Supporting Information

Antiaromaticity in Distal Bisfluorenyl Dications Separated by Multiple Discrete Spacer Units

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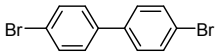
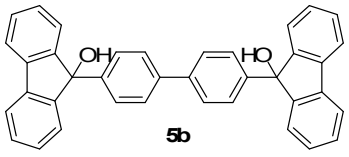
Synthetic Procedures

All starting materials were purchased commercially and used without further purification or prepared with known literature procedures as indicated in the text. Tetrahydrofuran and diethyl ether were distilled from Na and benzophenone before use. SO_2ClF was synthesized from NH_4F and SO_2Cl_2 according to literature methods.[1] Other reagent grade solvents were used as received. All IR spectra were recorded with a Thermo Nicolet Nexus 470 FT-IR spectrometer. All ^1H and ^{13}C NMR spectra were recorded on a Varian Inova 400 (100) MHz instrument or a Varian Mercury 300 (75) MHz instrument. Chemical shifts are reported in parts per million (ppm) and referenced to the appropriate residual solvent peak. Column chromatography was performed on silica gel 40-64 mesh using technical grade solvents.



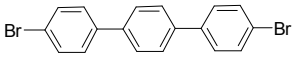
4,4'-dibromo-p-biphenyl. Prepared by literature method from biphenyl.[2] mp = 160-163 °C, lit mp = 162-163 °C. ^1H NMR (400 MHz, $CDCl_3$): δ 7.56 (d, J = 8.4 Hz, 4H), 7.41 (d, J = 8.4 Hz, 4H).



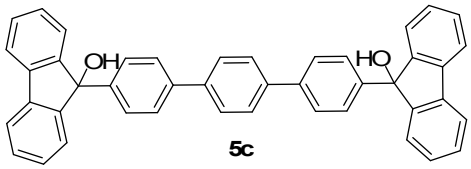
5b

9,9'-(biphenyl-4,4'-diyl)bis(9H-fluoren-9-ol (5b).[3] 4,4'-Dibromo-p-biphenyl (1.0 g, 3.2 mmol) was dissolved in 100 mL of anhydrous Et_2O in an oven dried and Ar flushed

flask. The reaction was cooled to -78 °C and 1.5 M *t*-BuLi in pentane (9.00 mL, 13.4 mmol) was added dropwise and then stirred 30 min. The cooling bath was removed and the reaction was stirred at rt for 1 hr. The reaction was cooled back to -78 °C and 1.15 g of 9-fluorenone (6.40 mmol) dissolved in 75 mL of anhydrous Et_2O was transferred into the reaction vessel via a canula. The reaction was allowed to slowly warm to rt stirring for 16 hrs. An Ar flushed reflux condenser was then attached to the reaction and it was refluxed for 4 hrs. The reaction was quenched with 50 mL of 5% HCl and the layers were separated. The aqueous layer was extracted 2 x with 100 mL EtOAc. The combined organics were washed with 100 mL of brine, dried with $MgSO_4$, filtered, and the solvents were removed under reduced pressure. Purification was achieved by recrystallization in EtOAc resulting in 1.55 g (94%) of white powder. ^{1}H NMR (400 MHz, d^6-acetone): δ 7.78 (d, *J* = 6.8 Hz, 4H), 7.50 (d, *J* = 10.4 Hz, 4H), 7.41-7.31 (m, 12H), 7.25 (t, *J* = 7.6 Hz, 4H). ^{13}C NMR (100 MHz, d^6-acetone): δ 153.4, 153.3, 145.9, 141.6, 130.5, 130.0, 128.3, 127.8, 126.6, 121.8, 84.9. IR (neat, cm^{-1}): 3533, 3045, 1489, 1164, 1029.

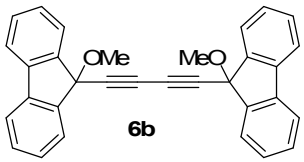


4,4'-dibromo-p-terphenyl.[4] Terphenyl (2.0 g, 8.7 mmol) was suspended in 200 mL glacial acetic acid and heated to 100 °C. Bromine (4.5 g, 28 mmol) and a crystal of iodine were added and the reaction was heated to reflux for 16 hrs. The reaction was then cooled slightly below reflux temperatures and the reaction was filtered. The filtered solid was washed with several portions of EtOH and dried on a vacuum pump. No further purification was performed and the solid was obtained as a white powder (1.90 g, 56%). mp = 314-317 °C, lit mp = 314-315 °C.[5] ^{1}H NMR (400 MHz, d^8-THF): δ 7.72 (s, 4H), 7.60 (s, 8H).



5c

9,9'-(terphenyl-4,4'-diyl)bis(9H-fluoren-9-ol (5c).[3] 4,4'-Dibromo-p-terphenyl (1.00 g, 2.58 mmol) was suspended in 150 mL of anhydrous THF in an over dried and Ar flushed flask. The reaction was cooled to -78 °C and 1.6 M *t*-BuLi in pentane (6.70 mL, 10.8 mmol) was added dropwise and stirred for 30 min. The cooling bath was removed and the reaction was stirred for 4 hrs at rt. The reaction was cooled back to -78 °C and 930 mg of 9-fluorenone (6.16 mmol) dissolved in 50 mL of anhydrous Et_2O was transferred into the reaction vessel via a canula. The reaction was allowed to slowly warm to rt stirring for 36 hrs. The reaction was quenched with 50 mL of sat NH_4Cl and the layers were separated. The aqueous layer was extracted 2 x with 100 mL Et_2O. The combined organics were washed with 100 mL of brine, dried with $MgSO_4$, filtered, and the solvents were removed under reduced pressure. Purification was achieved by column chromatography (5%→25%→50% EtOAc:hexane) resulting in 110 mg (7%) of white powder. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, J = 8.0 Hz, 4H), 7.59 (s, 4H), 7.52 (d, J = 8.4 Hz, 4H), 7.45 (d, J = 8.8 Hz, 4H), 7.39 (t, J = 6.8 Hz, 8H), 7.28 (t, J = 6.8 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) : δ 150.4, 142.3, 139.6, 139.5, 129.2, 128.5, 127.3, 126.8, 125.9, 124.8, 120.1, 83.6. IR (neat, cm^{-1}): 3545, 3033, 1489, 1448, 1165, 1031.



6b

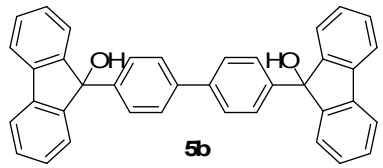
1,4-bis(9-methoxy-*9H*-fluoren-9-yl)buta-1,3-diyne (6b).

9-Ethynyl-9H-fluoren-9-ol[6] (600 mg, 2.91 mmol) was dissolved in 30 mL of pyridine and 10 mL of methanol and warmed to 50 °C. $Cu(OAc)_2 \cdot H_2O$ (1.45 g, 7.28 mmol) was added and the reaction was stirred overnight resulting in a color change from blue to green. The pyridine was removed under reduced pressure the crude solid was taken up in 150 mL of Et_2O. The organics were washed 2 x 50 mL of 10% HCl followed by 50 mL of sat. $NaHCO_3$. The organics were then dried with $MgSO_4$, filtered, and the solvents removed under reduced pressure. Purification was achieved by column chromatography (25%→75% EtOAc:hexane) resulting in 360 mg (60%) of tan powder. ^{1}H NMR (400 MHz, d^6-acetone): δ 7.73 (d, *J* = 7.2 Hz, 4H), 7.67 (s, *J* = 7.6 Hz, 4H), 7.41 (t, *J* = 7.2 Hz, 4H), 7.35 (d, *J* = 7.6 Hz, 4H). ^{13}C NMR (100 MHz, d^6-acetone): δ 148.9, 140.9, 131.4, 130.2, 126.2, 122.1, 82.8, 76.3, 67.6. IR (neat, cm^{-1}): 3272, 3010, 1450, 1394, 1195, 1056, 1031.

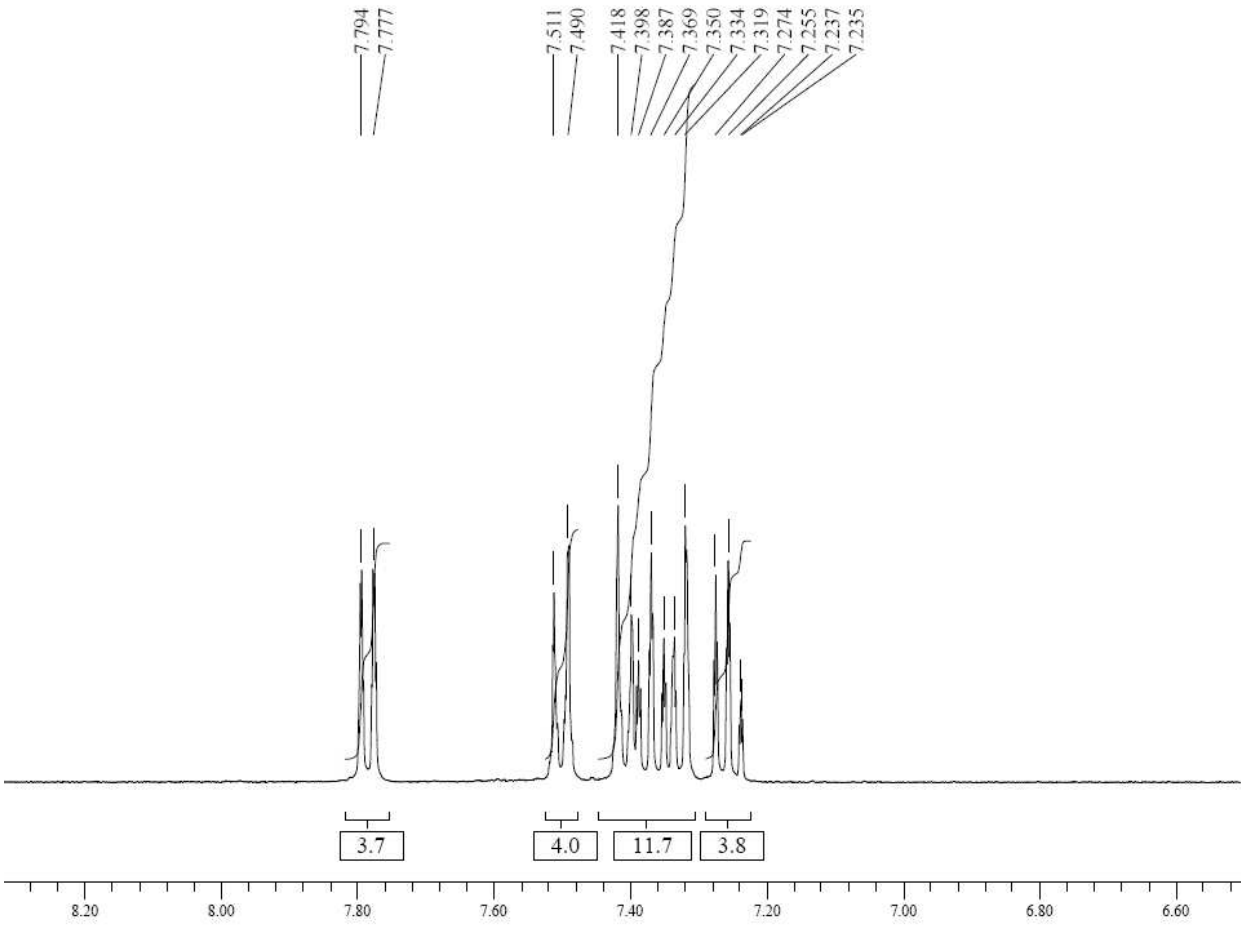
The purified diol (200 mg, 0.485 mmol) was dissolved in 5 mL of DMF and cooled to 0 °C. 60% NaH in mineral oil (58.0 mg, 1.45 mmol) was added and stirred for 15 minutes followed by MeI (181 μL, 291 mmol). The reaction was stirred for 2 hrs and then was taken up in 75 mL of Et_2O. The organics were washed with 75 mL of water followed by 75 mL of brine. The organics were then dried with $MgSO_4$, filtered, and the solvents removed under reduced pressure. Purification was achieved by column chromatography (5%→10% EtOAc:hexane) resulting in 140 mg (67%) of tan powder. ^{1}H NMR (400 MHz $CDCl_3$): δ 7.61-7.58 (m, 8H), 7.39 (t, *J* = 7.2 Hz, 4H), 7.41 (t, *J* = 7.2 Hz, 4H), 3.10 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.1, 140.0, 129.9, 128.3, 125.1, 120.2, 80.2, 78.1, 67.9, 52.0. IR (neat, cm^{-1}): 2926, 1450, 1231, 1091, 1034. mp = 151 °C dec.

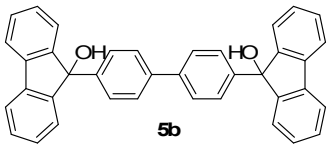
General Preparation of Dications by Superacid Ionization. Fluorosulfonic acid (0.5 mL) and SbF_5 (0.5 mL) were added to an oven dried graduated centrifuge tube in an inert atmosphere drybox. The tube was taken out of the drybox, placed under in Ar bubbler, and cooled to -78 °C. SO_2ClF (1 mL) at -78° was pressure transferred to the centrifuge tube using Teflon tubing and the reagents were mixed on a vortex stirrer. 10 mg of the neutral dimethoxy ether or diol (dried on a drying pistol) was placed in an NMR tube and the sample was flushed with Ar for 15 minutes and cooled to -78 °C. Approximately 1 mL of the reagent solution was Ar pressure transferred to the NMR tube using Teflon tubing and the reagents were mixed on a vortex stirrer. A Teflon insert containing a glass capillary filled with d^6-acetone was placed in the NMR tube and the solution was quickly analyzed by ^1H NMR at -50°.

NMR Spectra for **5b**, **5c**, and **6b**.

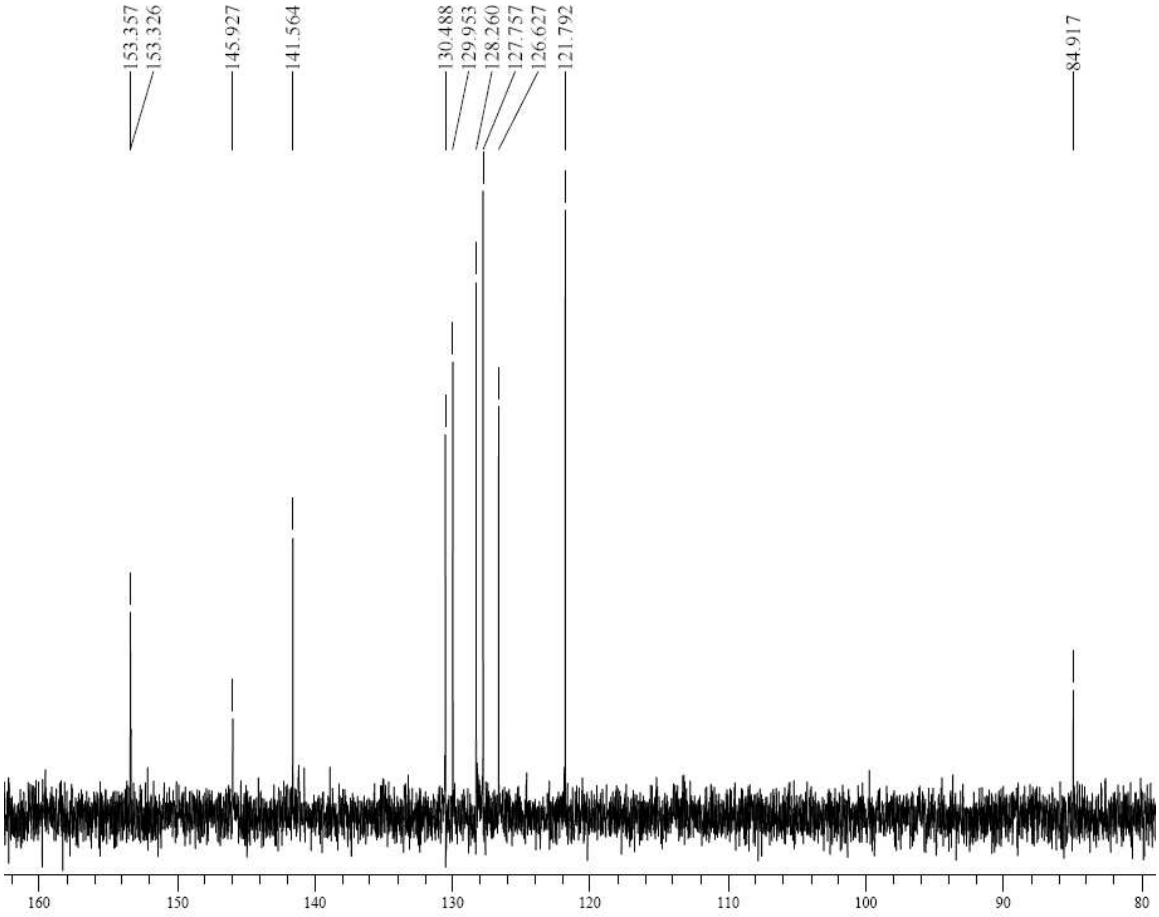


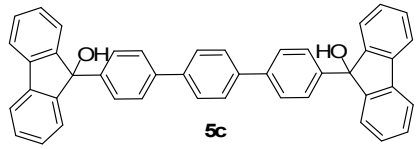
5b



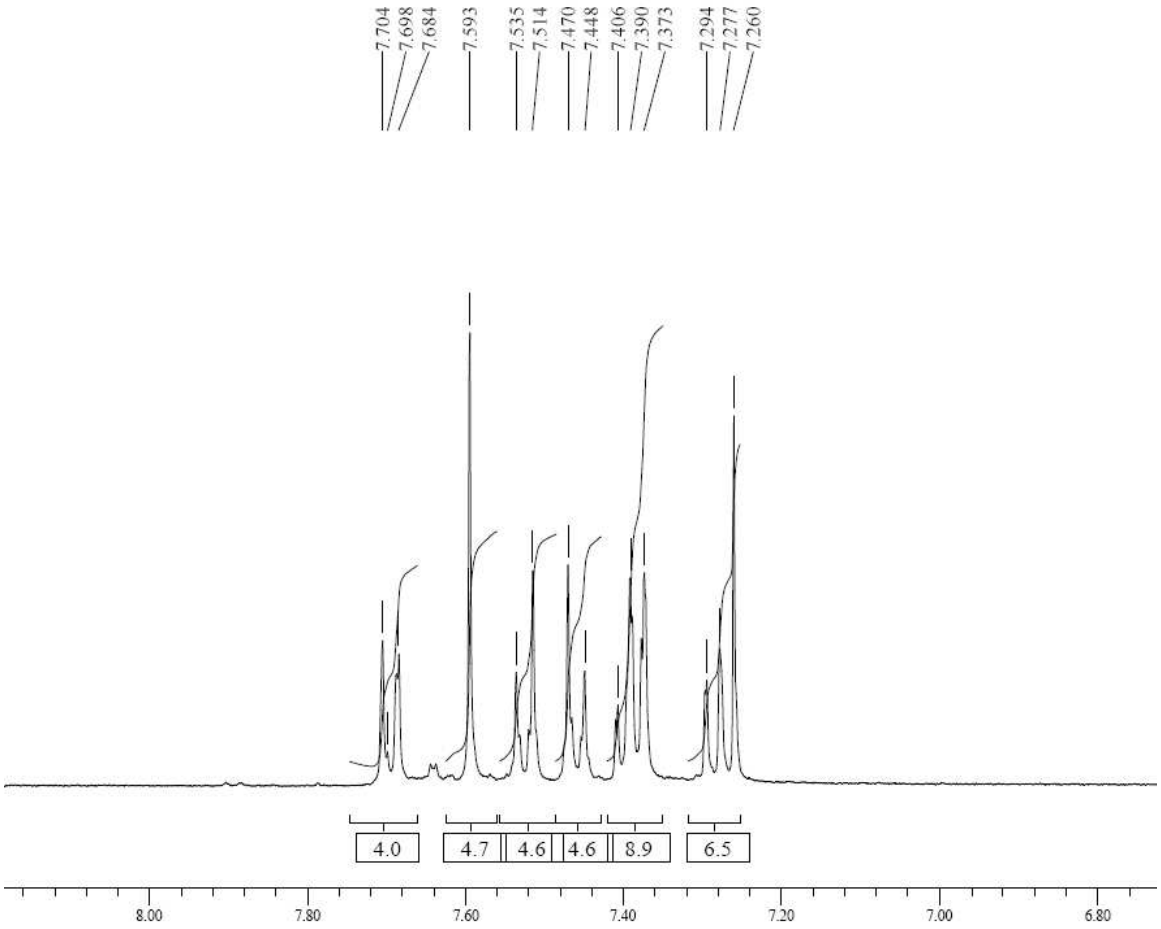

OH
HO

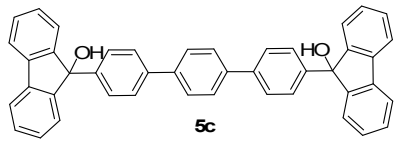
5b


153.357
153.326
145.927
141.564
130.488
129.953
128.260
127.757
126.627
121.792
84.917
160
150
140
130
120
110
100
90
80

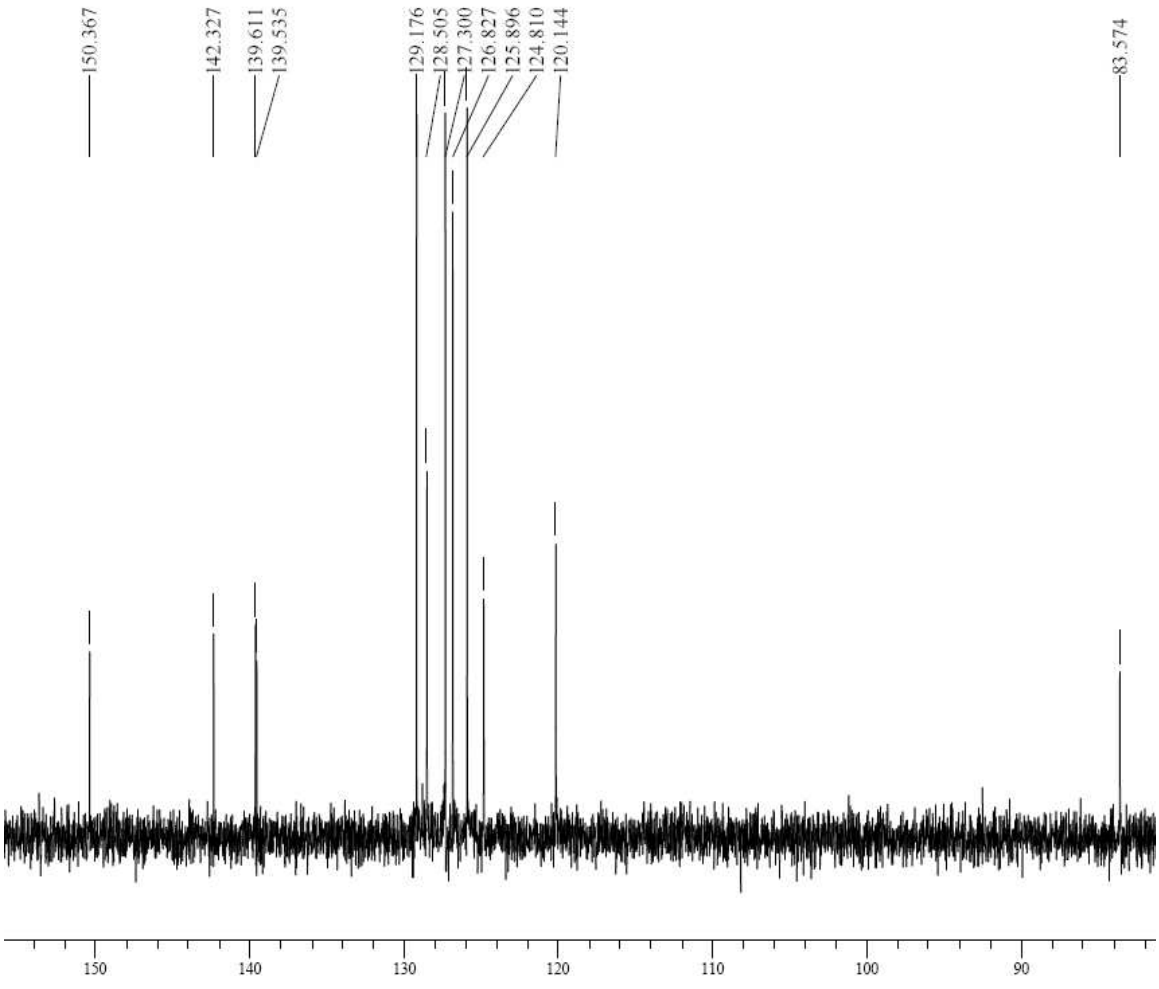

OH
HO

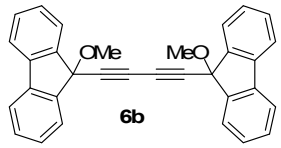
5c


7.704
7.698
7.684
7.593
7.535
7.514
7.470
7.448
7.406
7.390
7.373
7.294
7.277
7.260
4.0
4.7
4.6
4.6
8.9
6.5
8.00
7.80
7.60
7.40
7.20
7.00
6.80

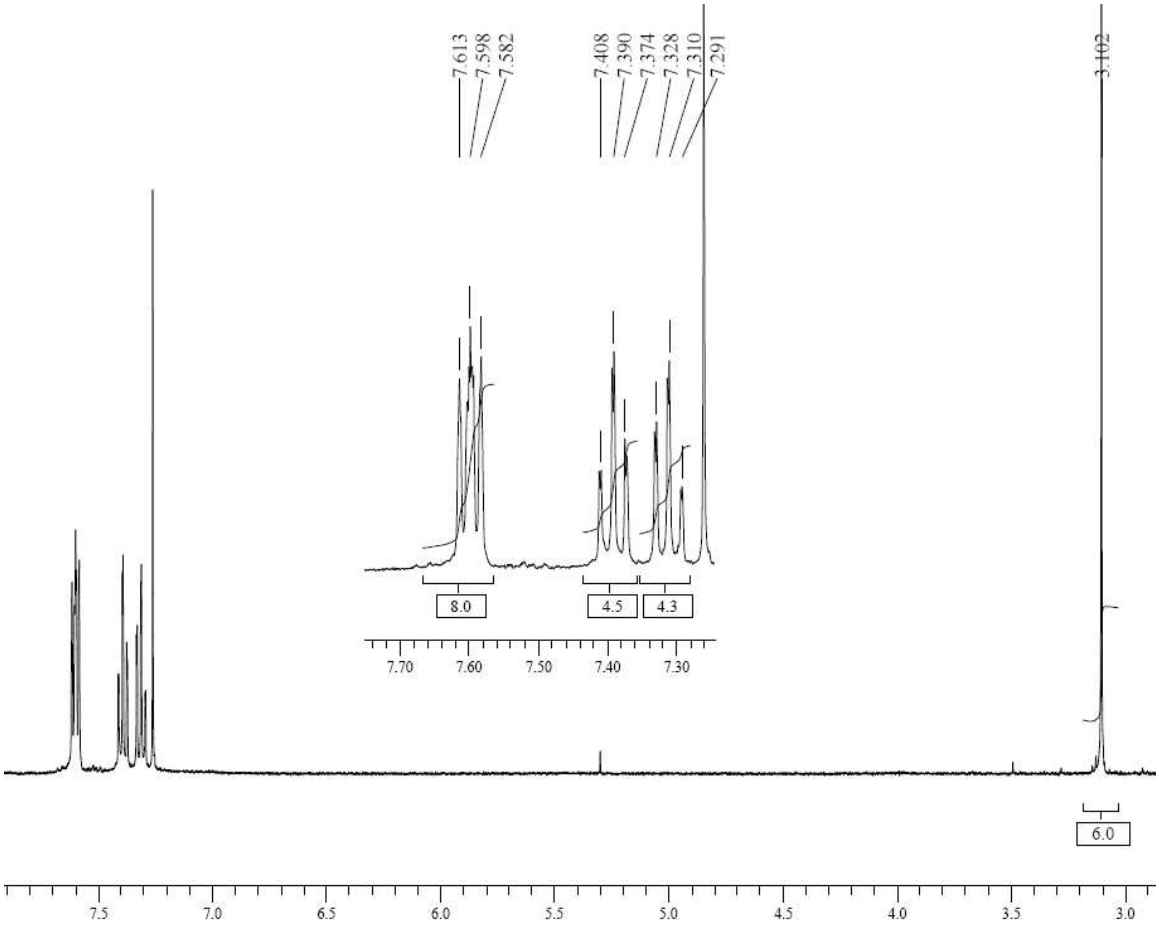

OH
HO

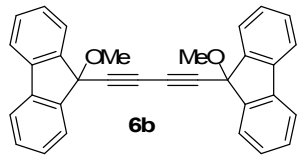
5c


150.367
142.327
139.611
139.535
129.176
128.505
127.300
126.827
125.896
124.810
120.144
83.574
150
140
130
120
110
100
90

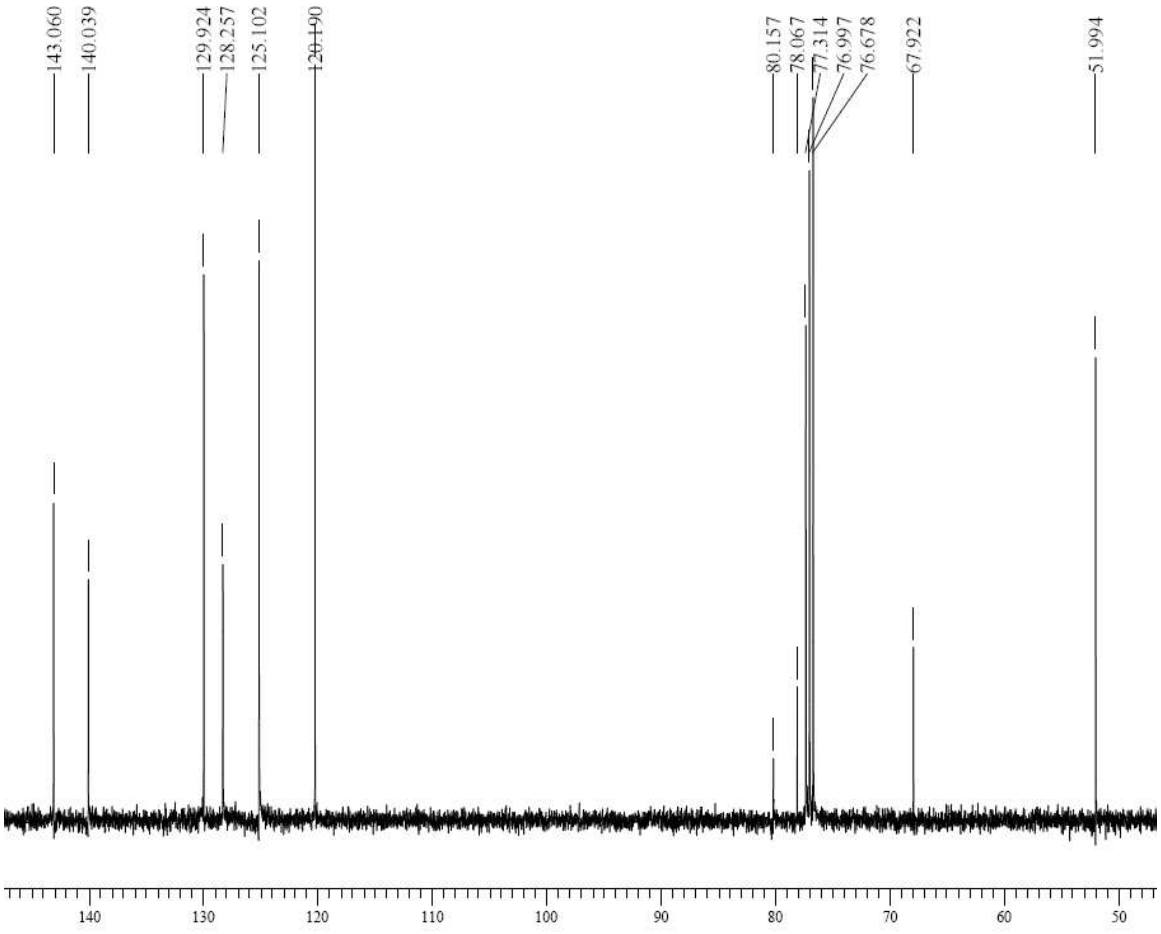

OMe
MeO

6b

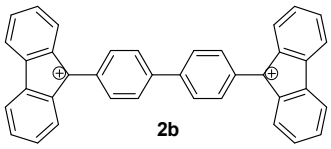

7.613
7.598
7.582
7.408
7.390
7.374
7.328
7.310
7.291
3.102
8.0
4.5
4.3
6.0
7.70
7.60
7.50
7.40
7.30
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0


OMe
MeO

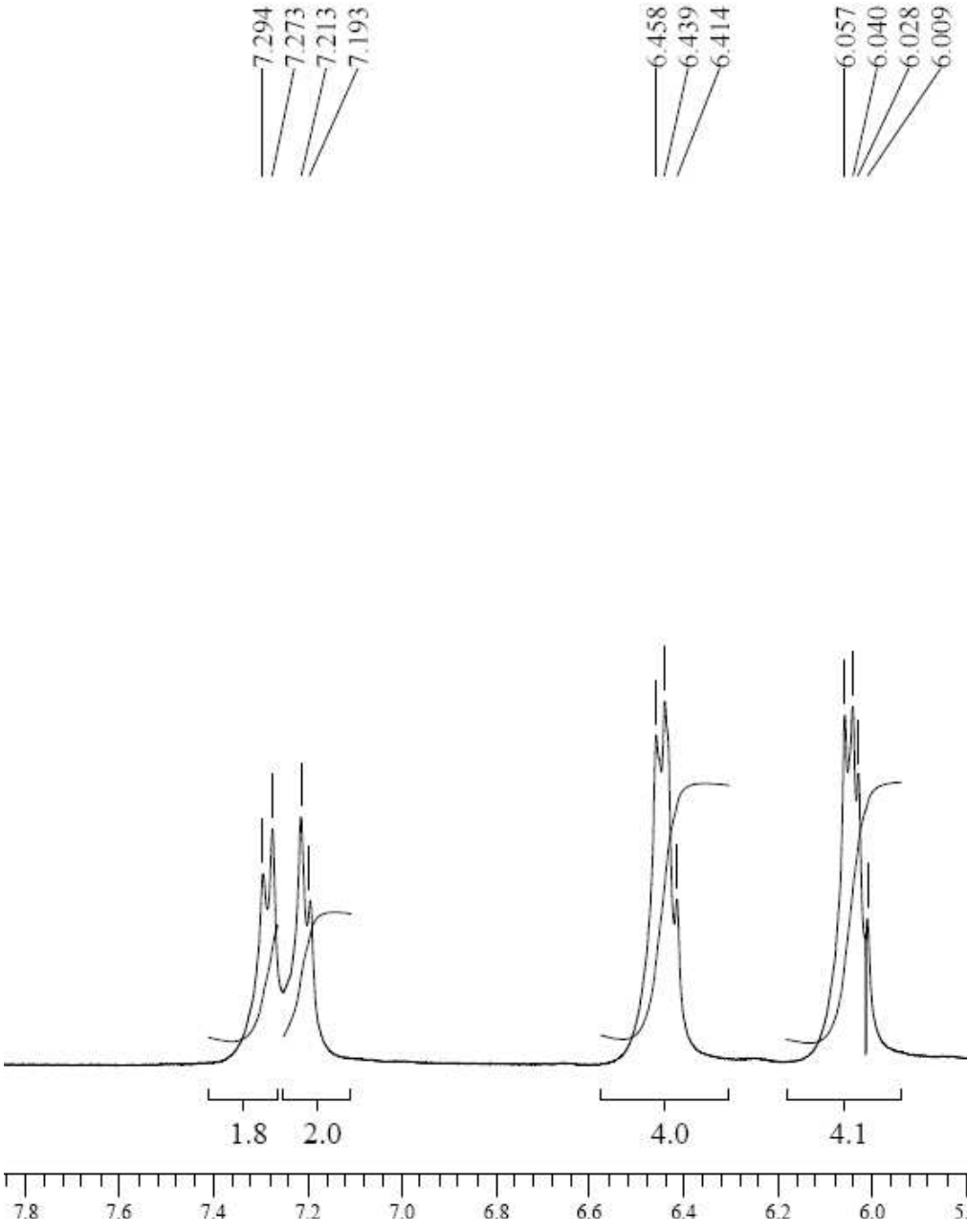
6b

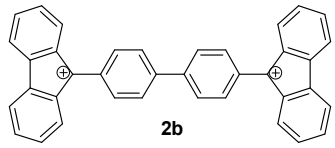

143.060
140.039
129.924
128.257
125.102
120.190
80.157
78.067
77.314
76.997
76.678
67.922
51.994
140
130
120
110
100
90
80
70
60
50

NMR Spectra for Dications **2b**, **2c**, and **3b**.

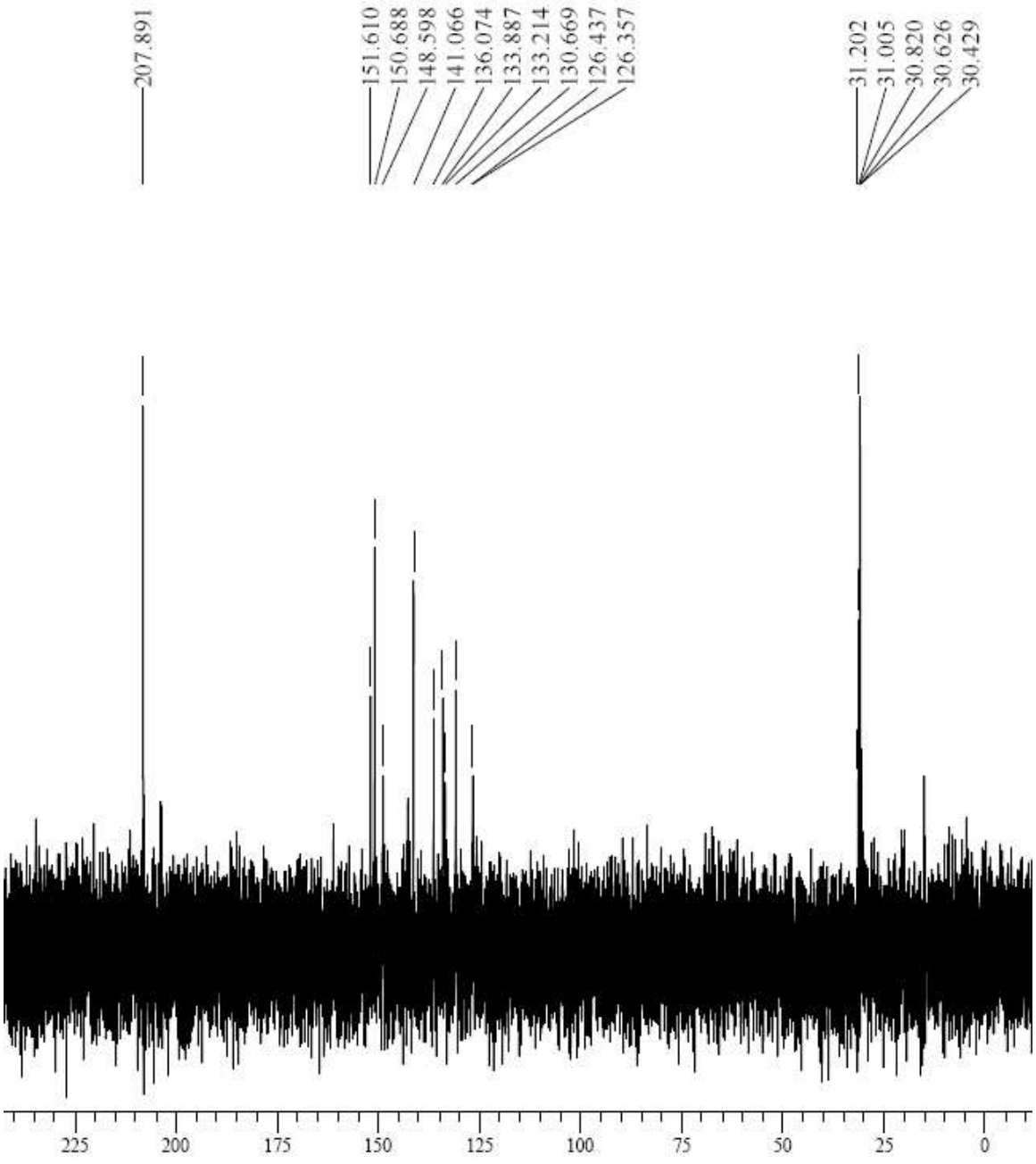


2b





2b


207.891
151.610
150.688
148.598
141.066
136.074
133.887
133.214
130.669
126.437
126.357
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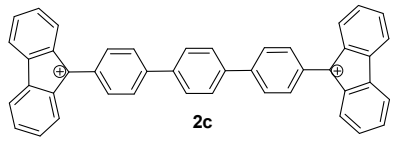
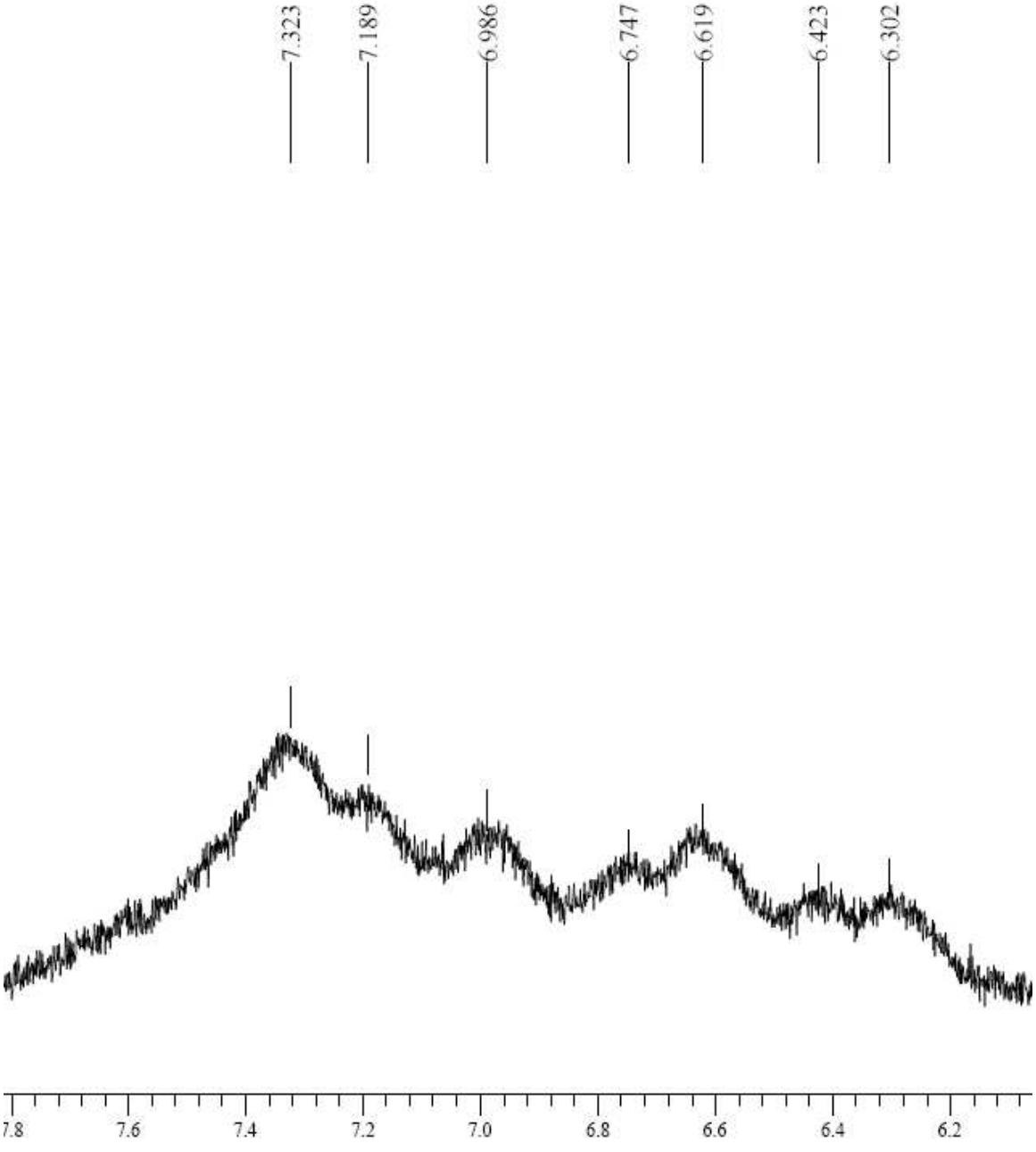
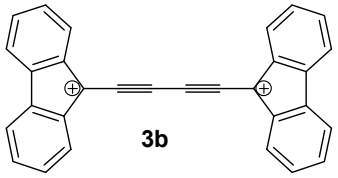
31.005
30.820
30.626
30.429
225
200
175
150
125
100
75
50
25
0

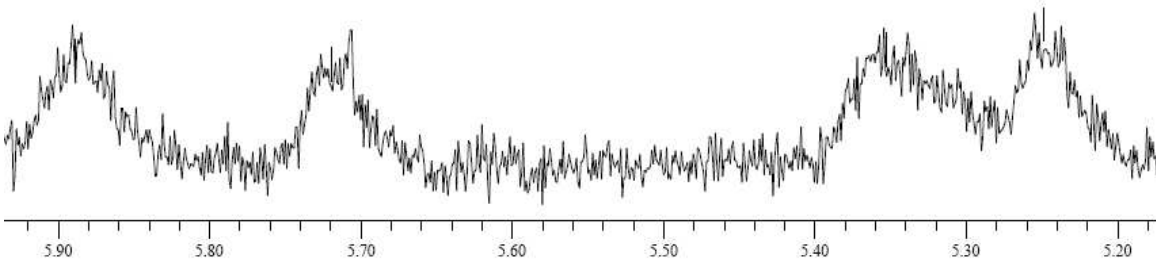


2c





3b



Dihedral angles between fluorenyl systems of **1, 2a-c, 3a-c,** and **4a-c,** between the fluorenyl system and phenylene spacers of **3a, 3b** and **3c** and between the phenylene spacers of **3b** and **3c.** If the dihedral angles varied by more than a degree, both dihedral angles were listed.

	1	**2a**	**2b**	**2c**	**3a**	**3b**	**3c**	**4a**	**4b**	**4c**
Fluorenyl sysems	61.07	89.87	90.00	90.00	90.12	144.09	169.47	38.29	42.21, 35.48	24.68, 14.08
Fluorenyl systems and phenylene spacers					135.74	139.78	142.87			
Phenylene spacers						145.14	147.49			

Calculated total energies, and [x,y,z] coordinates for **2b-c**, **3b-c**, and **4a-c**

2b
Total energy, -1152.1694983 hartrees
C -3.295184 -0.000030 -0.000042
C -4.132060 -0.829024 0.828934
C -4.132039 0.829006 -0.828996
C -3.791041 -1.791088 1.790954
C -5.493229 -0.523958 0.523892
C -3.790997 1.791081 -1.790997
C -5.493216 0.523963 -0.523964
C -4.825191 -2.456000 2.455838
H -2.752567 -2.015671 2.015517
C -6.505336 -1.183092 1.183001
C -4.825131 2.456017 -2.455882
H -2.752517 2.015645 -2.015554
C -6.505307 1.183125 -1.183072
C -6.156081 -2.156186 2.156044
H -4.595430 -3.205566 3.205364
H -7.551568 -0.978376 0.978307
C -6.156028 2.156222 -2.156102
H -4.595352 3.205587 -3.205400
H -7.551544 0.978430 -0.978381
H -6.950470 -2.679794 2.679634
H -6.950404 2.679853 -2.679689
C -1.902432 -0.000035 -0.000030
C 4.132063 -0.828994 -0.828963
C 4.132036 0.828982 0.829020
C 3.791048 -1.791031 -1.791012

C 5.493231 -0.523935 -0.523909
C 3.790990 1.791021 1.791056
C 5.493214 0.523951 0.523982
C 4.825200 -2.455922 -2.455914
H 2.752574 -2.015609 -2.015584
C 6.505341 -1.183049 -1.183036
C 4.825122 2.455935 2.455967
H 2.752510 2.015576 2.015618
C 6.505303 1.183090 1.183116
C 6.156089 -2.156114 -2.156109
H 4.595442 -3.205465 -3.205463
H 7.551572 -0.978339 -0.978331
C 6.156020 2.156152 2.156180
H 4.595340 3.205477 3.205511
H 7.551540 0.978403 0.978421
H 6.950479 -2.679706 -2.679711
H 6.950394 2.679765 2.679788
C 3.295184 -0.000022 0.000030
C -0.672987 -0.000035 -0.000014
C 0.672988 -0.000034 0.000003
C 1.902432 -0.000032 0.000018

2c

Total energy, -1462.0027511 hartrees
C 4.575796 -0.000024 -0.000023
C 5.416173 0.809024 -0.849350
C 5.416166 -0.809042 0.849338
C 5.076543 1.746635 -1.834103
C 5.076528 -1.746640 1.834101
C 6.111761 2.394687 -2.514393
C 6.111741 -2.394679 2.514411
C 7.442345 2.102329 -2.206554
C 7.442327 -2.102316 2.206589
C 7.789567 1.153957 -1.210551
C 7.789557 -1.153951 1.210582
C 6.775970 0.511007 -0.536245
C 6.775965 -0.511016 0.536253
C -4.575789 0.000010 -0.000014
C -5.416176 -0.849345 -0.809030
C -5.416164 0.849358 0.809022
C -5.076552 -1.834111 -1.746630
C -5.076526 1.834126 1.746616
C -6.111775 -2.514420 -2.394658
C -6.111739 2.514428 2.394666
C -7.442357 -2.206590 -2.102286
C -7.442326 2.206590 2.102322

C -7.789576 -1.210577 -1.153922
C -7.789559 1.210576 1.153965
C -6.775975 -0.536251 -0.510997
C -6.775968 0.536256 0.511018
C 3.188436 -0.000021 -0.000026
C 1.956228 -0.000015 -0.000026
C 0.617324 -0.000009 -0.000026
C -0.617312 -0.000003 -0.000026
C -1.956209 0.000005 -0.000026
C -3.188417 0.000012 -0.000026
H 4.038090 1.965442 -2.064444
H 4.038073 -1.965455 2.064426
H 5.882506 3.125807 -3.282147
H 5.882480 -3.125794 3.282169
H 8.237234 2.612926 -2.742076
H 8.237211 -2.612900 2.742129
H 8.835306 0.953409 -0.999104
H 8.835298 -0.953393 0.999153
H -4.038100 -2.064447 -1.965454
H -4.038071 2.064468 1.965417
H -5.882523 -3.282181 -3.125772
H -5.882476 3.282191 3.125774
H -8.237249 -2.742127 -2.612862
H -8.237210 2.742123 2.612914
H -8.835315 -0.999142 -0.953362
H -8.835301 0.999135 0.953426

3b

Total energy, -1462.0027511 hartrees
C -5.024168 0.000000 0.000000
C -5.875883 1.120877 0.332415
C -5.875883 -1.120877 -0.332415
C -5.559639 2.453058 0.639400
C -5.559639 -2.453058 -0.639400
C -6.602804 3.353417 0.880753
C -6.602804 -3.353417 -0.880753
C -7.929979 2.932757 0.784796
C -7.929978 -2.932757 -0.784796
C -8.260932 1.602640 0.432260
C -8.260932 -1.602640 -0.432260
C -7.236465 0.710614 0.205458
C -7.236465 -0.710614 -0.205458
C 5.024710 0.000000 0.000000
C 5.876243 -1.102697 0.388180
C 5.876243 1.102697 -0.388180
C 5.558719 -2.360892 0.921984

C 5.558719 2.360892 -0.921984
C 6.601377 -3.230766 1.258566
C 6.601377 3.230766 -1.258566
C 7.928792 -2.833688 1.091615
C 7.928792 2.833688 -1.091616
C 8.260736 -1.550607 0.594788
C 8.260736 1.550607 -0.594788
C 7.236894 -0.695825 0.251418
C 7.236894 0.695825 -0.251418
C -3.577043 0.000000 0.000000
C -2.849587 -0.678376 -1.007322
C -2.849587 0.678376 1.007322
C -1.463372 -0.663164 -1.011843
C -1.463372 0.663164 1.011843
C -0.739548 0.000000 0.000000
C 0.741013 0.000000 0.000000
C 1.464497 1.122368 0.451134
C 1.464497 -1.122368 -0.451134
C 2.850669 1.135104 0.431831
C 2.850669 -1.135105 -0.431831
C 3.577450 0.000000 0.000000
H -4.530590 2.794280 0.672153
H -4.530590 -2.794280 -0.672153
H -6.379843 4.385627 1.128844
H -6.379842 -4.385627 -1.128844
H -8.730167 3.644124 0.966218
H -8.730167 -3.644124 -0.966218
H -9.302582 1.311809 0.338067
H -9.302582 -1.311809 -0.338067
H 4.529189 2.656446 -1.093174
H 4.529189 -2.656446 1.093175
H 6.377781 4.211590 -1.664407
H 6.377781 -4.211590 1.664407
H 8.728547 3.515478 -1.365129
H 8.728548 -3.515478 1.365129
H 9.302549 1.259764 -0.502408
H 9.302549 -1.259763 0.502408
H -3.379521 -1.153834 -1.825475
H -3.379521 1.153834 1.825475
H -0.934804 -1.141194 -1.830087
H -0.934804 1.141194 1.830087
H 0.935363 2.005301 0.794949
H 0.935363 -2.005301 -0.794949
H 3.381235 2.003374 0.807014
H 3.381235 -2.003374 -0.807014

3c

Total energy, -1462.0027511 hartrees

C	7.181329	0.000000	0.000000
C	8.038413	1.165634	0.107435
C	8.038413	-1.165634	-0.107435
C	7.727880	2.515492	0.326224
C	7.727881	-2.515492	-0.326224
C	8.773937	3.437619	0.440601
C	8.773937	-3.437619	-0.440601
C	10.100230	3.009369	0.371666
C	10.100230	-3.009369	-0.371667
C	10.425281	1.644736	0.200300
C	10.425281	-1.644736	-0.200300
C	9.396988	0.735360	0.073942
C	9.396988	-0.735360	-0.073942
C	-7.181329	0.000000	0.000000
C	-8.038413	-1.165634	0.107435
C	-8.038413	1.165634	-0.107435
C	-7.727881	-2.515492	0.326223
C	-7.727880	2.515492	-0.326223
C	-8.773937	-3.437619	0.440601
C	-8.773937	3.437619	-0.440601
C	-10.100230	-3.009369	0.371666
C	-10.100230	3.009369	-0.371666
C	-10.425281	-1.644736	0.200299
C	-10.425281	1.644737	-0.200300
C	-9.396988	-0.735360	0.073942
C	-9.396988	0.735361	-0.073942
C	5.742586	0.000000	0.000000
C	5.009795	-1.031831	0.641198
C	5.009795	1.031831	-0.641197
C	3.626300	-1.017249	0.654381
C	3.626300	1.017249	-0.654381
C	2.897373	0.000000	0.000000
C	1.420355	0.000000	0.000000
C	0.694212	1.206318	-0.005187
C	0.694212	-1.206319	0.005187
C	-0.694212	1.206318	0.005185
C	-0.694212	-1.206319	-0.005185
C	-1.420355	0.000000	0.000000
C	-2.897373	0.000000	0.000000
C	-3.626300	-1.017250	-0.654380
C	-3.626300	1.017250	0.654380
C	-5.009795	-1.031832	-0.641196
C	-5.009795	1.031832	0.641196
C	-5.742586	0.000000	0.000000

H 6.700892 2.848277 0.428833
H 6.700892 -2.848277 -0.428833
H 8.552796 4.487708 0.599658
H 8.552796 -4.487708 -0.599658
H 10.902224 3.734636 0.471596
H 10.902225 -3.734636 -0.471596
H 11.465344 1.334011 0.181813
H 11.465344 -1.334011 -0.181813
H -6.700892 2.848277 -0.428832
H -6.700892 -2.848277 0.428832
H -8.552796 4.487708 -0.599657
H -8.552796 -4.487708 0.599657
H -10.902224 3.734637 -0.471595
H -10.902225 -3.734636 0.471595
H -11.465344 1.334011 -0.181814
H -11.465344 -1.334011 0.181813
H 5.538458 -1.796474 1.199516
H 5.538458 1.796474 -1.199516
H 3.097817 -1.783803 1.211105
H 3.097817 1.783803 -1.211105
H 1.219389 2.156096 0.010899
H 1.219389 -2.156096 -0.010899
H -1.219389 2.156096 -0.010903
H -1.219389 -2.156096 0.010903
H -3.097817 -1.783805 -1.211102
H -3.097817 1.783805 1.211102
H -5.538458 -1.796476 -1.199513
H -5.538458 1.796476 1.199513

4a

Total energy, -1311.9253656 Hartrees
C -2.850765 0.034007 -0.078802
C -3.623890 -1.114056 0.375638
C -3.790009 1.089072 -0.394903
C -3.240558 -2.382767 0.849663
C -3.621387 2.421702 -0.830444
C -4.224536 -3.302181 1.227976
C -4.746555 3.217587 -1.063305
C -5.574967 -2.968829 1.133696
C -6.028556 2.705042 -0.870338
C -5.981064 -1.696925 0.666652
C -6.224051 1.376461 -0.422980
C -5.010593 -0.792085 0.301461
C -5.118509 0.594762 -0.187026
C -0.769065 -0.099791 1.292190
C -0.801418 -1.124373 -1.034843

C	0.769186	0.099772	1.292099
C	0.711617	-1.334648	-0.763738
C	2.850769	-0.033981	-0.078955
C	3.623902	1.114080	0.375507
C	3.790030	-1.089029	-0.395070
C	3.240597	2.382838	0.849438
C	3.621391	-2.421590	-0.830791
C	4.224585	3.302217	1.227820
C	4.746526	-3.217574	-1.063450
C	5.575006	2.968792	1.133708
C	6.028525	-2.705152	-0.870153
C	5.981083	1.696846	0.666771
C	6.224045	-1.376600	-0.422712
C	5.010605	0.792042	0.301510
C	5.118523	-0.594811	-0.186953
H	-2.201145	-2.672386	0.939205
H	-2.645828	2.857897	-0.982312
H	-3.933058	-4.280137	1.595823
H	-4.618055	4.241635	-1.397099
H	-6.329527	-3.692971	1.425869
H	-6.893547	3.333613	-1.060372
H	-7.037439	-1.454204	0.607106
H	-7.230582	0.999465	-0.270960
H	-1.233660	0.637968	1.954446
H	-1.340616	-2.054196	-0.858567
H	1.233886	-0.637845	1.954443
H	1.195357	-1.591897	-1.709807
H	2.645791	-2.857521	-0.983049
H	2.201196	2.672525	0.938886
H	4.618015	-4.241578	-1.397374
H	3.933114	4.280204	1.595591
H	6.893506	-3.333783	-1.060036
H	6.329570	3.692910	1.425931
H	7.230579	-0.999693	-0.270498
H	7.037449	1.454062	0.607351
H	1.023807	1.083236	1.690251
H	-1.023695	-1.083196	1.690470
H	0.851344	-2.176597	-0.076386
H	-0.969584	-0.871067	-2.087104
C	1.345055	-0.055836	-0.162413
C	0.801279	1.124401	-1.034908
H	0.969246	0.871101	-2.087204
H	1.340531	2.054210	-0.858742
C	-1.345062	0.055842	-0.162244
C	-0.711690	1.334693	-0.763512
H	-0.851294	2.176549	-0.075996

H -1.195672 1.592127 -1.709397

4b

Total energy, -1624.0313979 Hartrees

C -4.975688 -0.064280 0.065626
C -5.955491 -1.079105 0.403218
C -5.715124 1.113526 -0.379302
C -5.830553 -2.412810 0.843882
C -5.289746 2.362315 -0.864947
C -6.982851 -3.162266 1.101735
C -6.243967 3.319824 -1.227525
C -8.246448 -2.600805 0.928595
C -7.604339 3.042164 -1.106300
C -8.397024 -1.268619 0.478430
C -8.051492 1.789865 -0.627768
C -7.265093 -0.532418 0.217976
C -7.110611 0.847381 -0.277687
C 4.975686 -0.064251 -0.065644
C 5.715145 1.113539 0.379292
C 5.955468 -1.079101 -0.403211
C 5.289798 2.362321 0.864986
C 5.830495 -2.412810 -0.843851
C 6.244040 3.319810 1.227555
C 6.982774 -3.162294 -1.101705
C 7.604406 3.042137 1.106287
C 8.246385 -2.600854 -0.928590
C 8.051530 1.789837 0.627729
C 8.396993 -1.268663 -0.478450
C 7.110627 0.847371 0.277657
C 7.265080 -0.532435 -0.217997
H -4.868586 -2.882319 0.980886
H -4.240890 2.606662 -0.974663
H -6.888566 -4.188855 1.439293
H -5.919864 4.284166 -1.604165
H -9.131984 -3.193815 1.137331
H -8.334506 3.795477 -1.386444
H -9.389989 -0.851381 0.342889
H -9.115221 1.588639 -0.547101
H 4.240949 2.606676 0.974749
H 4.868514 -2.882296 -0.980843
H 5.919961 4.284148 1.604227
H 6.888465 -4.188885 -1.439248
H 8.334590 3.795434 1.386429
H 9.131907 -3.193885 -1.137327
H 9.115255 1.588593 0.547047
H 9.389969 -0.851443 -0.342925

C -3.480705 -0.150482 0.115854
C -2.857657 1.018406 0.960153
C -2.882564 -1.450603 0.704491
C -2.939230 -0.036326 -1.362612
C -1.356926 1.170343 0.611389
C -1.348023 -1.299802 0.900784
C -1.415822 -0.326995 -1.382346
C -0.786634 -0.150160 0.025602
C 0.786634 -0.150155 -0.025607
C 1.356907 1.170196 -0.611753
C 1.415823 -0.326596 1.382391
C 1.348043 -1.300025 -0.900477
C 2.939227 -0.035911 1.362582
C 2.882584 -1.450756 -0.704130
C 2.857637 1.018178 -0.960483
C 3.480704 -0.150464 -0.115851
H -3.381476 1.962674 0.812353
H -2.986137 0.762921 2.018179
H -3.471093 -0.744377 -2.006426
H -3.149425 0.961175 -1.753712
H -3.090274 -2.289574 0.030732
H -3.343772 -1.678275 1.670060
H -0.816988 1.468874 1.516126
H -1.223905 1.982449 -0.112778
H -1.242504 -1.348351 -1.736349
H -0.946105 0.342060 -2.111459
H -1.132385 -1.100910 1.955655
H -0.864926 -2.251843 0.659607
H 0.864955 -2.252007 -0.659050
H 1.132413 -1.101418 -1.955404
H 0.946096 0.342650 2.111322
H 1.242517 -1.347858 1.736672
H 1.223881 1.982497 0.112196
H 0.816961 1.468477 -1.516567
H 3.471097 -0.743781 2.006590
H 3.149411 0.961699 1.753409
H 3.343809 -1.678702 -1.669627
H 3.090293 -2.289533 -0.030128
H 2.986108 0.762384 -2.018435
H 3.381443 1.962495 -0.812970

4c

Total energy, -1936.1251654 Hartrees

C 7.105896 -0.050881 -0.048960
C 7.827761 1.209770 -0.209552

C 8.102092 -1.083925 0.170080
C 7.381457 2.528584 -0.399627
C 7.996055 -2.466592 0.420668
C 8.319905 3.560419 -0.518446
C 9.159311 -3.225671 0.587738
C 9.684384 3.285333 -0.452034
C 10.414321 -2.626058 0.506452
C 10.151619 1.967001 -0.253569
C 10.544879 -1.239457 0.263965
C 9.226193 0.954135 -0.131189
C 9.402041 -0.490479 0.105188
C -7.105898 -0.050904 0.049025
C -7.827787 1.209708 0.209842
C -8.102067 -1.083918 -0.170312
C -7.381521 2.528480 0.400336
C -7.996042 -2.466557 -0.421094
C -8.319994 3.560280 0.519278
C -9.159302 -3.225567 -0.588456
C -9.684460 3.285210 0.452566
C -10.414308 -2.625940 -0.507283
C -10.151655 1.966928 0.253698
C -10.544861 -1.239379 -0.264580
C -9.226208 0.954096 0.131217
C -9.402024 -0.490466 -0.105491
H 6.328394 2.773934 -0.451131
H 7.040167 -2.961522 0.497714
H 7.979555 4.580129 -0.664180
H 9.079363 -4.289882 0.782286
H 10.402041 4.094333 -0.550128
H 11.308357 -3.229091 0.634664
H 11.218135 1.772141 -0.197146
H 11.531039 -0.788844 0.209880
H -6.328469 2.773825 0.452097
H -7.040201 -2.961608 -0.497986
H -7.979668 4.579952 0.665340
H -9.079352 -4.289755 -0.783128
H -10.402133 4.094185 0.550737
H -11.308340 -3.228928 -0.635734
H -11.218161 1.772075 0.197049
H -11.531011 -0.788738 -0.210567
C 5.617957 -0.177835 -0.080290
C 5.047537 0.626455 1.157043
C 5.002700 0.434892 -1.390883
C 5.039028 -1.608931 0.021336
C 3.525928 0.360256 1.290159
C 3.496089 0.712426 -1.175402

C 3.507614 -1.592549 -0.243202
C 2.921525 -0.172558 -0.035785
C 1.348461 -0.171243 -0.015409
C 0.777287 -0.756799 1.303661
C 0.760572 1.258564 -0.156963
C 0.748100 -1.015081 -1.171597
C -0.760538 1.258510 0.157506
C -0.777252 -0.756349 -1.303816
C -0.748064 -1.015484 1.171350
C -1.348432 -0.171251 0.015454
H 5.571917 0.318987 2.067867
H 5.247915 1.691619 1.024390
H 5.521308 -2.266459 -0.708646
H 5.240355 -2.015222 1.019256
H 5.152740 -0.296961 -2.192865
H 5.520525 1.340076 -1.707826
H 3.037491 1.292363 1.593821
H 3.349928 -0.363254 2.092376
H 3.308212 -1.926392 -1.266577
H 3.024372 -2.317796 0.418666
H 3.342996 1.769891 -0.931627
H 2.968873 0.530911 -2.117522
H 1.238773 -0.786725 -2.124558
H 0.929345 -2.078705 -0.979017
H 1.269708 1.963312 0.510577
H 0.929397 1.622753 -1.177019
H 0.964987 -0.056373 2.125841
H 1.282130 -1.691245 1.573394
H -1.269672 1.963496 -0.509785
H -0.929363 1.622340 1.177690
H -1.282103 -1.690699 -1.573869
H -0.964951 -0.055639 -2.125754
H -0.929298 -2.079043 0.978401
H 1.238739 -0.787462 2.124389
C -2.921509 -0.172564 0.035830
C -3.496067 0.712032 1.175744
C -3.525909 0.360679 -1.289942
C -5.002703 0.434473 1.391113
H -3.342932 1.769575 0.932351
H -2.968870 0.530152 2.117803
C -5.047522 0.626854 -1.156745
H -3.037450 1.292878 -1.593286
H -3.349920 -0.362570 -2.092396
C -5.617947 -0.177821 0.080313
H -5.520501 1.339589 1.708296
H -5.152804 -0.297606 2.192882

H	-5.247897	1.691978	-1.023782
H	-5.571924	0.319649	-2.067646
C	-5.039022	-1.608867	-0.021808
H	-5.521316	-2.266592	0.707982
H	-5.240417	-2.014820	-1.019848
C	-3.507611	-1.592598	0.242787
H	-3.024316	-2.317636	-0.419272
H	-3.308283	-1.926737	1.266077

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