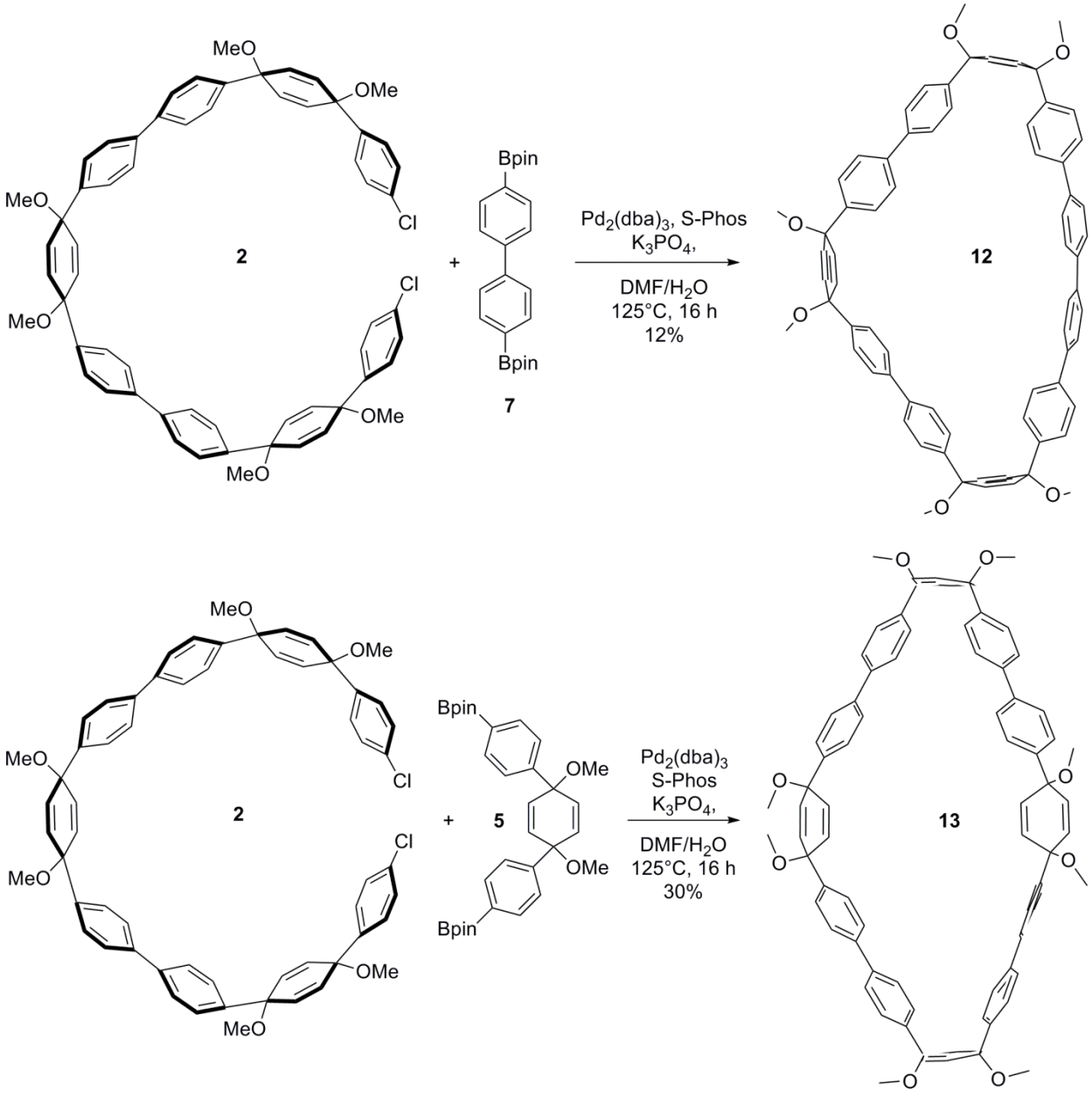


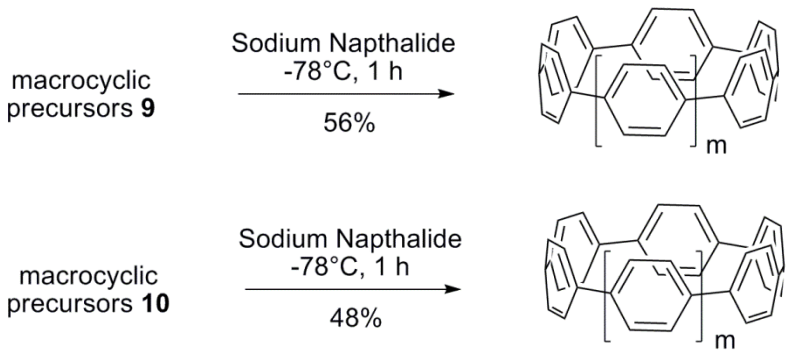


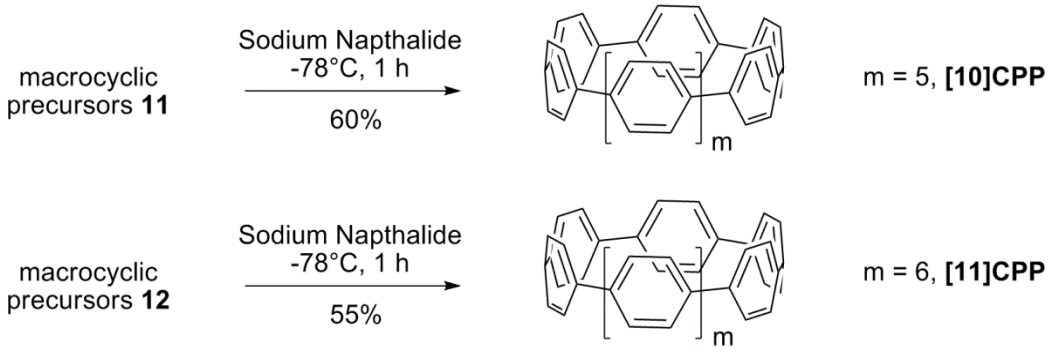

MeO
OMe
Cl
Cl
MeO
OMe
1
+
Bpin
Bpin
7
Pd2(dba)3, S-Phos
K3PO4,
DMF/H2O
125°C, 16 h
14%
O
O
O
O
9


MeO
OMe
Cl
Cl
MeO
OMe
1
+
Bpin
OMe
OMe
Bpin
5
Pd2(dba)3, S-Phos
K3PO4,
DMF/H2O
125°C, 16 h
23%
O
O
O
O
O
10

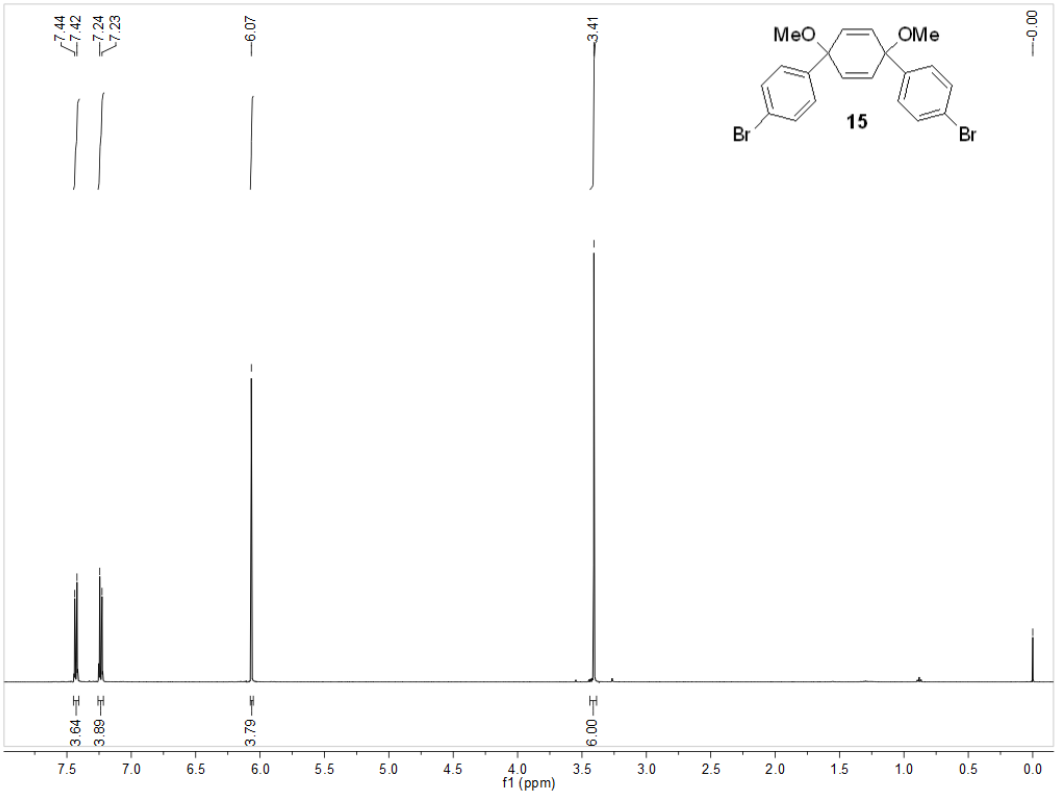

MeO
OMe
MeO
Cl
Cl
MeO
OMe
2
+
Bpin
Bpin
6
Pd2(dba)3, S-Phos
K3PO4,
DMF/H2O
125°C, 16 h
20%
O
O
O
O
O
O
11

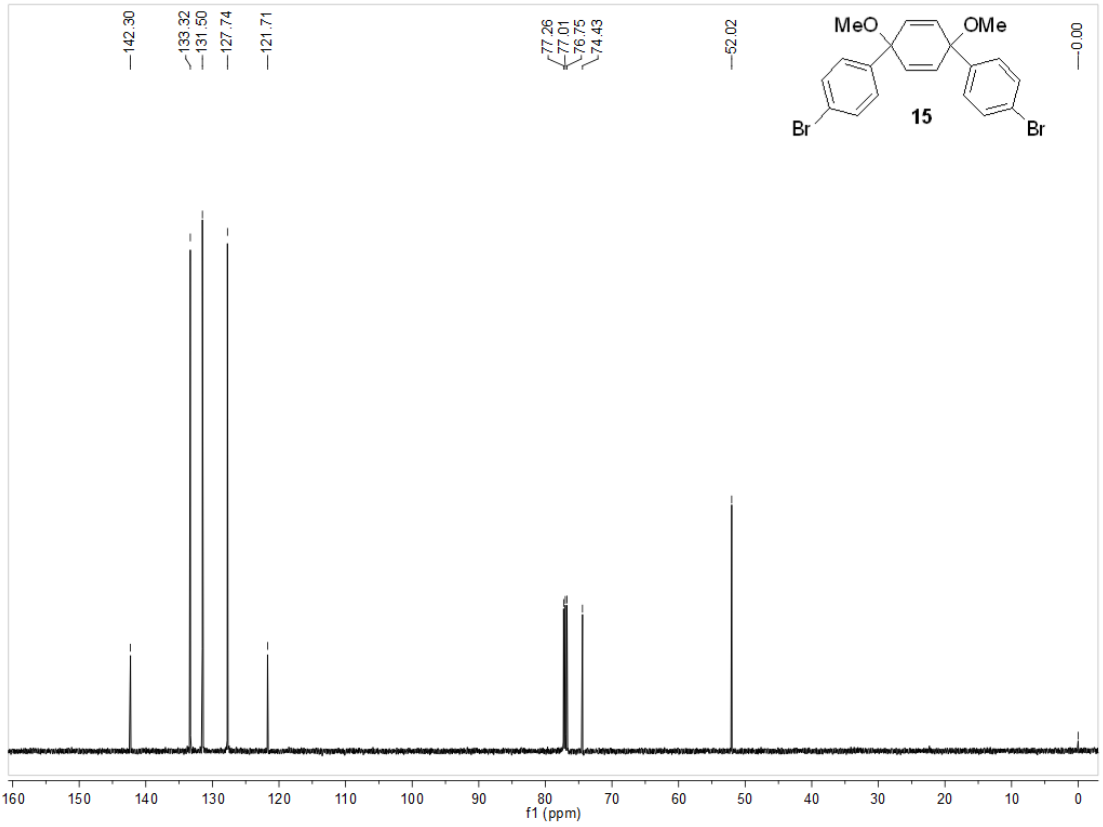

MeO
OMe
Cl
2
Bpin
7
$Pd_2(dba)_3$, S-Phos
K_3PO_4,
DMF/H_2O
125°C, 16 h
12%
12
5
30%
13

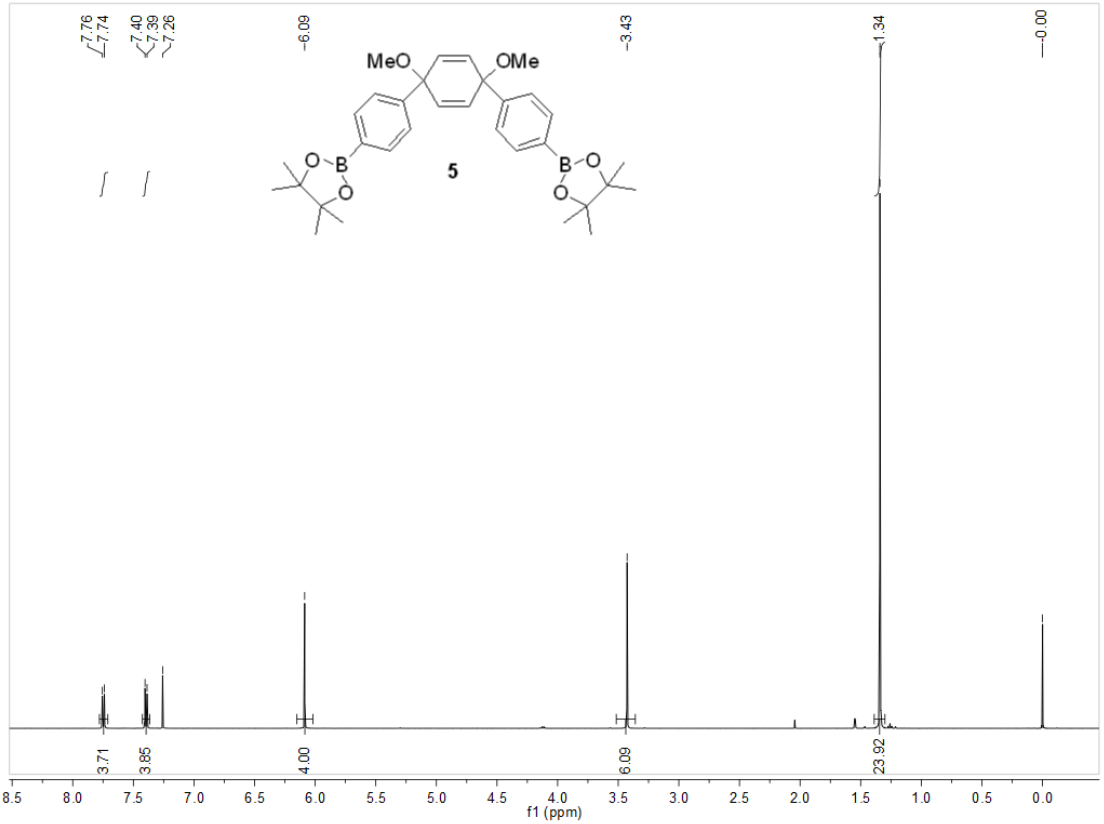

macrocyclic
precursors **9**
Sodium Napthalide
-78°C, 1 h
56%
m = 3, **[8]CPP**
macrocyclic
precursors **10**
48%
m = 4, **[9]CPP**

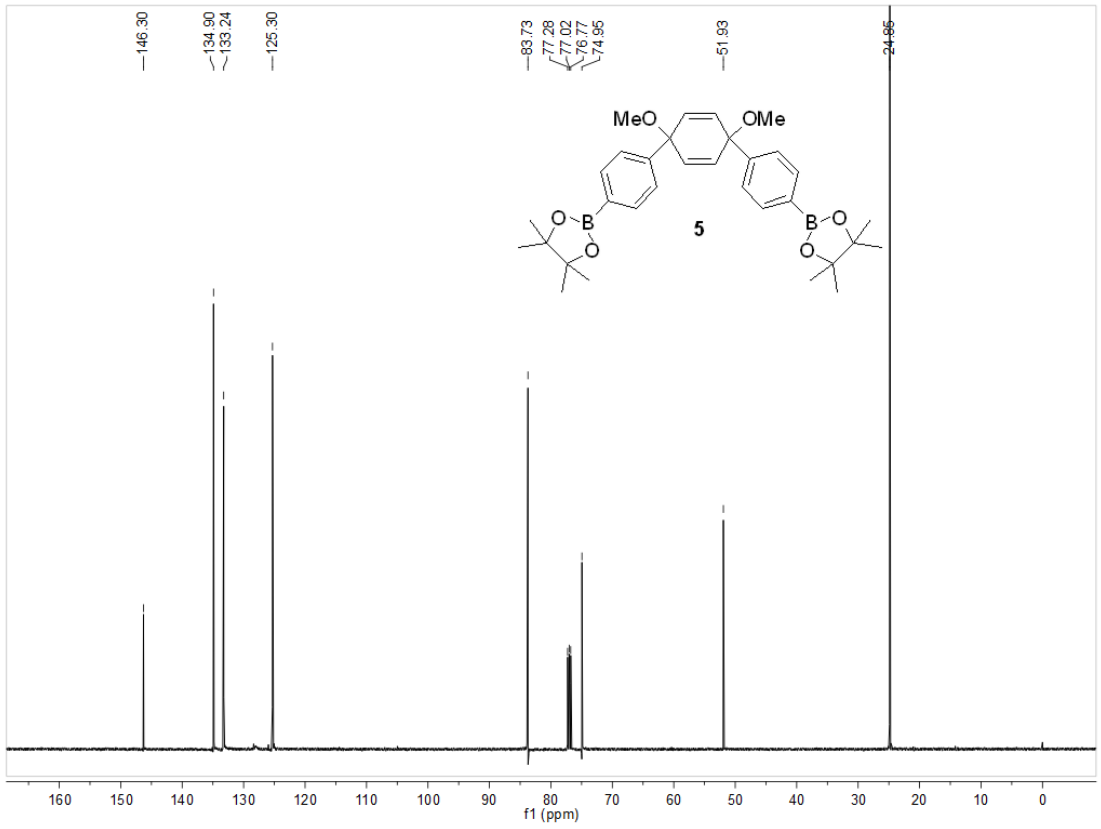

macrocyclic
precursors **11**
Sodium Napthalide
-78°C, 1 h
60%
m
m = 5, **[10]CPP**
macrocyclic
precursors **12**
Sodium Napthalide
-78°C, 1 h
55%
m
m = 6, **[11]CPP**

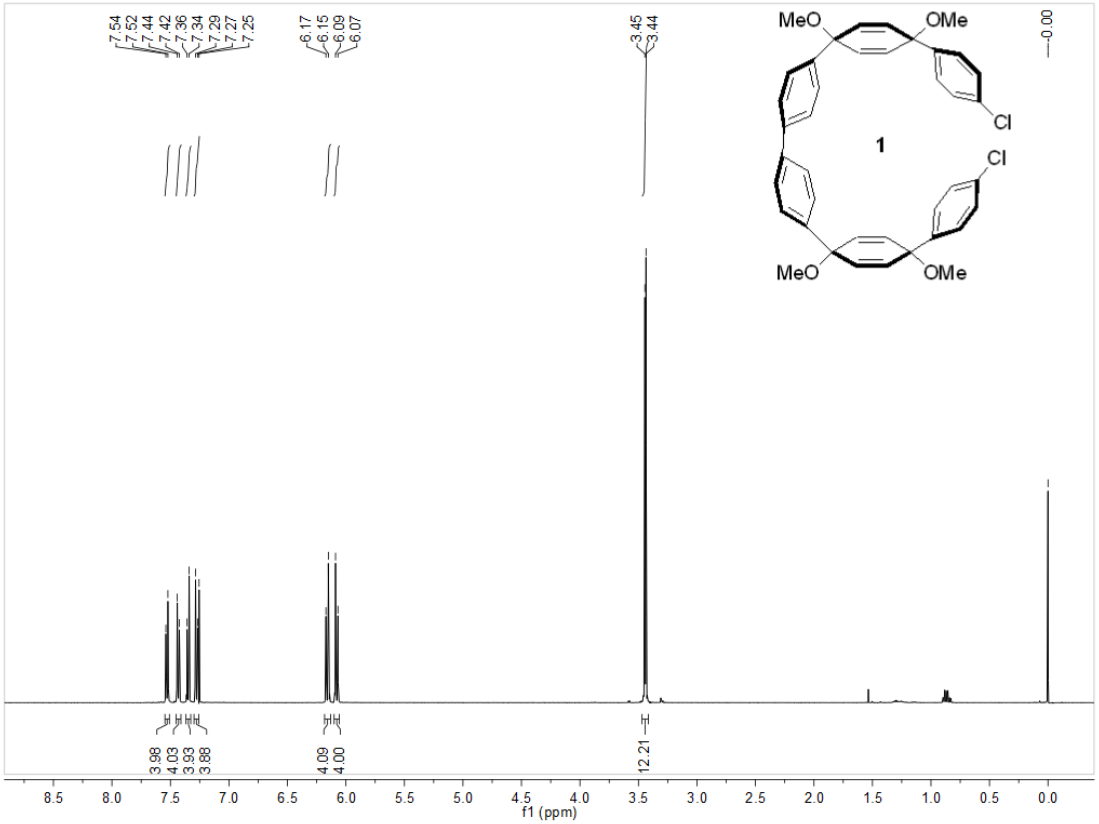
NMR Spectra

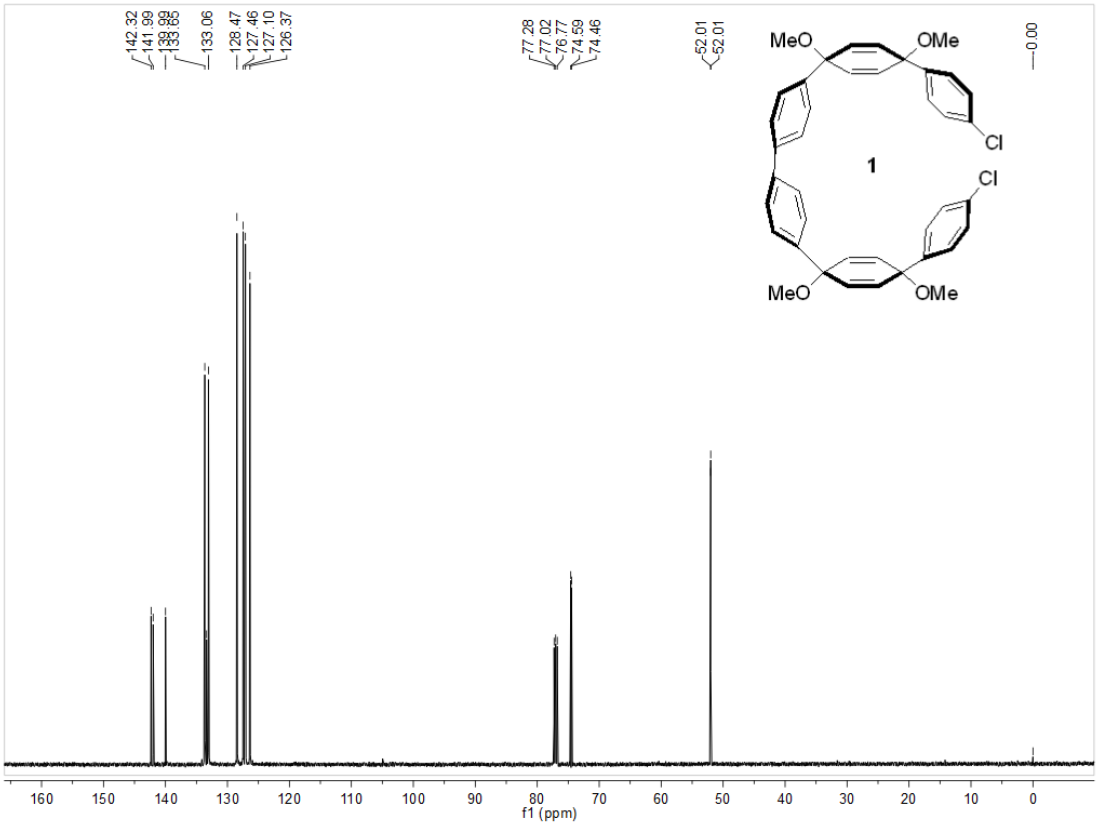

7.44
7.42
7.24
7.23
6.07
3.41
0.00
MeO
OMe
Br
Br
15
3.64
3.89
3.79
6.00
f1 (ppm)

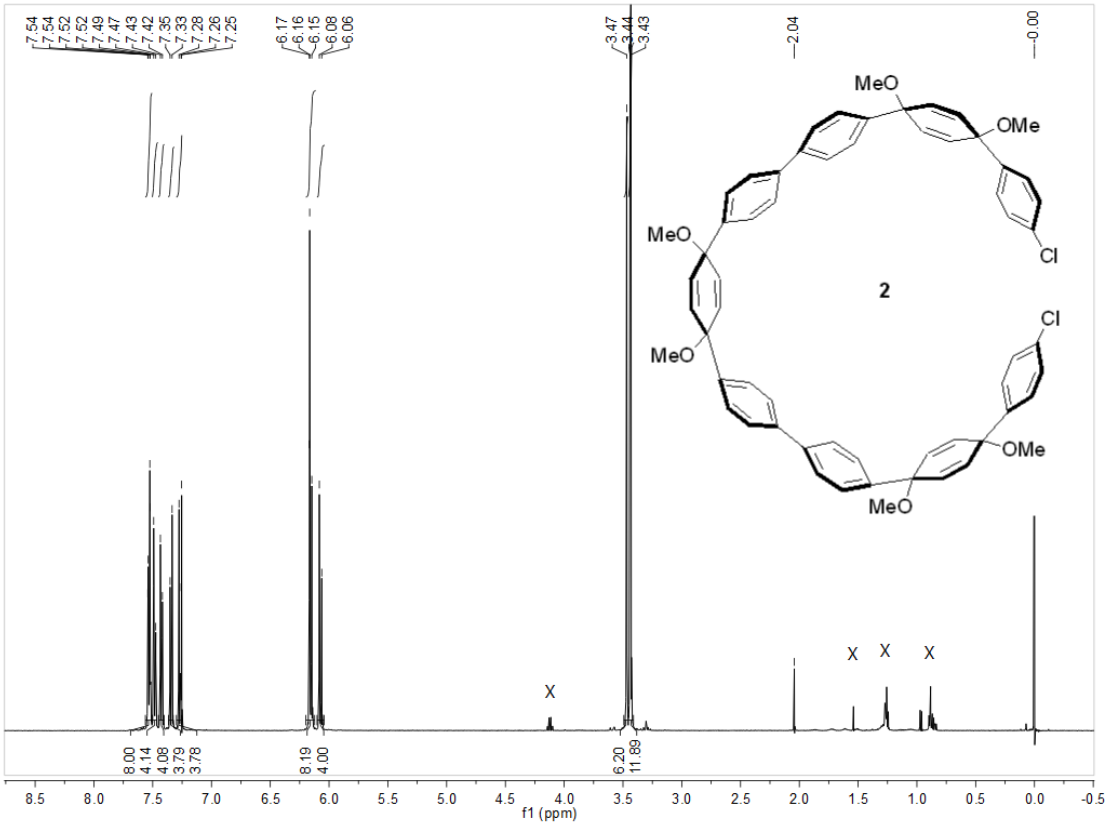

142.30
133.32
131.50
127.74
121.71
77.26
77.01
76.75
74.43
52.02
0.00
MeO
OMe
Br
Br
15
f1 (ppm)

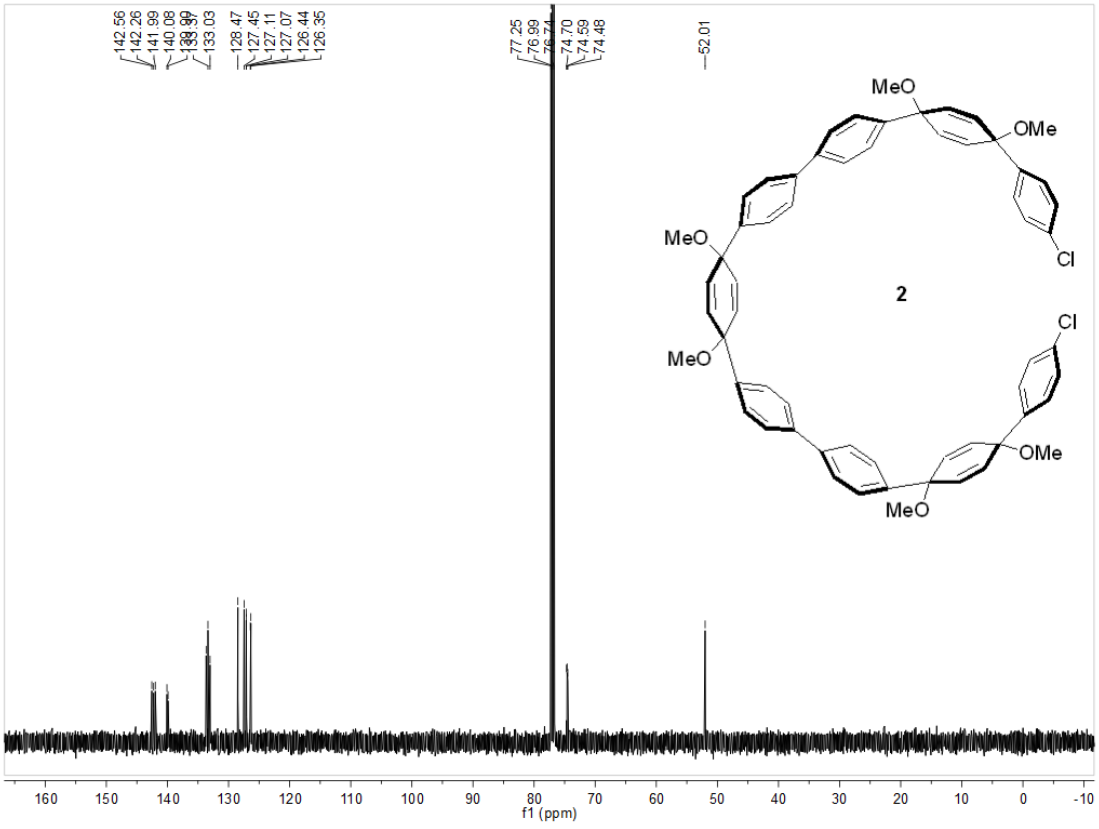

7.76
7.74
7.40
7.39
7.26
6.09
3.43
1.34
0.00
MeO
OMe
5
3.71
3.85
4.00
6.09
23.92
f1 (ppm)

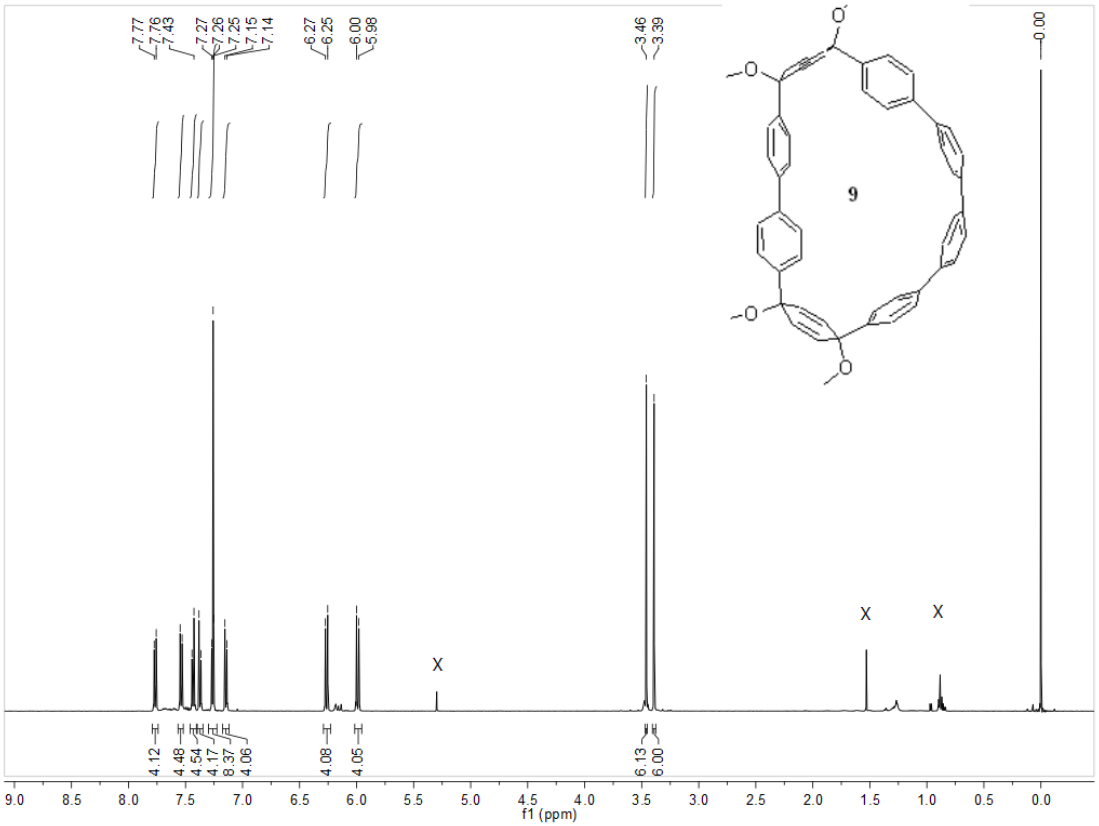

146.30
134.90
133.24
125.30
83.73
77.28
77.02
76.77
74.95
51.93
24.86
MeO
OMe
5
f1 (ppm)

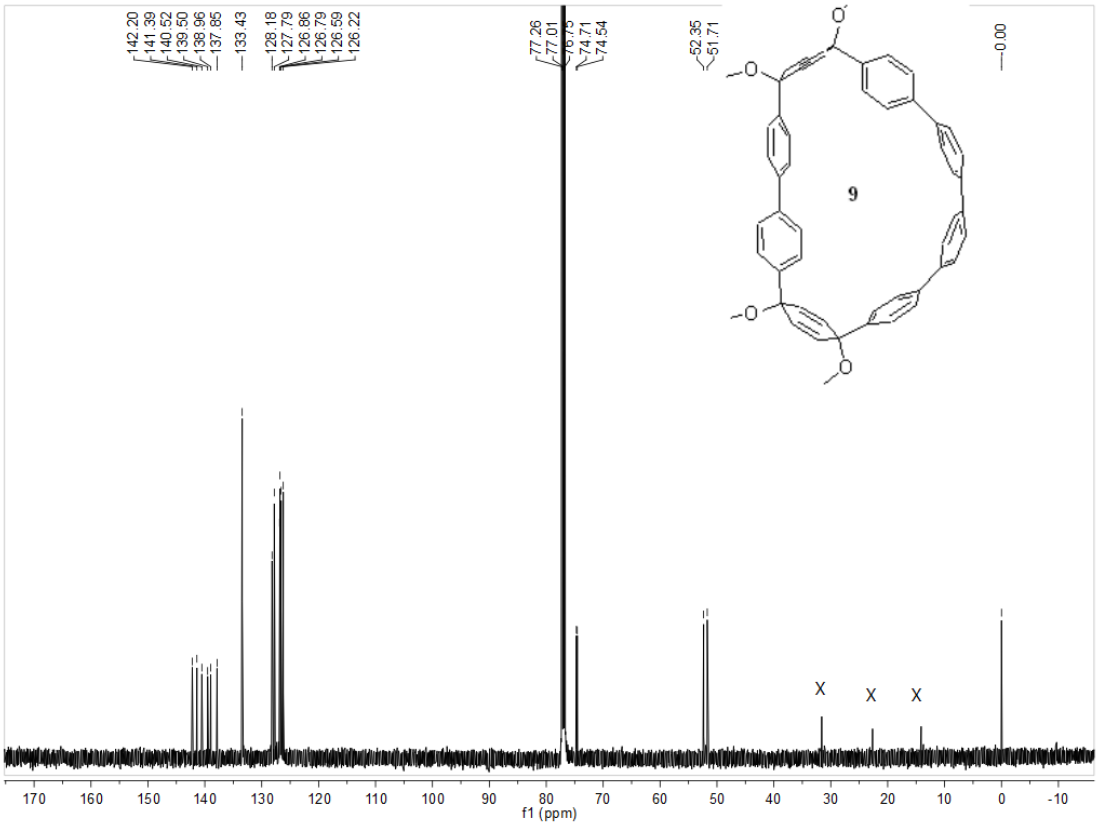

7.54
7.52
7.44
7.42
7.36
7.34
7.29
7.27
7.25
6.17
6.15
6.09
6.07
3.45
3.44
0.00
MeO
OMe
Cl
1
Cl
MeO
OMe
3.98
4.03
3.93
3.88
4.09
4.00
12.21
f1 (ppm)

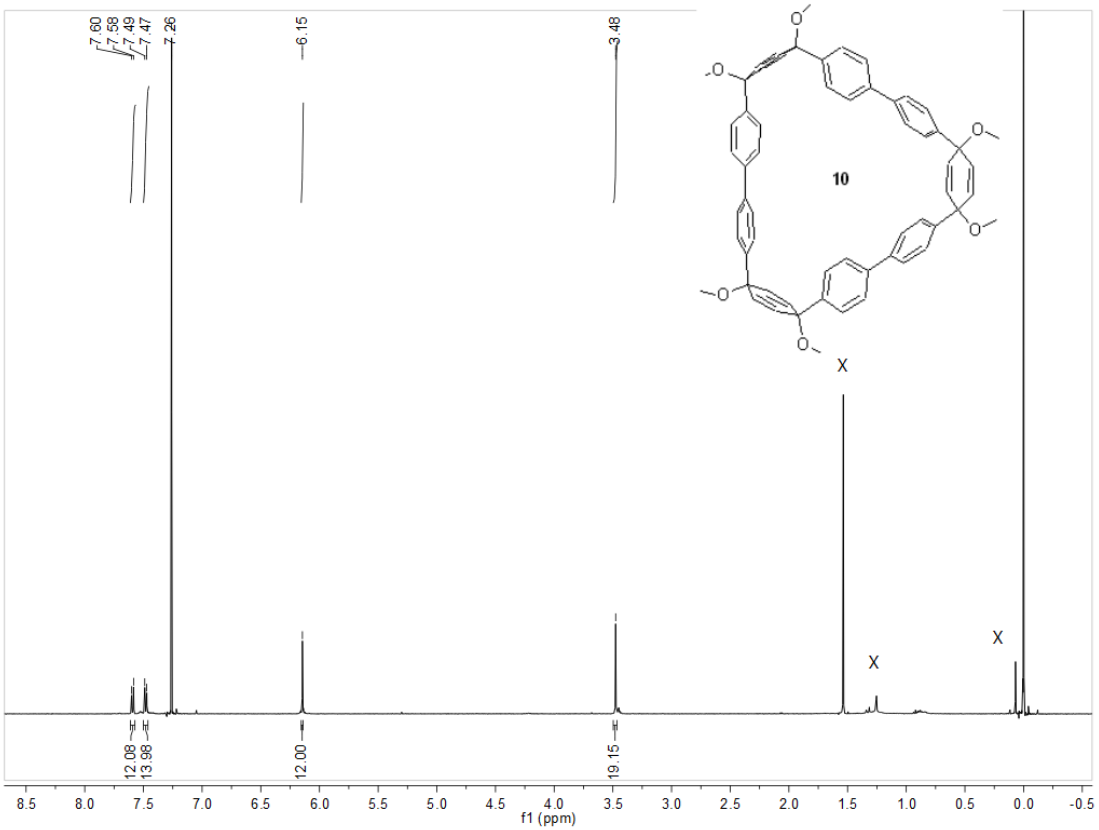

142.32
141.99
133.89
133.65
133.06
128.47
127.46
127.10
126.37
77.28
77.02
76.77
74.59
74.46
52.01
52.01
0.00
MeO
OMe
Cl
1
Cl
MeO
OMe
f1 (ppm)

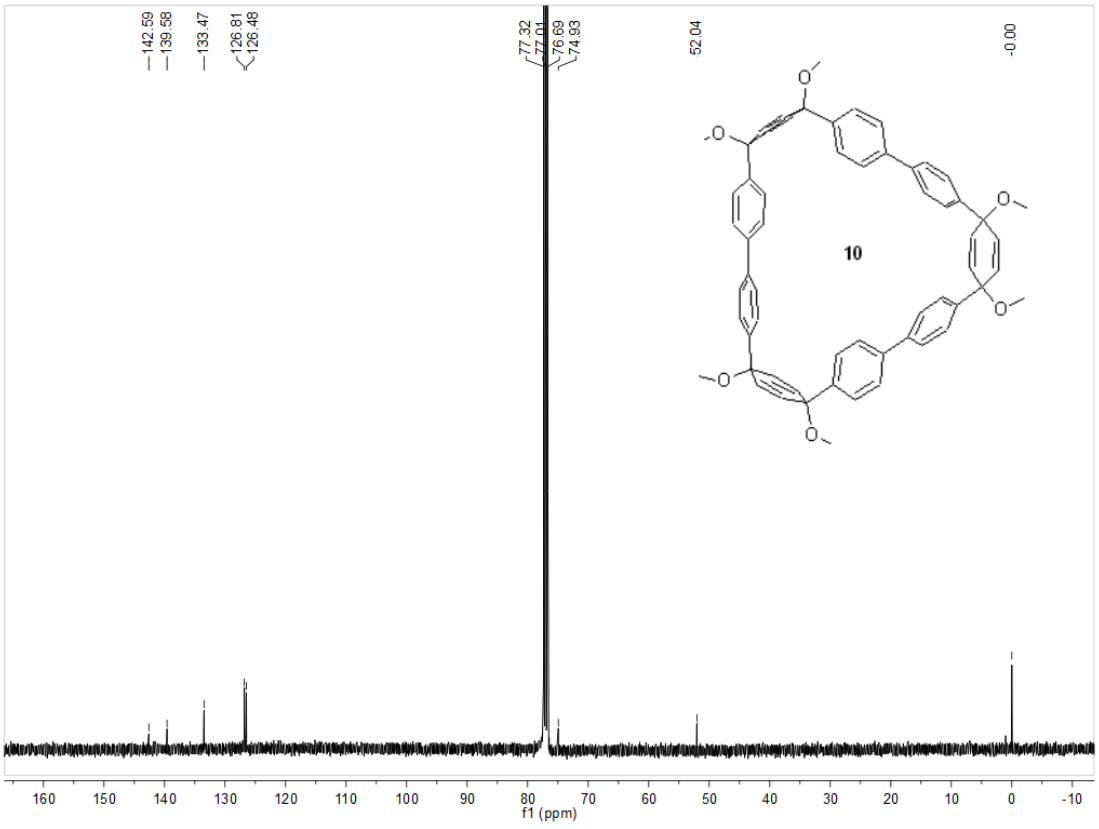

MeO
OMe
Cl
MeO
2
Cl
MeO
OMe
MeO
X
X
X
X
f1 (ppm)

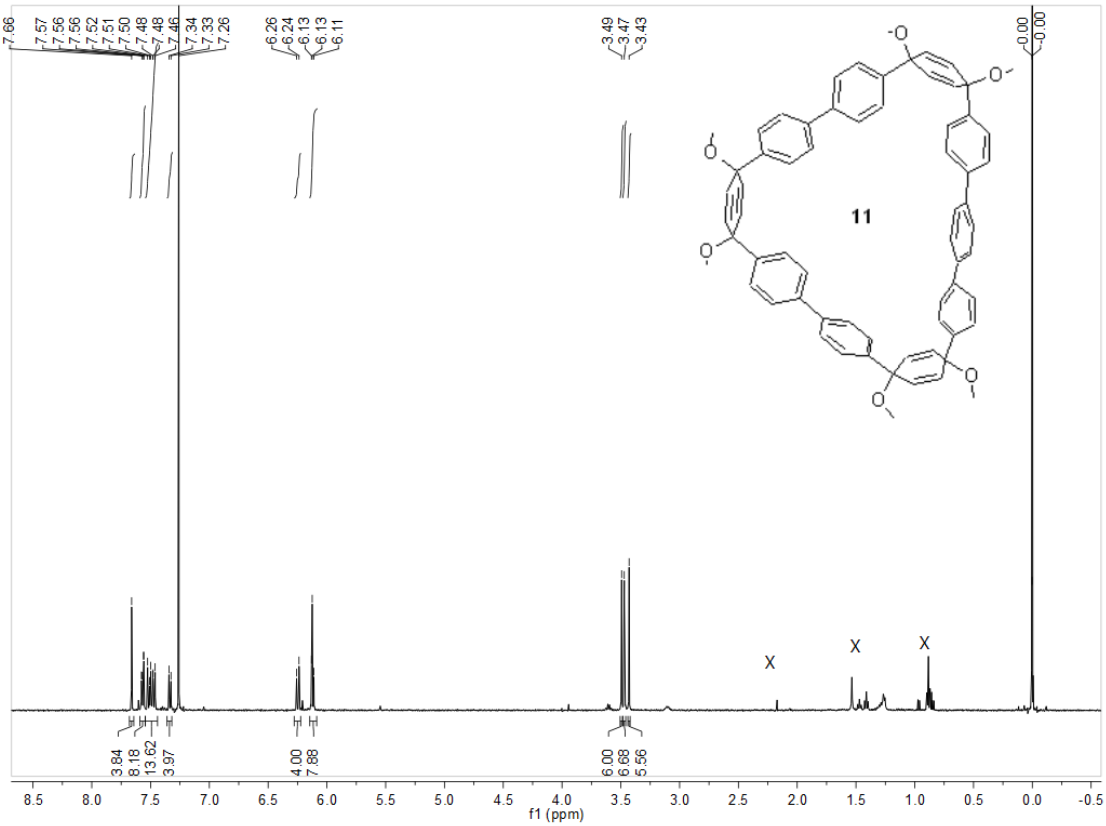

MeO
OMe
Cl
MeO
2
Cl
MeO
OMe
MeO
f1 (ppm)

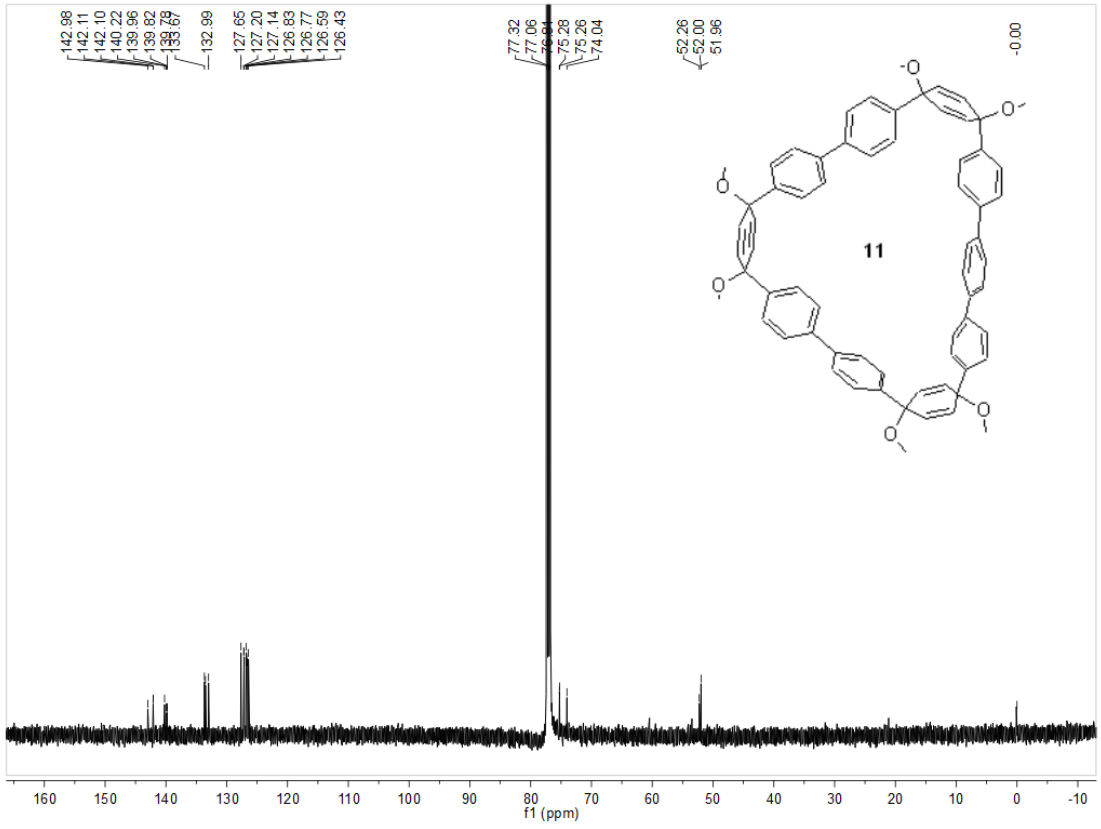

7.77
7.76
7.43
7.27
7.26
7.25
7.15
7.14
6.27
6.25
6.00
5.98
3.46
3.39
0.00
9
X
X
X
4.12
4.48
4.54
4.17
8.37
4.06
4.08
4.05
6.13
6.00
f1 (ppm)

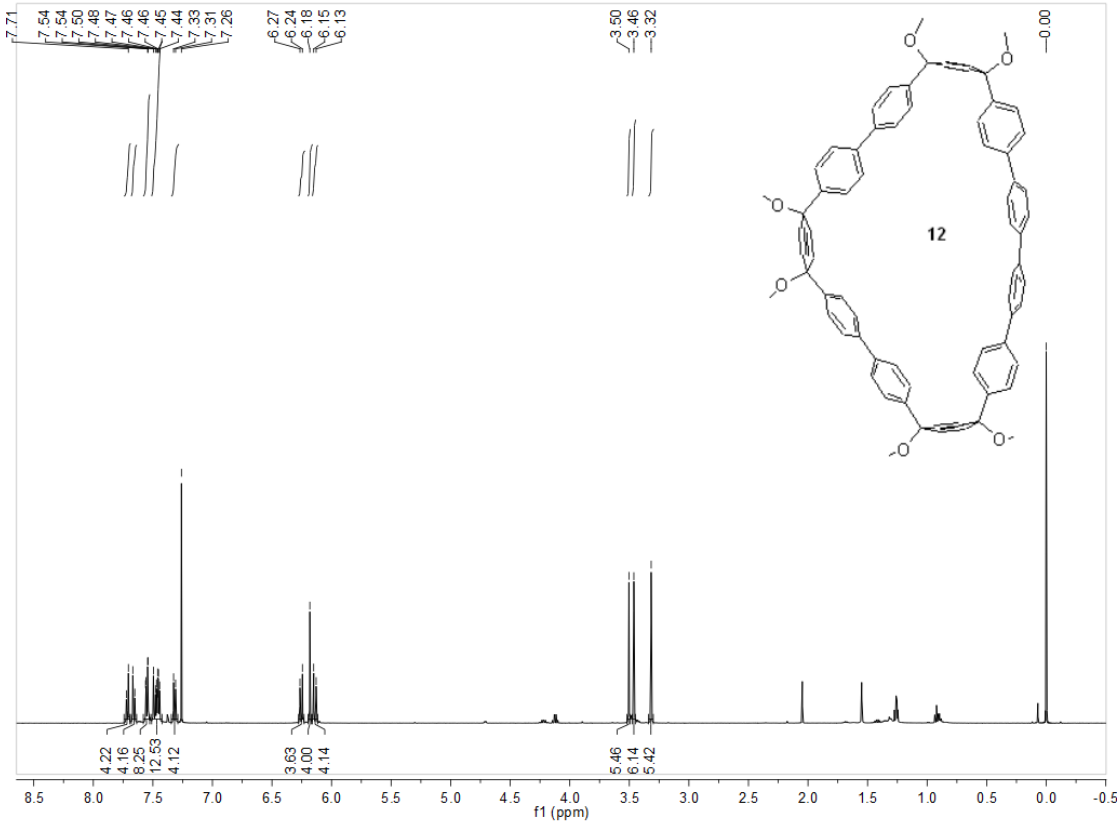

142.20
141.39
140.52
139.50
138.96
137.85
133.43
128.18
127.79
126.86
126.79
126.59
126.22
77.26
77.01
76.75
74.71
74.54
52.35
51.71
0.00
9
X
X
X
f1 (ppm)

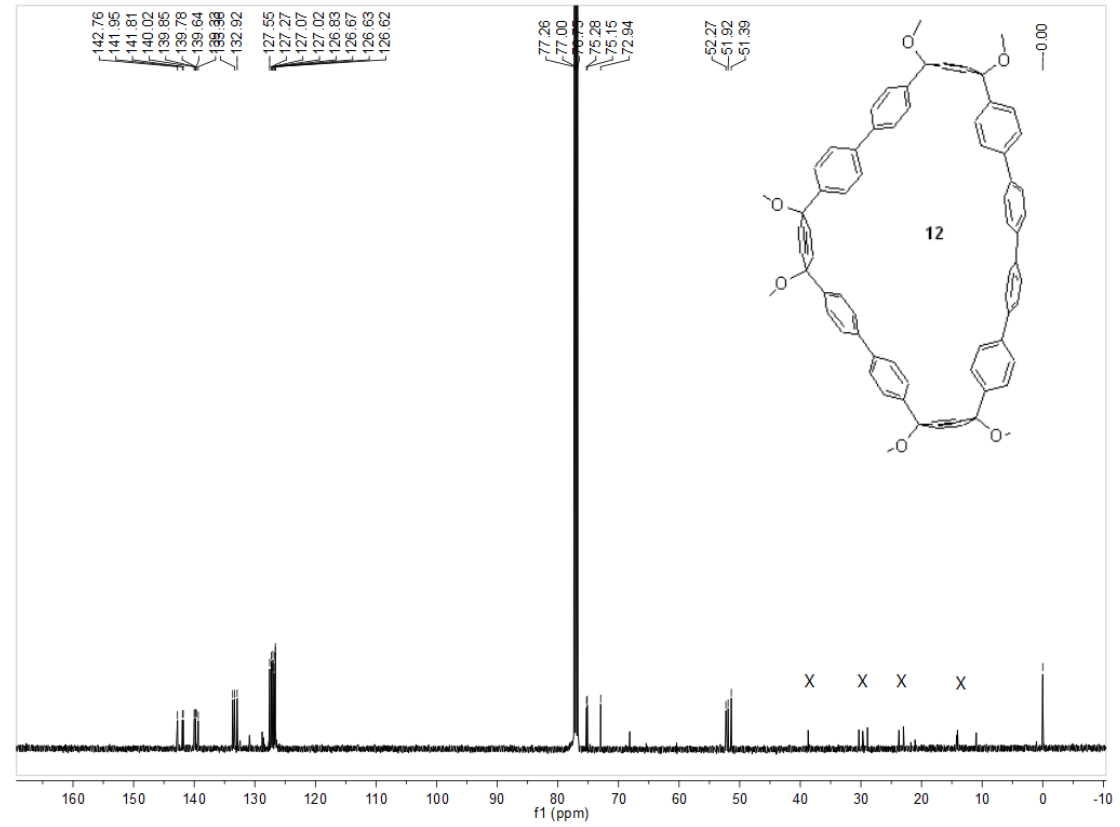

7.60
7.58
7.49
7.47
7.26
6.15
3.48
10
X
X
X
12.08
13.98
12.00
19.15
f1 (ppm)


142.59
139.58
133.47
126.81
126.48
77.32
77.01
76.69
74.93
52.04
-0.00
10
f1 (ppm)


11
X
X
X
f1 (ppm)


11
f1 (ppm)


7.71
7.54
7.54
7.50
7.48
7.47
7.46
7.46
7.45
7.44
7.33
7.31
7.26
6.27
6.24
6.18
6.15
6.13
3.50
3.46
3.32
0.00
12
4.22
4.16
8.25
12.53
4.12
3.63
4.00
4.14
5.46
6.14
5.42
f1 (ppm)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139.85
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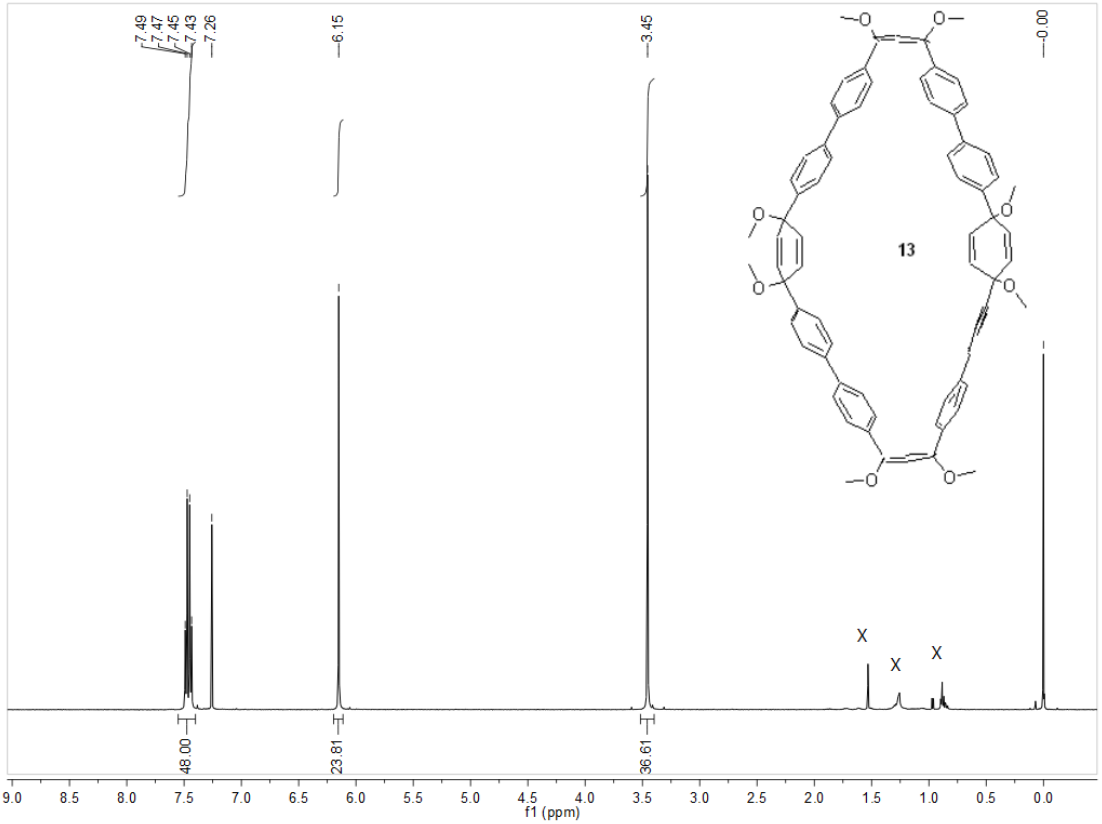
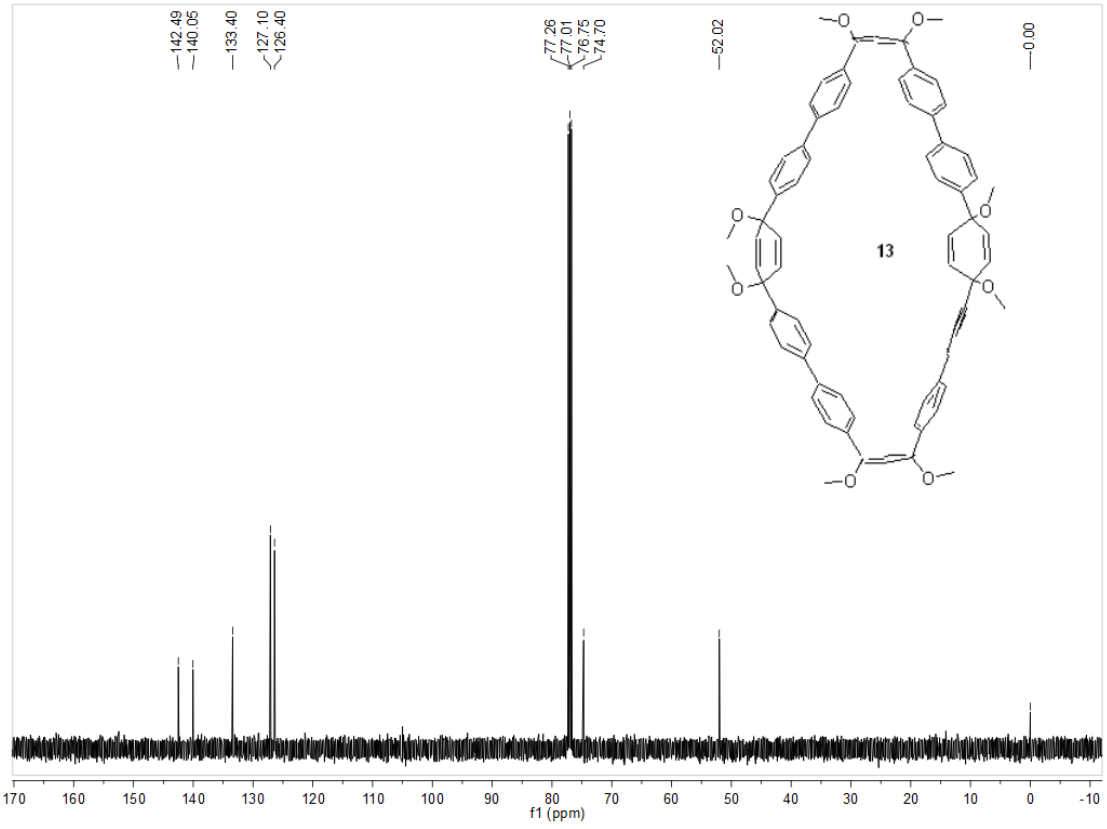
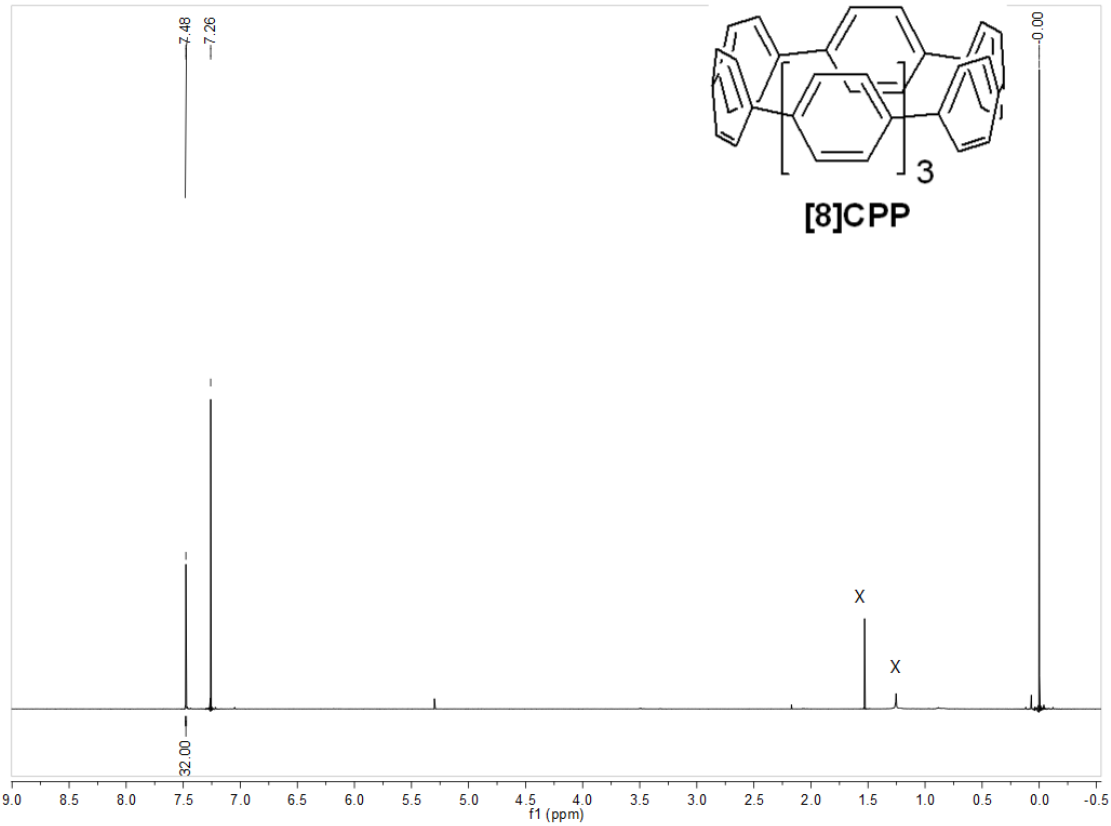
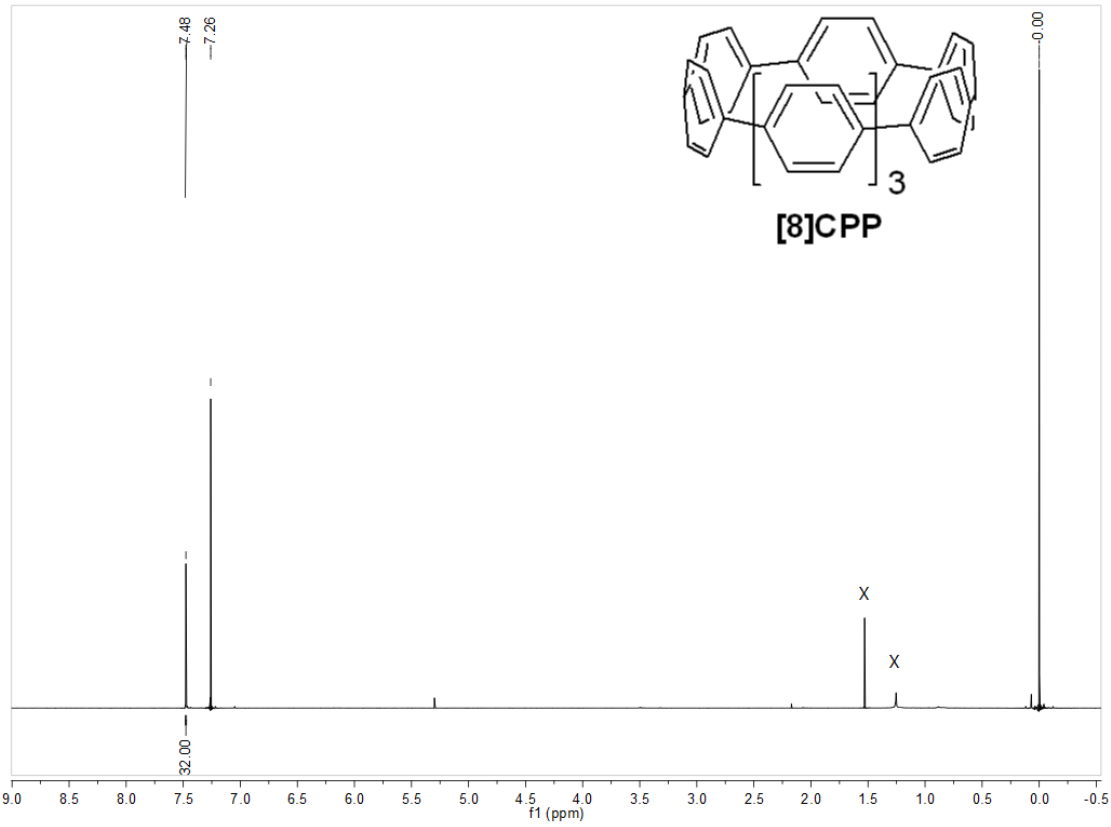
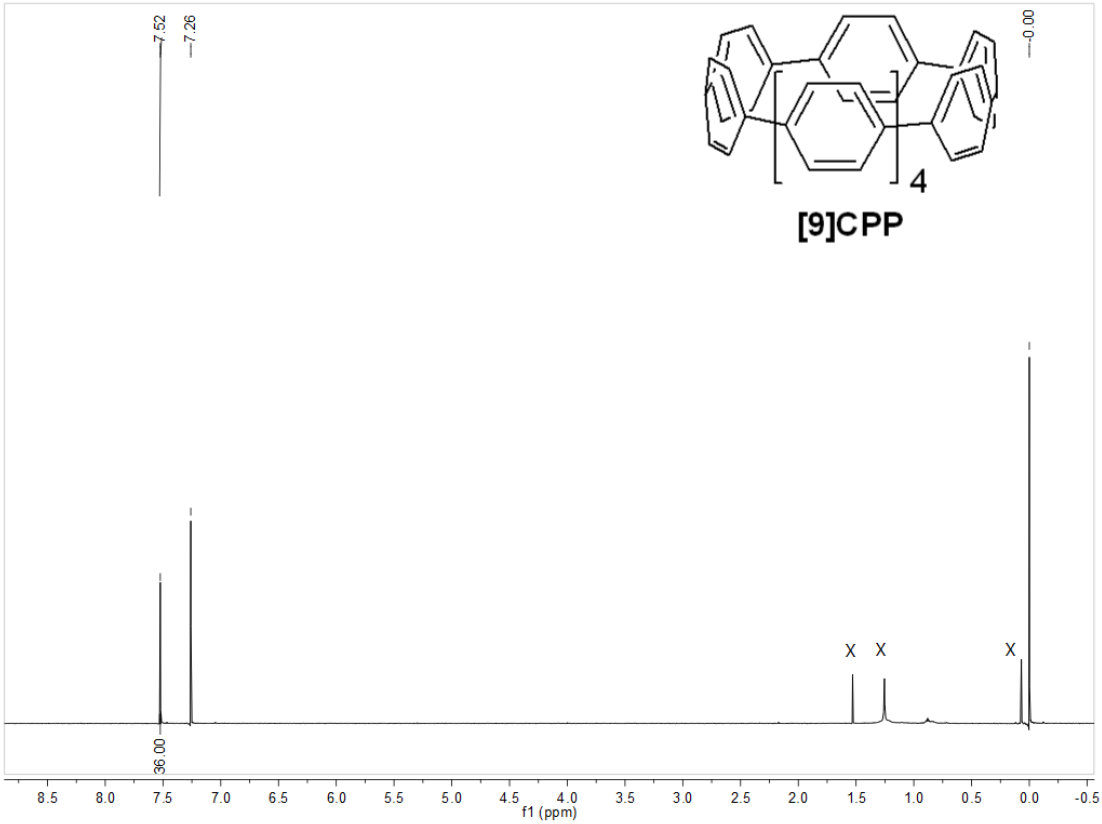
132.92
127.55
127.27
127.07
127.02
126.83
126.67
126.63
126.62
77.26
77.00
75.28
75.15
72.94
52.27
51.92
51.39
0.00
12
X
X
X
X
f1 (ppm)

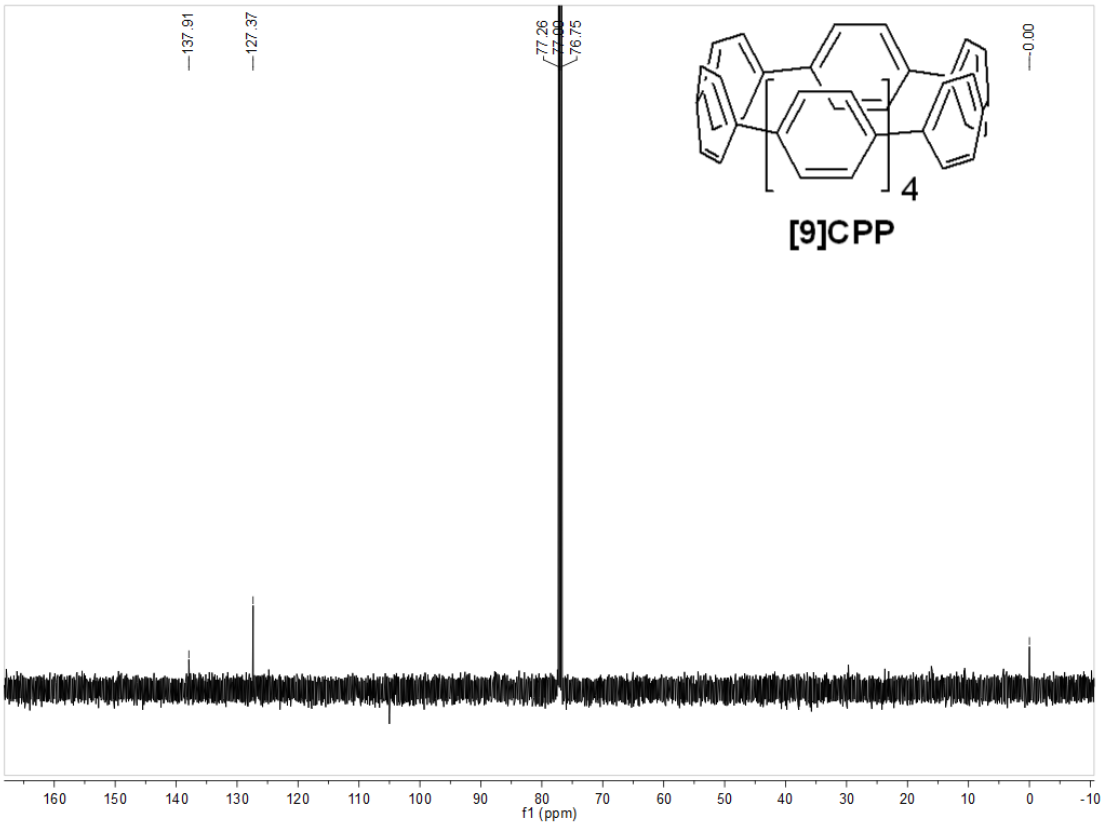

7.49
7.47
7.45
7.43
7.26
6.15
3.45
0.00
13
X
X
X
48.00
23.81
36.61
f1 (ppm)

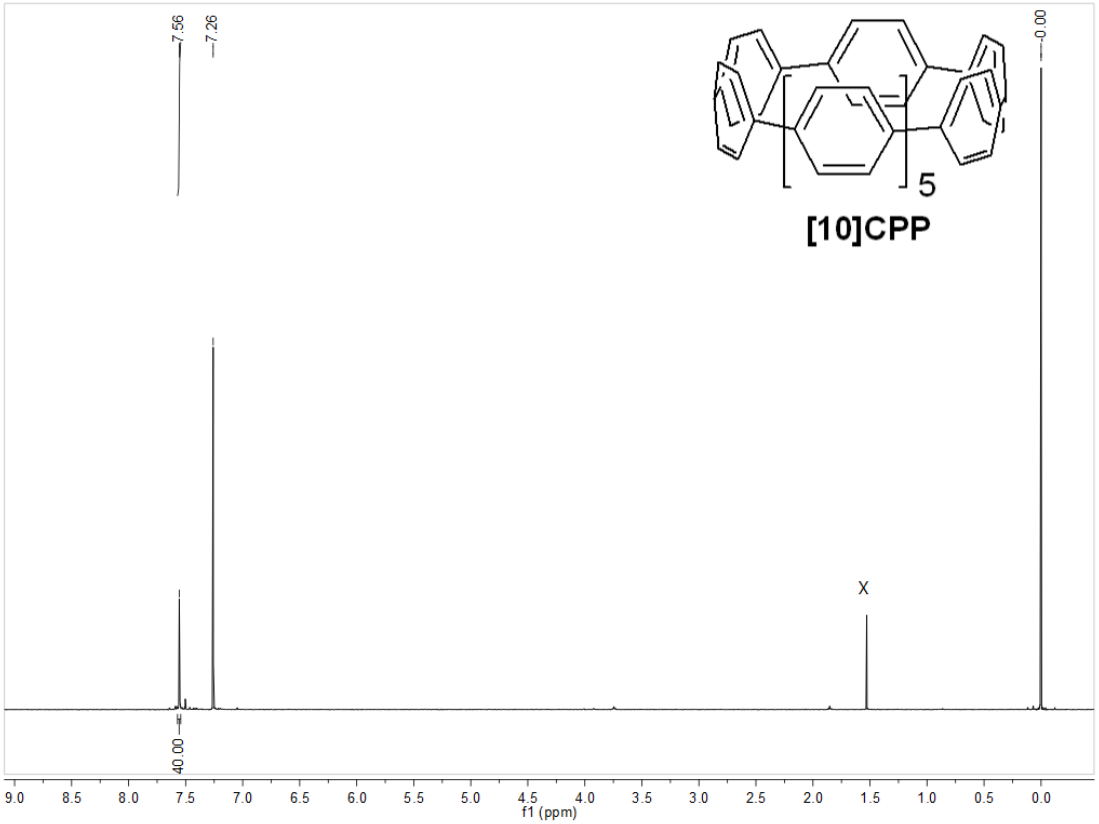

142.49
140.05
133.40
127.10
126.40
77.26
77.01
76.75
74.70
52.02
0.00
13
f1 (ppm)

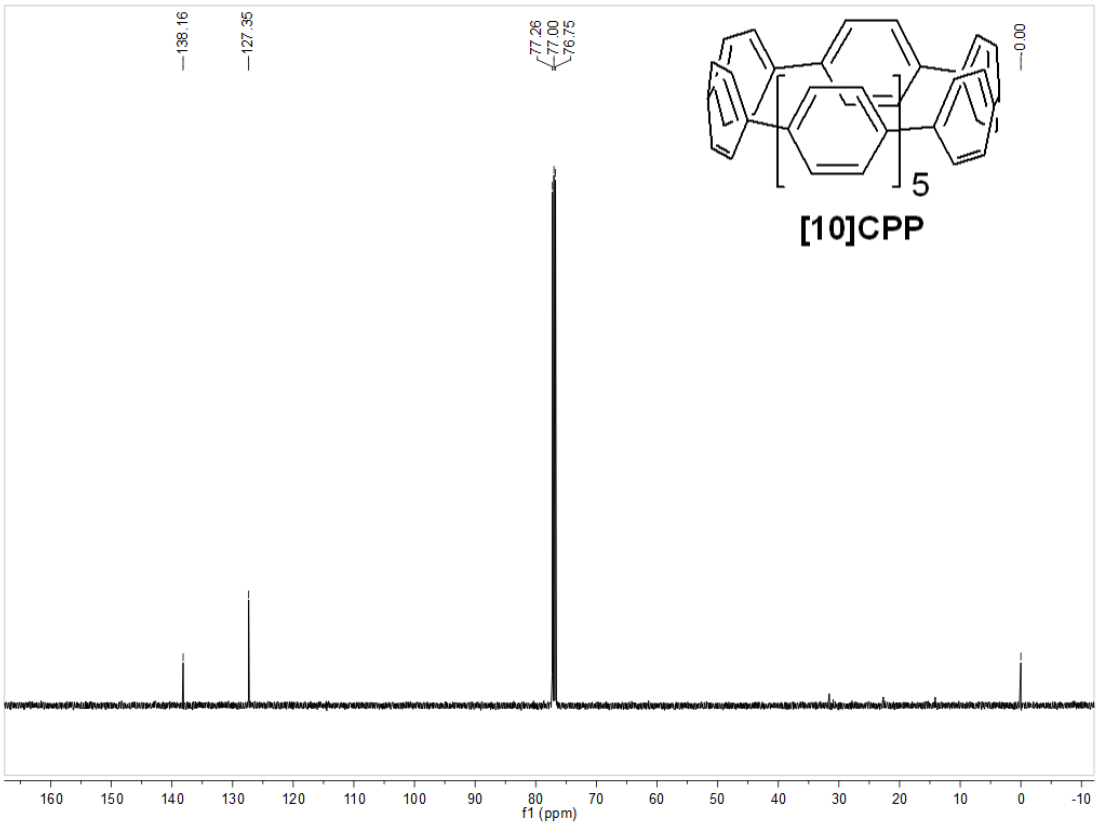

7.48
7.26
0.00
3
[8]CPP
X
X
32.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

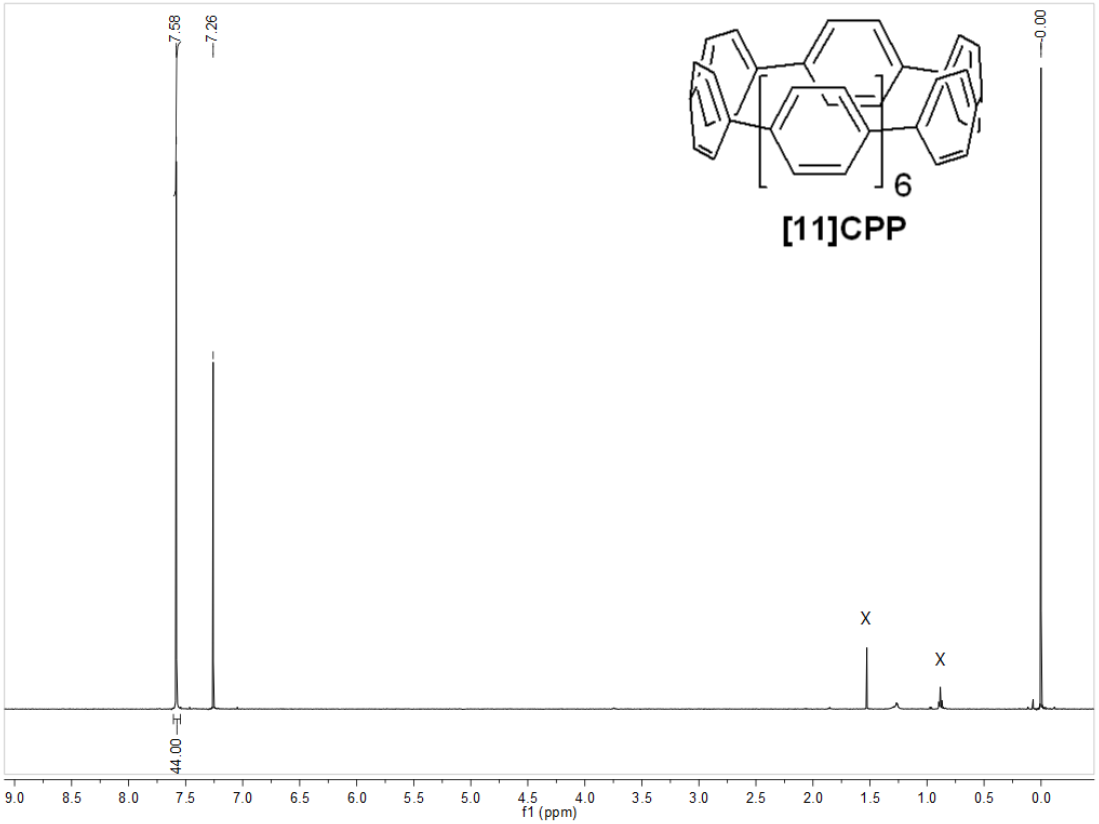

7.48
7.26
0.00
3
[8]CPP
X
X
32.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

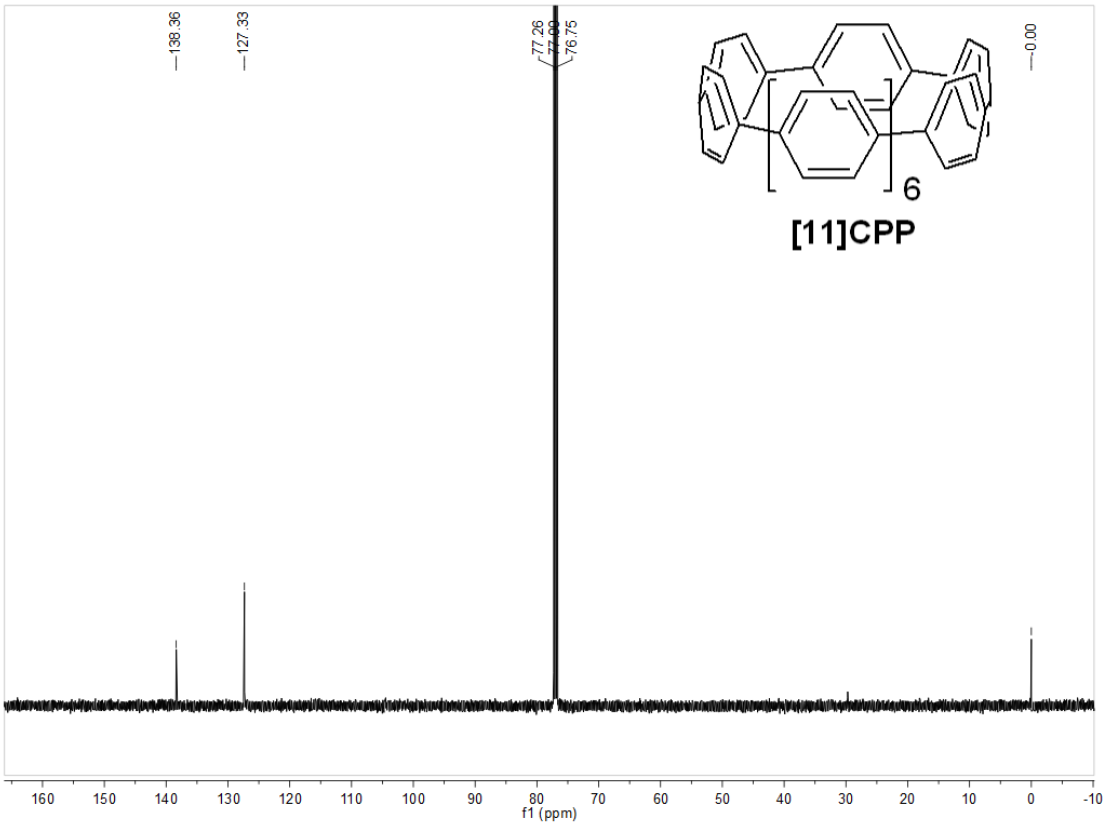

7.52
7.26
0.00
4
[9]CPP
X X X
36.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


137.91
127.37
77.26
77.00
76.75
0.00
4
[9]CPP
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.56
7.26
0.00
5
[10]CPP
X
40.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

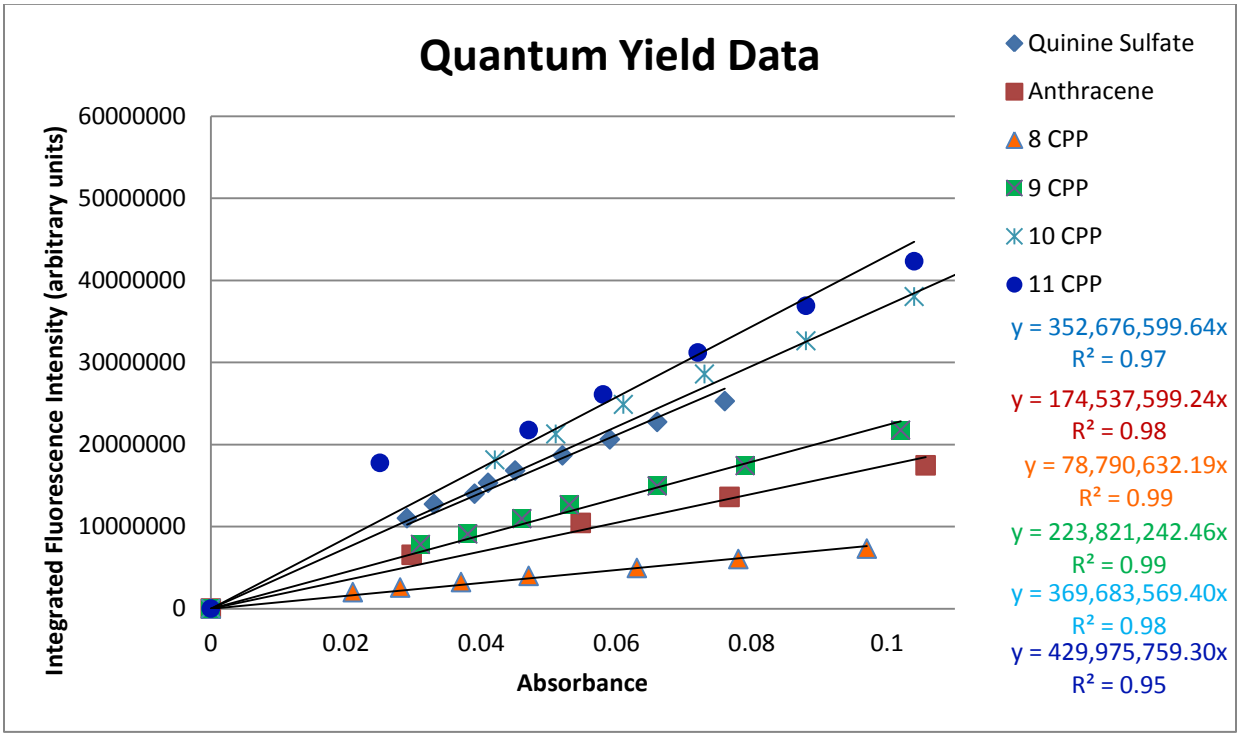

138.16
127.35
77.26
77.00
76.75
0.00
5
[10]CPP
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.58
7.26
0.00
6
[11]CPP
X
X
44.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


138.36
127.33
77.26
77.00
76.75
0.00
6
[11]CPP
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Optical Characterization

Relative quantum yields for [8]cycloparaphenylene, [9]cycloparaphenylene, [10]cycloparaphenylene and [11]cycloparaphenylene (dichloromethane) were determined as described by Williams[1] using anthracene (ethanol) and quinine sulfate (0.1 M H_2SO_4) as standards. All CPP samples were purified by preparative TLC followed by slow crystallization from chloroform with hexanes to give fine crystalline material. The NMR of each crystalline sample was greatly enhanced to make sure there were no traces of impurities. Excitation occurred at 339 nm for all standards and cycloparaphenylene samples. The fluorescence of [8]cycloparaphenylene was integrated from 450 – 650 nm. The fluorescence of [9]cycloparaphenylene was integrated from 400 – 650 nm. The fluorescence of [10]cycloparaphenylene was integrated from 375 – 625 nm. The fluorescence of [11]cycloparaphenylene was integrated from 400 – 600 nm. The fluorescence of [7]cycloparaphenylene and [12]cycloparaphenylene were as previously reported. The fluorescence of anthracene was integrated from 360 – 480 nm. The fluorescence of quinine sulfate was integrated from 400 – 600 nm.



1 Williams, A. T. R.and Winfield, S. A., Miller, J. N., *Analyst*, 1983, *108*, pp. 1067-1071.

1 Williams, A. T. R.and Winfield, S. A., Miller, J. N., *Analyst*, 1983, *108,* pp. 1067-1071.

Computational Details

The Gaussian 03 program[2] running on an IBM pSeries 655 system was used for optimization of structure 8, 9, 10, 11, 12, and 13 at the (B3LYP/6-31G*) level of theory. Structures were minimized with no symmetry restrictions.

Energy minimized structure of the ground state of [7] macrocycle (**8**):

C	-6.11167400	-0.07121700	-1.09765400
C	-3.75193500	-3.53227900	-0.47652400
C	0.63410500	-3.80603600	-1.30293100
C	4.28418400	-1.41238000	-1.29289100
C	5.78908900	1.81919400	-0.88830900
C	1.46815600	1.89665300	-1.00005200
C	-2.82139000	1.15783800	-0.67747300
C	-5.64665300	1.15882400	-1.32023100
C	-4.92585700	-2.78114900	-0.43981100
C	-0.74407600	-3.81107800	-1.10767600
C	3.14858300	-2.21564100	-1.34387200
C	6.33629600	0.60847700	-1.02716300
C	2.86035100	1.88199200	-0.92955600
C	-1.43356100	1.24046800	-0.59843700
C	-5.18287600	2.08560800	-0.21557000
C	-5.06108200	-1.69422500	0.43987600
C	-1.29182000	-3.73179200	0.18453000
C	2.90153400	-3.19226400	-0.36654200
C	6.28177200	-0.47241700	0.03462100
C	3.53373000	2.38073800	0.18962200
C	-0.79671800	2.34583100	-0.01150500
C	-3.63675300	2.17397600	-0.16474900
C	-6.22809900	-0.70213100	0.28142500
C	-2.67614600	-3.23313500	0.37874500
C	1.51887200	-3.71002300	-0.21437000
C	5.21535800	-1.54877800	-0.26085700
C	5.06702000	2.29118600	0.35920600
C	0.68725700	2.41029800	0.04720100

2 Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

C	-6.19196300	0.37938100	1.34096000
C	-2.87383300	-2.22921000	1.33943000
C	0.96989200	-3.84032400	1.07354500
C	5.05466800	-2.62872200	0.62387100
C	5.37426900	1.35537700	1.50911800
C	1.36872200	2.95428900	1.15103300
C	-3.00906900	3.27516600	0.43711400
C	-5.71333700	1.60491900	1.12283900
C	-4.03900900	-1.47134200	1.36529800
C	-0.40625800	-3.85678100	1.26844100
C	3.92140700	-3.43502300	0.57272400
C	5.91990700	0.14978900	1.36872400
C	2.75977000	2.94228300	1.21847400
C	-1.61868200	3.36056500	0.51008600
O	-5.75149400	3.40578000	-0.34288100
O	-7.42471100	-1.49324000	0.37771500
O	5.58959900	3.56271600	0.80765200
O	7.57499500	-1.06785600	0.25692800
C	-8.64082000	-0.78256800	0.18946200
C	-5.52280800	4.09328700	-1.56321300
C	5.41101400	4.67445700	-0.05508500
C	8.12083100	-1.82318300	-0.81211800
H	-6.39384500	-0.71460200	-1.92868400
H	-3.65759400	-4.33911100	-1.19922300
H	1.02417000	-3.78614200	-2.31702100
H	4.40017300	-0.62001500	-2.02393500
H	5.86291700	2.53129500	-1.70714700
H	0.98023700	1.51183300	-1.89114100
H	-3.27114600	0.28166000	-1.13109800
H	-5.53272000	1.51609100	-2.34056200
H	-5.73455100	-3.01889400	-1.12466200
H	-1.40157600	-3.75896900	-1.97142800
H	2.39129000	-2.00232100	-2.09190200
H	6.84294400	0.35766900	-1.95652000
H	3.42534700	1.46917500	-1.75811900
H	-0.83558000	0.41630300	-0.97625200
H	-6.54314100	0.08713300	2.32868800
H	-2.06312300	-1.96373000	2.01048500
H	1.62284000	-3.80554600	1.94070500
H	5.80362300	-2.80504200	1.39108300
H	5.11573200	1.73623200	2.49331700
H	0.80037000	3.35838200	1.98465200
H	-3.61922600	4.08242900	0.83144400
H	-5.67517700	2.34598600	1.91766400
H	-4.11244700	-0.65025100	2.06893500
H	-0.79839600	-3.87180300	2.28160100

H	3.80197200	-4.22974400	1.30465200
H	6.11195900	-0.47783700	2.23449300
H	3.25688400	3.36486600	2.08695900
H	-1.16495600	4.24270600	0.95449300
H	-9.44073100	-1.51998900	0.29407700
H	-8.77800100	0.00629900	0.94143300
H	-8.70350000	-0.32299800	-0.80670900
H	-4.46389400	4.08558800	-1.85408700
H	-6.12391300	3.68466900	-2.38711300
H	-5.83352800	5.12724700	-1.39014200
H	5.70777900	5.55404200	0.52261700
H	6.04921900	4.61787100	-0.94821500
H	4.36610500	4.79252900	-0.37159400
H	9.01443000	-2.30987200	-0.41234900
H	7.42519400	-2.59299200	-1.17251900
H	8.42251700	-1.19273100	-1.66072600

Total energy: -2077.72961824 a.u.

Energy minimized structure of the ground state of [8] macrocycle (9):

C	6.55463300	-1.06732100	-1.20184400
C	4.38253300	2.56557300	-1.05158100
C	1.45344700	5.59819600	-0.87881400
C	-2.70351400	4.48626400	-1.36225000
C	-5.10668800	0.88438800	-1.12598400
C	-5.80199200	-2.67994400	-0.91294500
C	-1.46817600	-2.40823200	-0.98576000
C	2.91101200	-1.88678400	-0.68040800
C	5.84960700	-2.19897800	-1.26852400
C	5.17976700	1.42492500	-1.09019700
C	2.75529000	5.10688200	-0.88452400
C	-1.43898400	5.04378500	-1.22575700
C	-4.33512300	2.03851800	-1.20137600
C	-6.58246700	-1.59969700	-0.99600200
C	-2.86169400	-2.42841500	-0.89892700
C	1.51733900	-1.91436900	-0.64032200
C	5.21189900	-2.88082600	-0.07482700
C	6.02110100	1.09961200	-0.02270300
C	3.25525700	4.37060400	0.20355800
C	-0.89033100	5.31043000	0.04298000
C	-4.52622300	3.10889000	-0.31137600
C	-6.78643700	-0.60408400	0.12676300
C	-3.51229300	-3.07642600	0.15645300
C	0.82034500	-3.00322900	-0.08746300
C	3.66943000	-2.94329100	-0.15984200
C	6.75121100	-0.25138900	0.05721600
C	4.38131800	3.41346600	0.06634300

C	0.58684700	5.34607100	0.20245000
C	-3.47196500	4.14951600	-0.23484400
C	-6.10290800	0.74930400	-0.15613400
C	-5.04643200	-3.09979500	0.33020300
C	-0.66505600	-3.02758300	-0.01466600
C	6.23906100	-1.01206000	1.26591800
C	5.30283600	3.14112000	1.09169400
C	1.16328600	4.79833300	1.36321100
C	-3.01997100	4.62413500	1.00903400
C	-6.37118000	1.85487400	0.66763800
C	-5.42623000	-2.21972800	1.50084600
C	-1.32656000	-3.67666300	1.04462900
C	2.98174500	-4.03172400	0.39321200
C	5.57532300	-2.16622500	1.20909800
C	6.11647800	2.01163100	1.04029600
C	2.47155100	4.32812400	1.36717500
C	-1.76187900	5.20451900	1.14276000
C	-5.59877400	3.01196000	0.59297200
C	-6.19956300	-1.14013400	1.41489300
C	-2.71455900	-3.70681200	1.12397500
C	1.58957200	-4.06532400	0.41839600
O	5.75454900	-4.20891000	0.10318900
O	8.14278900	0.09014100	0.23074100
O	-5.46193600	-4.42001200	0.75862200
O	-8.18449800	-0.41428800	0.42723000
C	9.02906700	-1.00866100	0.40110100
C	5.72085900	-5.07773500	-1.01989700
C	-5.26554300	-5.48644300	-0.15695600
C	-8.99580200	0.10439700	-0.61504600
H	7.01850100	-0.65789900	-2.09777100
H	3.68048700	2.75011700	-1.85958300
H	1.08324400	6.11044000	-1.76244300
H	-3.05766500	4.21910200	-2.35398000
H	-4.88430800	0.05782800	-1.79244200
H	-5.70042500	-3.32668500	-1.78189800
H	-1.00077500	-1.92101800	-1.83709000
H	3.41132600	-1.01444900	-1.09062600
H	5.72575400	-2.69404300	-2.22895800
H	5.09884700	0.75911800	-1.94296600
H	3.36952500	5.23401500	-1.77242900
H	-0.82471400	5.15308400	-2.11380500
H	-3.50962600	2.06946700	-1.90533700
H	-7.09359700	-1.38667600	-1.93256700
H	-3.44501400	-1.93623700	-1.67112900
H	0.96357000	-1.05750400	-1.01374200
H	6.44473900	-0.54921700	2.22846800

H	5.35964500	3.80336600	1.95209300
H	0.54323000	4.59754500	2.23064700
H	-3.60513200	4.42883300	1.90344200
H	-7.17483600	1.78979200	1.39576700
H	-5.02978600	-2.53841000	2.46126000
H	-0.74402400	-4.14513100	1.83263200
H	3.54797400	-4.85903200	0.80808500
H	5.23551300	-2.66082700	2.11582300
H	6.81363300	1.81774900	1.84984000
H	2.83555400	3.78628900	2.23573200
H	-1.41813000	5.48068700	2.13549600
H	-5.81172400	3.83759600	1.26738200
H	-6.43954400	-0.55899800	2.30137200
H	-3.19399100	-4.22851000	1.94689200
H	1.09299200	-4.94078500	0.82725300
H	10.02509900	-0.57392000	0.51769700
H	8.78699300	-1.60360300	1.29154200
H	9.02808500	-1.67746500	-0.47042700
H	4.73695100	-5.09258600	-1.50804700
H	6.48613200	-4.81837400	-1.76381400
H	5.93726800	-6.07801800	-0.63465000
H	-5.43954500	-6.40557100	0.40919200
H	-5.97971800	-5.45392500	-0.99140400
H	-4.24425900	-5.50708500	-0.56076900
H	-9.95390000	0.35936000	-0.15420500
H	-8.56530800	1.00943300	-1.06483300
H	-9.17906900	-0.63517500	-1.40704400

Total energy: -2308.77760787 a.u.

Energy minimized structure of the ground state of [9] macrocycle (**10**):

C	-5.54463100	-4.32845100	-1.06146300
C	-1.26526600	-3.94414400	-0.85310200
C	3.05243700	-3.46888500	-0.46118100
C	6.44188600	-2.50246900	-1.28095800
C	5.47920700	1.67225700	-0.67077800
C	2.18568500	4.67487900	-0.84063200
C	-0.76146700	7.03924700	-1.16123700
C	-2.59243500	3.07919200	-0.74366700
C	-4.88107300	-0.63632400	-1.12397300
C	-6.26752000	-3.20816900	-1.13827700
C	-2.65666400	-3.96751600	-0.80307100
C	1.66474800	-3.51951900	-0.38107000
C	5.82272600	-3.67290200	-1.42422300
C	6.23013300	0.50154600	-0.70663800

C	2.97340100	3.52322300	-0.85600100
C	0.55642600	7.04453100	-0.95274200
C	-1.91934600	4.29703600	-0.70391600
C	-4.27785800	0.61726700	-1.21928400
C	-6.51218200	-2.26991800	0.02359400
C	-3.33068000	-4.82516300	0.07105600
C	0.99299800	-4.71254000	-0.06171700
C	5.37282800	-4.53907400	-0.26933500
C	5.96572100	-0.55430400	0.17961300
C	3.63856000	3.08788000	0.29717400
C	1.21428900	6.74057500	0.37564600
C	-2.57524200	5.46982400	-0.30872100
C	-4.64634000	1.67084800	-0.36838200
C	-5.88847500	-0.88148900	-0.18638500
C	-4.86226000	-4.81975700	0.19745200
C	-0.48966000	-4.76360400	-0.01726600
C	3.83076000	-4.60584800	-0.20749000
C	6.77728600	-1.86095900	0.04837200
C	4.45461900	1.84527100	0.27499200
C	2.05380600	5.44605000	0.32012600
C	-1.79625000	6.78448700	-0.08707800
C	-3.95316300	2.98326100	-0.40282600
C	-5.23594600	-3.96292000	1.39050600
C	-1.17477800	-5.62486100	0.85734100
C	3.17274000	-5.78941900	0.14617000
C	6.51648900	-2.82419100	1.18499800
C	4.21271600	0.80324600	1.17985500
C	2.74209600	5.02393900	1.46856400
C	-1.14048800	6.69235300	1.27229000
C	-4.61156600	4.17039500	-0.04245600
C	-6.29117000	0.17785600	0.63935800
C	-5.95936400	-2.84470900	1.31388200
C	-2.56564300	-5.66033000	0.89732900
C	1.78078400	-5.84393600	0.20631800
C	5.90322300	-3.99923000	1.04179600
C	4.94694900	-0.38286600	1.12367500
C	3.50378500	3.85879900	1.46385500
C	0.17449200	6.64844200	1.47117700
C	-3.93428800	5.38634800	0.01671800
C	-5.67764200	1.42246600	0.55557100
O	-7.92917700	-2.00823000	0.15235200
O	-5.21137500	-6.20164900	0.43537400
O	-2.70908100	7.89494400	0.03469000
O	2.05328500	7.83780000	0.81479300
O	5.92765900	-5.86922900	-0.33589700
C	-6.58093200	-6.46966200	0.69091800

C	-8.74792100	-3.12599900	0.45911200
C	-3.31521100	8.37043900	-1.15789900
C	3.15619700	8.17995000	-0.00881900
C	5.85328200	-6.54214100	-1.58365300
O	8.18423300	-1.54920900	-0.07601900
C	8.80638400	-0.93989200	1.04445700
H	-5.41694900	-4.96710900	-1.93389100
H	-0.77547900	-3.29168100	-1.57000400
H	3.53646400	-2.53046200	-0.71403700
H	6.73536400	-1.92451000	-2.15364700
H	5.70008300	2.47576000	-1.36876000
H	1.66526000	4.96447700	-1.74798700
H	-1.14195500	7.23216600	-2.16140600
H	-2.03871000	2.18041800	-0.99962000
H	-4.56377300	-1.42696300	-1.79640200
H	-6.74229800	-2.91867700	-2.07437000
H	-3.22051900	-3.31378500	-1.46006100
H	1.09395400	-2.61147100	-0.55224500
H	5.58358700	-4.03140200	-2.42208200
H	7.04079000	0.40423200	-1.42287100
H	3.05405800	2.94037400	-1.76985000
H	1.22046300	7.25649700	-1.78762600
H	-0.85950100	4.32495500	-0.93984100
H	-3.51534500	0.77894700	-1.97587100
H	-4.84282400	-4.30472600	2.34606400
H	-0.61176500	-6.26057600	1.53509300
H	3.75863300	-6.67706000	0.36032500
H	6.84844000	-2.51474800	2.17319700
H	3.41909200	0.90819800	1.91504300
H	2.69171300	5.62297000	2.37293000
H	-1.83342700	6.64248000	2.10829700
H	-5.67130600	4.14636100	0.19530000
H	-7.08845700	0.01842400	1.35780000
H	-6.16644400	-2.25936700	2.20741400
H	-3.06848400	-6.34248700	1.57408900
H	1.29969300	-6.78997600	0.43863400
H	5.74992500	-4.65642600	1.89455200
H	4.70780200	-1.18715500	1.81246300
H	4.02547200	3.55294600	2.36706600
H	0.57176200	6.57466000	2.47961200
H	-4.45901500	6.28100900	0.33433000
H	-5.98050600	2.20568800	1.24427200
H	-6.64680900	-7.54669200	0.86603200
H	-6.94974200	-5.93823100	1.57844700
H	-7.22044100	-6.20772600	-0.16319100
H	-8.70455500	-3.89707000	-0.32223900

H	-8.47906900	-3.58780300	1.41879800
H	-9.76879100	-2.74018300	0.52169300
H	-4.12823100	9.02954300	-0.84108500
H	-2.61468100	8.95262400	-1.77167200
H	-3.73611300	7.55869000	-1.76735100
H	3.73656100	8.91327500	0.55757400
H	3.79652400	7.31544900	-0.23057100
H	2.84352600	8.64361200	-0.95514300
H	6.11869000	-7.58322500	-1.38011500
H	4.84367300	-6.51386500	-2.01639400
H	6.56736000	-6.13577000	-2.31223300
H	9.79149200	-0.61241800	0.70133200
H	8.24803200	-0.06562400	1.40584200
H	8.94526600	-1.64446000	1.87595800

Total energy: -2770.04797540 a.u.

Energy minimized structure of the ground state of [10] macrocycle (**11**):

C	4.25549100	-3.29008600	-1.08103400
C	7.66943700	-2.39927300	-0.26188100
C	6.41827700	1.75811500	0.55306600
C	2.20484000	3.99122700	-0.50616400
C	-0.36827200	6.48107900	-1.65433900
C	-2.85037900	3.10623400	-0.66045800
C	-5.86952700	-0.05028600	-0.37529600
C	-7.60677600	-2.50011000	0.13595200
C	-4.43979000	-3.12972200	-0.79424200
C	2.90097200	-3.22794000	-1.39706600
C	7.15139400	-3.51827500	-0.76755100
C	7.17913200	0.60612600	0.73812600
C	2.97463200	2.85778100	-0.25840500
C	0.96266800	6.42938100	-1.57831600
C	-1.98327400	4.17826600	-0.85989200
C	-5.09151100	1.07690800	-0.64052700
C	-7.30085500	-1.46236800	1.26300600
C	-5.57521100	-3.85561300	-0.69736700
C	2.03608300	-4.30110200	-1.12728900
C	6.26609600	-4.46408900	0.01284600
C	6.57052800	-0.61684300	1.05420200
C	4.19718700	2.94390700	0.42752600
C	1.75275700	6.51189600	-0.28930700
C	-2.27196800	5.44586700	-0.34290700
C	-4.93975400	2.10089700	0.30592800
C	-6.53544900	-0.19762300	0.84568700
C	-6.66320300	-3.73764700	0.35870800

C	-3.67962000	-3.52138200	-2.04238500
C	4.79983000	-4.42592500	-0.47086200
C	7.42709900	-1.89921800	1.14739100
C	5.01808600	1.73116100	0.66899100
C	2.62273600	5.25575900	-0.07539200
C	-1.28922000	6.62796400	-0.46266800
C	-4.04627800	3.25961600	0.05913800
C	-6.07750900	-3.45939500	1.73015800
C	-4.52525300	-4.65400500	-2.59067700
C	3.94757000	-5.50961500	-0.21498300
C	6.76708700	-2.97215300	1.98419000
C	4.41655000	0.50700100	1.00150100
C	3.83502500	5.34648100	0.62158800
C	-0.49652100	6.73368500	0.82269700
C	-4.34016100	4.53925600	0.56126800
C	-6.41897600	0.84521700	1.77924600
C	-6.41927700	-2.26522200	2.21176800
C	-5.62148900	-4.80965700	-1.82539600
C	2.59471700	-5.45038300	-0.54172700
C	6.27361000	-4.10476900	1.48433300
C	5.17758700	-0.64430100	1.19311100
C	4.60975700	4.21370900	0.86305100
C	0.83155200	6.68214400	0.89880800
C	-3.46997600	5.60848800	0.36726900
C	-5.63808800	1.96548900	1.51826000
O	-8.48645100	-0.94963600	1.89960500
O	-7.33897200	-5.00542200	0.28877600
O	-2.02131500	7.87418000	-0.51388300
O	2.57981200	7.69666000	-0.25198300
O	6.76663500	-5.81669600	-0.01530400
C	-8.33351800	-5.28474900	1.25461600
C	-9.27300700	-1.84732900	2.66066400
C	-2.78044600	8.12332500	-1.68754500
C	3.42563000	7.92702400	-1.36879900
C	6.96354600	-6.39913000	-1.29474100
O	8.74929500	-1.58060400	1.62996700
C	8.85551600	-1.17284900	2.98555800
H	-8.64730800	-2.81829800	0.23281800
H	-3.75913400	-2.68451600	-2.75858700
H	4.88825800	-2.43224900	-1.28414400
H	8.30064400	-1.75348700	-0.86781800
H	6.91393800	2.68625600	0.28080100
H	1.26788800	3.88859700	-1.04491000
H	-0.84797200	6.39932800	-2.62748600
H	-2.57723200	2.12611500	-1.04110600
H	-5.93167800	-0.82191500	-1.13385200

H	-7.50700300	-2.08373700	-0.86680300
H	-4.09837600	-2.35856600	-0.11484200
H	2.50205200	-2.31367500	-1.82693800
H	7.34412600	-3.77382500	-1.80645800
H	8.25860400	0.64605900	0.62860400
H	2.63636300	1.89330200	-0.62709300
H	1.54258800	6.30490700	-2.49035400
H	-1.06266300	4.01777300	-1.41290400
H	-4.60309600	1.16372700	-1.60726100
H	-5.41365000	-4.17521300	2.20688300
H	-4.26820700	-5.20613600	-3.48754000
H	4.35526500	-6.40637300	0.24165400
H	6.68393700	-2.77815500	3.05059200
H	3.33888000	0.45886000	1.13179200
H	4.16689500	6.31642200	0.97777500
H	-1.09610400	6.87563900	1.71834500
H	-5.27140000	4.70326400	1.09668600
H	-6.94482900	0.76803500	2.72482400
H	-6.07912400	-1.83691200	3.15072300
H	-6.42726100	-5.51619500	-1.97664700
H	1.96418100	-6.31419100	-0.34890000
H	5.81067800	-4.84552000	2.13201800
H	4.67934500	-1.57479300	1.44551300
H	5.53789000	4.31209800	1.41998200
H	1.33590400	6.78210800	1.85670800
H	-3.72027600	6.58906400	0.76024600
H	-5.53704200	2.73035300	2.28325600
H	-8.57149700	-6.34634500	1.14441200
H	-7.98549000	-5.10221400	2.27993300
H	-9.25466600	-4.70710800	1.09072400
H	-9.77788300	-2.59950600	2.03823600
H	-8.69124900	-2.37028100	3.43183900
H	-10.03813500	-1.23615900	3.14699200
H	-3.39864300	8.99759000	-1.46649500
H	-2.14127000	8.35759400	-2.54978400
H	-3.43748300	7.28167200	-1.94678700
H	4.10595700	8.72953400	-1.07095300
H	4.01918000	7.04127900	-1.63463500
H	2.86095600	8.25794000	-2.25094800
H	7.12190300	-7.46686000	-1.12034100
H	6.08960000	-6.27244200	-1.94817300
H	7.85088100	-5.99439900	-1.80002200
H	9.86599200	-0.77187100	3.10249800
H	8.13086000	-0.38808800	3.24206700
H	8.73311400	-2.01466800	3.68040800
C	-1.73780300	-4.59261900	-0.78709100

C	-0.37540200	-4.77969500	-0.57245400
C	0.58423600	-4.18812100	-1.41394600
C	0.11611600	-3.43352100	-2.50105200
C	-1.24781500	-3.23888600	-2.70735000
C	-2.19799800	-3.79900400	-1.84679300
H	-2.45759700	-5.03753700	-0.10493200
H	-0.04879200	-5.35538300	0.28916600
H	0.82676700	-2.99299800	-3.19459900
H	-1.57813800	-2.63234500	-3.54813300

Total energy: -2924.86235588 a.u.

Energy minimized structure of the ground state of [11] macrocycle (**12**):

Total energy: -3232.15665363 a.u.

C	-9.23894800	-2.53320200	-1.26378000
C	-5.84436000	-5.32385400	-0.12891800
C	6.83707600	-2.86660800	-0.91360800
C	9.71932400	-0.84325100	-1.29529300
C	6.94979600	2.52286900	-0.95910300
C	2.73404500	4.13140800	-0.91339300
C	-0.71920100	6.21665200	-1.10484300
C	-3.66625900	3.05886100	-0.40904300
C	-7.17881100	0.49733100	-1.02464000
C	-9.45363200	-1.22596800	-1.42428200
C	-7.18580600	-4.94485600	-0.18823500
C	5.51070700	-3.28171700	-0.85371800
C	9.59072000	-2.16573500	-1.39079200
C	8.10567300	1.74579000	-0.95713300
C	3.83436700	3.27055500	-0.95334900
C	0.61221500	6.13655900	-1.06659900
C	-2.60005300	3.95445200	-0.36941400
C	-6.10398800	1.38444800	-0.97920900
C	-9.53439600	-0.23851900	-0.28139700
C	-7.58368600	-3.66127700	0.20688500
C	5.12623800	-4.38794200	-0.08030600
C	9.30205800	-3.06385300	-0.20868200
C	8.31505400	0.76256100	0.02266600
C	4.77524700	3.25402200	0.08355600
C	1.42072200	6.06438100	0.21155700
C	-2.79429400	5.29163400	0.00117700
C	-6.12448300	2.52032000	-0.15473500
C	-8.33213100	0.72199800	-0.26562600
C	-9.04883300	-3.20583100	0.08413100
C	-4.85852700	-4.43624500	0.33055400

C	7.83472000	-3.54558800	-0.20574300
C	9.62071300	-0.06378700	-0.00027300
C	5.97471600	2.37057800	0.04073500
C	2.55541700	5.02526700	0.14807800
C	-1.60469600	6.26157300	0.12494200
C	-4.97836100	3.46577300	-0.10261100
C	-9.41027900	-2.26686300	1.21409100
C	-5.27006000	-3.15438000	0.72999500
C	7.46020900	-4.65790300	0.56282000
C	9.72379100	-1.00440100	1.18024600
C	6.18600100	1.39131100	1.01934000
C	3.49429200	5.00064800	1.19159500
C	-0.80961400	5.91967200	1.36896300
C	-5.16154000	4.81019300	0.26013000
C	-8.36695700	1.85992800	0.55298400
C	-9.61480300	-0.95837300	1.05336800
C	-6.60480000	-2.77268100	0.66669600
C	6.13035100	-5.06989200	0.62746400
C	9.57967300	-2.32566900	1.08477000
C	7.32914400	0.59059500	1.00079800
C	4.57257900	4.12228500	1.16920900
C	0.51689900	5.81121700	1.40178800
C	-4.09150200	5.69911400	0.32876900
C	-7.28373300	2.72981400	0.61638900
O	-10.67912600	0.62803100	-0.44641600
O	-9.83406400	-4.40925900	0.15691300
O	-2.08673200	7.60260500	0.37442200
O	2.00299100	7.36132600	0.52304100
O	10.19791200	-4.19292400	-0.15174800
C	-11.23655400	-4.24142900	0.02170600
C	-11.94660600	-0.01135200	-0.43257700
C	-2.51840300	8.35517200	-0.74965800
C	2.84743800	7.93110500	-0.46504700
C	10.22429000	-5.05086300	-1.28180400
O	10.75651800	0.82982900	-0.07244200
C	10.94780600	1.72267800	1.01297600
H	-9.16249400	-3.19756500	-2.12274700
H	-5.56256200	-6.33140900	-0.42434900
H	7.09294600	-1.99275800	-1.50302000
H	9.91710100	-0.24010600	-2.17768100
H	6.81395500	3.28432700	-1.72292500
H	2.01460200	4.09910800	-1.72584400
H	-1.22468200	6.27793000	-2.06622500
H	-3.46827700	2.02062000	-0.65865700
H	-7.11630300	-0.37348500	-1.66899200
H	-9.56001400	-0.79613400	-2.41868800

H	-7.93448500	-5.65164900	-0.52754600
H	4.75319900	-2.71478400	-1.38721800
H	9.64930300	-2.64034200	-2.36692400
H	8.86802200	1.92109500	-1.71088900
H	3.95758700	2.59619900	-1.79688800
H	1.16811100	6.15224400	-2.00114500
H	-1.59861600	3.60338200	-0.60594400
H	-5.24647000	1.19661700	-1.61833800
H	-9.45267800	-2.72414200	2.20080800
H	-4.52820100	-2.43414900	1.06258700
H	8.22397500	-5.20988700	1.10277800
H	9.90238600	-0.55560300	2.15404100
H	5.44110900	1.24466100	1.79714700
H	3.39377200	5.70537000	2.01175600
H	-1.39710500	5.79227300	2.27469200
H	-6.15939300	5.17866700	0.47802800
H	-9.25549600	2.06820100	1.14049100
H	-9.83601100	-0.32316700	1.90896300
H	-6.88262300	-1.76881000	0.96900500
H	5.86962400	-5.94392000	1.21894200
H	9.65459000	-2.96287800	1.96259100
H	7.44895300	-0.17688200	1.75855500
H	5.29303100	4.13157000	1.98297900
H	1.02194700	5.59547200	2.33946900
H	-4.26133800	6.72305400	0.64152400
H	-7.33535500	3.57818000	1.29200500
H	-11.66838900	-5.24253000	0.09863300
H	-11.65407700	-3.60893900	0.81689700
H	-11.51091400	-3.80566100	-0.94877900
H	-12.05053400	-0.74031500	-1.24806800
H	-12.14325700	-0.52459900	0.51881100
H	-12.68464000	0.78334000	-0.56879700
H	-2.98038100	9.25916300	-0.34336000
H	-1.67865900	8.64796400	-1.39364700
H	-3.26355300	7.82014800	-1.35577500
H	3.29356900	8.81626700	-0.00374600
H	3.65154100	7.24855900	-0.77318600
H	2.28608000	8.24658300	-1.35566900
H	10.77995300	-5.94040100	-0.97280100
H	9.21716400	-5.35414800	-1.59796100
H	10.74609900	-4.59614500	-2.13495000
H	11.74662500	2.40250700	0.70454500
H	10.04647900	2.31029300	1.23317100
H	11.26890500	1.20553200	1.92793100
C	1.71143800	-5.29001400	1.31012200
C	3.08837700	-5.10511000	1.21819300

C	3.69298600	-4.75943300	-0.00135600
C	2.87159400	-4.68463800	-1.13855800
C	1.49760800	-4.87328600	-1.04772600
C	0.88152300	-5.14279900	0.18586200
H	1.26966000	-5.53206100	2.27299800
H	3.69754500	-5.17669500	2.11535500
H	3.31594300	-4.45475700	-2.10296200
H	0.88405700	-4.75297900	-1.93613000
C	-2.80086500	-5.47658900	-0.68903900
C	-1.41990400	-5.65095400	-0.72430300
C	-0.59687800	-5.14210400	0.29450400
C	-1.22244800	-4.51421600	1.38460600
C	-2.60050100	-4.33704800	1.41778300
C	-3.41695200	-4.78122900	0.36424200
H	-3.40580300	-5.83829800	-1.51626300
H	-0.97032500	-6.17244900	-1.56508300
H	-0.61461600	-4.10868000	2.18851000
H	-3.05224100	-3.82770100	2.26443500

Total energy: -3232.15665363 a.u.

Energy minimized structure of the ground state of [12] macrocycle (**13**):

C	-1.65680900	8.12608400	2.14298900
C	2.81909000	7.74204000	0.75676200
C	3.85158500	-5.22534700	0.67681400
C	1.65380000	-7.87283900	2.23115400
C	-2.52226800	-7.01334400	1.22901300
C	-5.74254700	-4.15569500	0.32480100
C	-8.92904000	-1.98621500	0.07876400
C	-6.16242000	1.43408100	0.19482600
C	-4.23438800	5.19821400	1.43299400
C	-2.92919600	7.72815500	2.16920400
C	1.62662300	8.43187900	0.96450400
C	4.46312900	-4.03467900	0.29078300
C	2.93642000	-7.51536100	2.25283800
C	-1.37515800	-7.73427500	1.54045000
C	-4.51762200	-4.75800000	0.61248400
C	-8.45365300	-3.22945700	-0.00653800
C	-6.86151300	0.26653000	-0.09936900
C	-4.93732100	4.01360400	1.20382200
C	-3.83872000	7.71458300	0.95989600
C	0.39289200	7.81788400	0.73017100
C	5.80641100	-4.00623800	-0.12037400
C	3.90539400	-7.75568100	1.11715300
C	-0.27656200	-7.75593100	0.66816000

C	-3.88483000	-5.59202400	-0.31952300
C	-7.77681800	-3.80560600	-1.23008100
C	-8.16574800	0.31517300	-0.61080600
C	-5.99758300	3.95673700	0.28474500
C	-4.57986200	6.38020900	0.77025000
C	-0.92854600	8.59165600	0.89855900
C	2.82943500	6.40132200	0.33859700
C	4.55717900	-6.43538700	0.66078500
C	0.97124900	-8.56380900	1.07113700
C	-2.62570000	-6.30226100	0.02109000
C	-6.38756600	-4.38237900	-0.89633800
C	-8.88793500	-0.97555200	-1.04721100
C	-6.74526200	2.70176500	0.01304000
C	-1.79041200	8.41102200	-0.33272500
C	1.58205100	5.77606700	0.15672500
C	5.87975200	-6.42237000	0.20172500
C	1.93019000	-8.76995200	-0.07954400
C	-1.52552800	-6.32136300	-0.84736900
C	-5.74315800	-5.19582400	-1.84080300
C	-8.17604600	-1.54073100	-2.25729400
C	-8.06309500	2.73638500	-0.47147200
C	-5.64462800	6.33220700	-0.14171200
C	-3.06574000	8.02889600	-0.30346100
C	0.39015800	6.47254300	0.33703800
C	6.49348700	-5.23047200	-0.17468200
C	3.21664200	-8.42213700	-0.05437300
C	-0.36534000	-7.02754400	-0.52316700
C	-4.51085800	-5.78005800	-1.56348700
C	-7.67287600	-2.77098400	-2.32951300
C	-8.75219000	1.57029700	-0.79582000
C	-6.32641300	5.14828500	-0.38889400
O	-4.80836300	8.79281100	1.02819600
O	-0.65121000	9.98499500	1.17224900
O	-10.21208400	-0.66104000	-1.53351200
O	-8.58760400	-4.84462400	-1.83731400
O	4.93103700	-8.70858000	1.48204400
C	-0.44006700	10.83937300	0.05805900
C	-5.64741400	8.81732600	2.17339200
C	-11.25980500	-0.56366000	-0.58135700
C	-8.94293400	-5.94314800	-1.01161200
C	5.59342500	-8.49697200	2.72027100
O	0.55719600	-9.83012700	1.64322200
C	-0.06443200	-10.75461700	0.76323300
H	-1.07067500	8.16670300	3.05816600
H	3.75753200	8.27164500	0.89043700
H	2.81423400	-5.21260200	0.99964500

H	1.01732600	-7.68517700	3.09243800
H	-3.36918000	-7.03045300	1.90994100
H	-6.20021200	-3.51096600	1.06903100
H	-9.37961900	-1.65031600	1.00987500
H	-5.13438900	1.35748500	0.53669800
H	-3.41139500	5.19597000	2.14207100
H	-3.37253200	7.42834800	3.11615000
H	1.64996000	9.46388100	1.29561300
H	3.88751400	-3.11330500	0.30599700
H	3.33418900	-7.00737000	3.12816400
H	-1.33474400	-8.31484100	2.45733300
H	-4.04310100	-4.57528700	1.57306100
H	-8.53672900	-3.88680200	0.85618000
H	-6.37253600	-0.69511400	0.03304600
H	-4.66476100	3.12644600	1.76813000
H	-1.31149300	8.60651700	-1.28920400
H	1.54053100	4.72758700	-0.12364600
H	6.43801300	-7.35234000	0.17457700
H	1.52682700	-9.24971500	-0.96844200
H	-1.57095700	-5.76460300	-1.77983700
H	-6.23652800	-5.40317000	-2.78578600
H	-8.10520400	-0.86165700	-3.10321900
H	-8.56718900	3.68989200	-0.59567400
H	-5.93936300	7.24044000	-0.65894600
H	-3.62975900	7.93807800	-1.22826400
H	-0.55630500	5.96451800	0.17056200
H	7.53833100	-5.24441000	-0.47174600
H	3.86334600	-8.63036300	-0.90361900
H	0.47822800	-7.00562600	-1.20700900
H	-4.04715400	-6.43165700	-2.29953200
H	-7.18759200	-3.11196900	-3.24046800
H	-9.75012000	1.63470700	-1.21358600
H	-7.11509600	5.14536000	-1.13470800
H	-0.13547400	11.80248800	0.47681800
H	0.35671900	10.47703300	-0.60754200
H	-1.35728100	10.98232400	-0.52740300
H	-6.14519100	7.85304800	2.34596200
H	-5.09810800	9.10491200	3.08005900
H	-6.40864600	9.57596900	1.97231800
H	-12.12449800	-0.18002400	-1.12990900
H	-11.52034100	-1.54116500	-0.15439900
H	-11.02656800	0.13197500	0.23781200
H	-9.39998800	-6.68209400	-1.67520100
H	-8.07050100	-6.39788500	-0.52276100
H	-9.67757000	-5.66272600	-0.24396500
H	6.43408200	-9.19597500	2.73393000

H	5.98289200	-7.47393600	2.81685800
H	4.94143200	-8.71564900	3.57623100
H	-0.45700900	-11.55490000	1.39634800
H	-0.89678700	-10.30389700	0.20538000
H	0.64945500	-11.19133800	0.05170100
C	8.24056600	-1.49055200	-1.60253700
C	7.51747000	-2.66227600	-1.39681800
C	6.50218300	-2.73154100	-0.42723200
C	6.21100700	-1.55992200	0.29055400
C	6.93058600	-0.38542000	0.08066700
C	7.97569000	-0.33874700	-0.84933400
H	9.03759600	-1.46796600	-2.33918000
H	7.74364500	-3.53788900	-1.99924400
H	5.44340100	-1.57928400	1.05908500
H	6.69227400	0.49757700	0.66672100
C	5.30787700	6.08422900	0.68974800
C	6.52056100	5.48835800	0.36331200
C	6.58981200	4.45707800	-0.58513800
C	5.39570500	4.03431200	-1.17807600
C	4.18265600	4.64981100	-0.86937600
C	4.10837400	5.69705200	0.06319400
H	5.29298300	6.86222900	1.44717300
H	7.43447300	5.83784700	0.83467800
H	5.40969000	3.22810800	-1.90553400
H	3.28718200	4.33215300	-1.39527200
C	8.47881600	3.05356600	0.24688100
C	8.85851000	1.77806200	0.19331100
C	8.82365300	0.93084400	-1.05862800
C	8.29438800	1.72213200	-2.23492300
C	7.91585700	2.99879400	-2.18118800
C	7.96142800	3.84900000	-0.93159600
H	8.54818500	3.60792700	1.17972500
H	9.21131500	1.28866700	1.09813300
H	8.26310200	1.17541400	-3.17459600
H	7.55552200	3.48385700	-3.08542400
O	10.15494400	0.55892200	-1.48958600
O	8.93821300	4.91408500	-1.05414800
C	11.00233000	-0.03080400	-0.51486800
H	10.52144300	-0.87208000	0.00328600
H	11.87288200	-0.40513400	-1.06032200
H	11.34344500	0.70162900	0.22882300
C	8.77725000	5.80581300	-2.14691600
H	9.02367300	5.33110200	-3.10636400
H	7.76082900	6.21919600	-2.20149000
H	9.48154900	6.62395500	-1.97347800

Total energy: -3693.38963079 a.u.