

Supporting Information for:

**Nesting Complexation of C₆₀ with Large, Rigid D₂ Symmetrical
Macrocycles**

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Figure S1. ^1H NMR spectra (CDCl_3 , 300 MHz, room temperature) of macrocycles a) (*RR*)-**8**; b) (*RR*)-**9**; c) (*RR*)-**10**; d) (*RR*)-**11**.

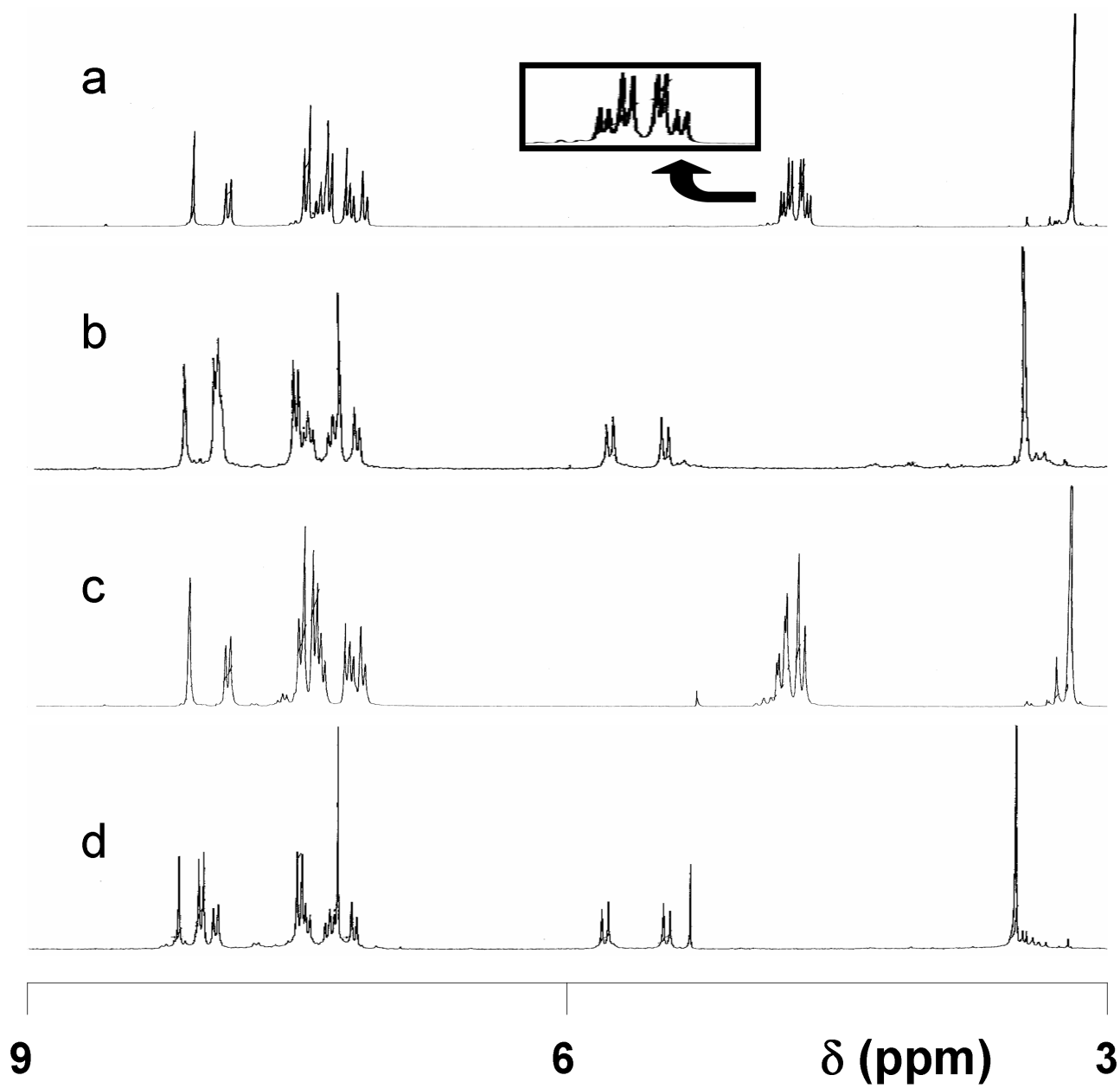
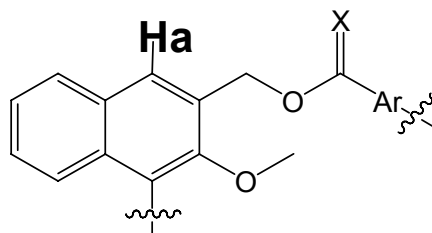


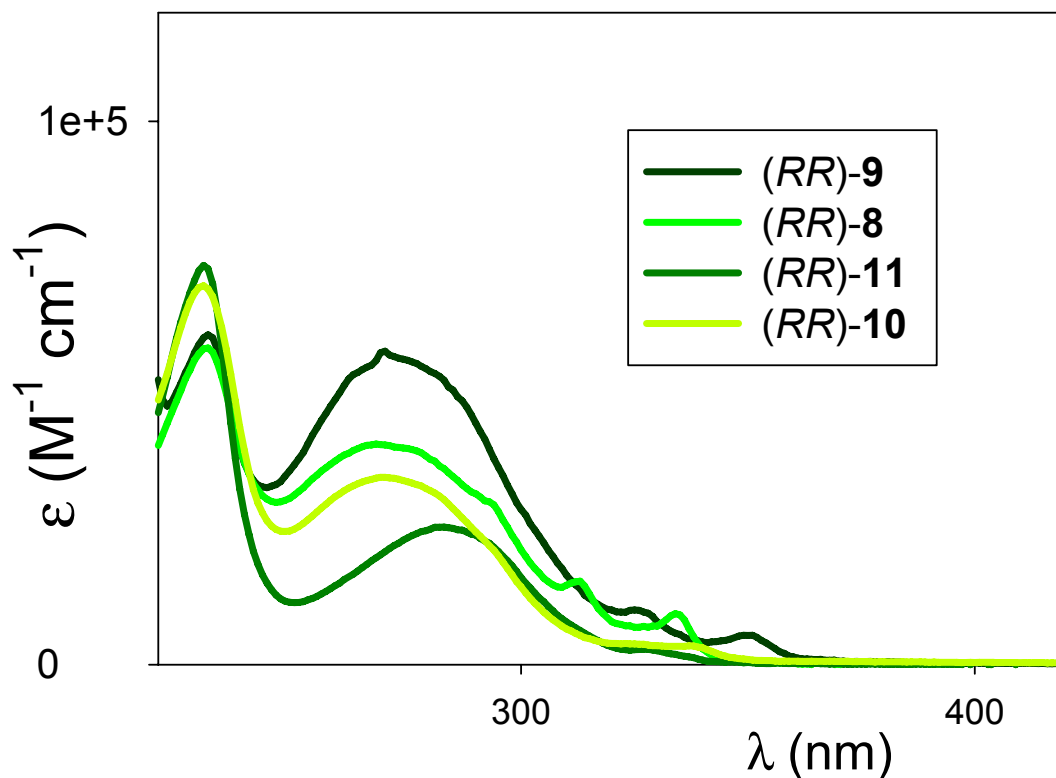
Table S1. Selected ^1H NMR chemical shifts for precursors (*R*)-**4-7** and macrocycles (*RR*)-**8-11**, in CDCl_3 at room temperature.^[a]



Compound	BINOL-OMe (s) ^[b]	BINOL-Ha (s) ^[b]	Ar-CH ₂ O	Binol-CH ₂ O
(<i>R</i>)- 1 ^[c]	3.30	8.03	-	4.98(dd)
(<i>R</i>)- 4	3.31	8.15	4.78(s)	4.91(dd)
(<i>R</i>)- 5	3.38	8.13	-	5.72(dd)
(<i>R</i>)- 6	3.38	8.22	4.85(s)	4.98(dd)
(<i>R</i>)- 7	3.36	8.11	-	5.69(dd)
(<i>RR</i>)- 8	3.22	8.13	4.68-4.85(m)	4.68-4.85(m)
(<i>RR</i>)- 9	3.47	8.14	-	5.62(dd)
(<i>RR</i>)- 10	3.24	8.15	4.72-4.95(m)	4.72-4.95(m)
(<i>RR</i>)- 11	3.51	8.16	-	5.61(dd)

[a] Spectra taken at 300 MHz with 5-10 mM sample concentration in CDCl_3 . [b] Peak multiplicity as follows: s singlet, bs broad singlet, d doublet, m multiplet, dd double doublet (AB system). [c] Data taken from reference 9.

Figure S2. Normalized UV/Vis spectra of macrocycles (*RR*)-**8-11** (6×10^{-6} - 2×10^{-5} in EtOH).



For UV/Vis of molecular fragments of the macrocycles (taken from literature):

- a) 4,4'-dimethylbiphenyl: $\lambda_{\text{max}}=254 \text{ nm}$ ($\epsilon=18400$ in petroleum ether)^{S1}
- b) 4,4'-dicarboxy dimehtyl ester: $\lambda_{\text{max}}=280 \text{ nm}$ ($\epsilon=30000$ in EtOH)^{S2}
- c) 1,4-bis(4-carbomethoxyphenyl)buta-1,3-diyne (MeCN): $\lambda_{\text{max}} (\epsilon \times 10^{-4}) = 284 (0.50), 302 (0.58), 322 (0.78), 345 (0.68)$.^{S3}
- d) 1,4-bis(phenylethynyl)buta-1,3-diyne (MeCN): $\lambda_{\text{max}} (\epsilon \times 10^{-4}) = 296 (2.16), 305 (3.62), 326 (3.50)$.^{S3}

Figure S3. Titration of C_{60} ($65 \mu\text{M}$) with macrocycle $(RR)\text{-}8$ ($0\text{-}485 \mu\text{M}$) in toluene at 25°C .

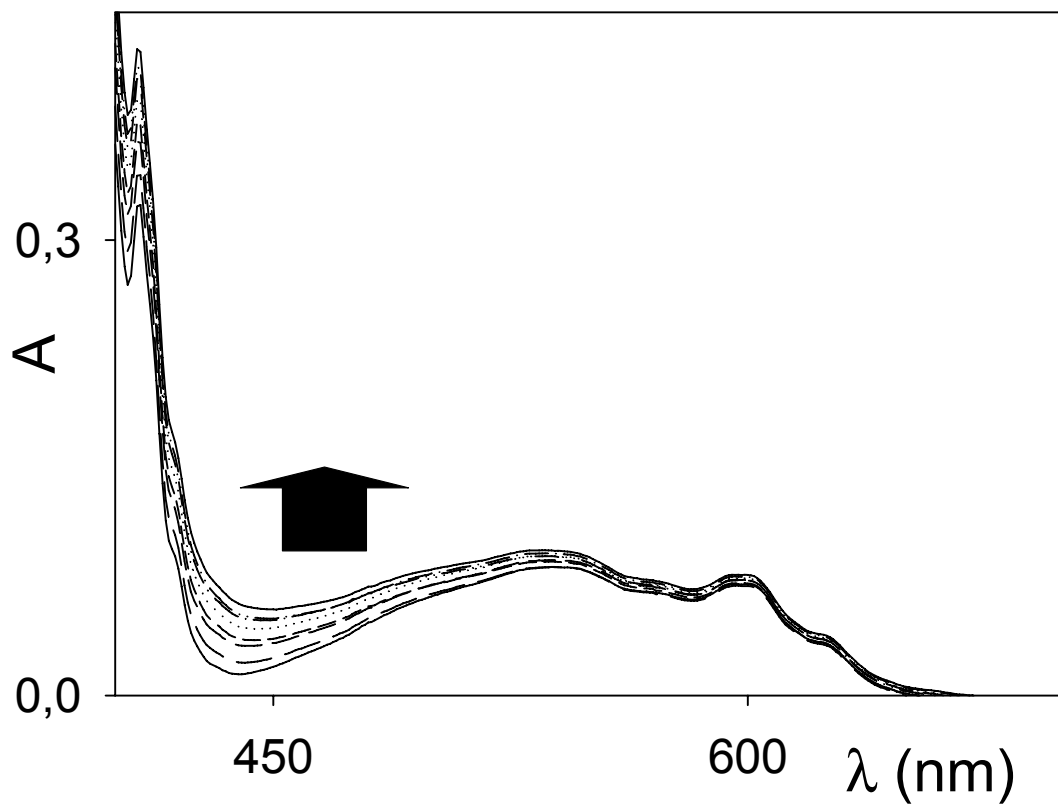


Figure S4. Titration of C_{60} (103 μM) with macrocycle (*RR*)-**9** (0-500 μM) in toluene at 25°C.

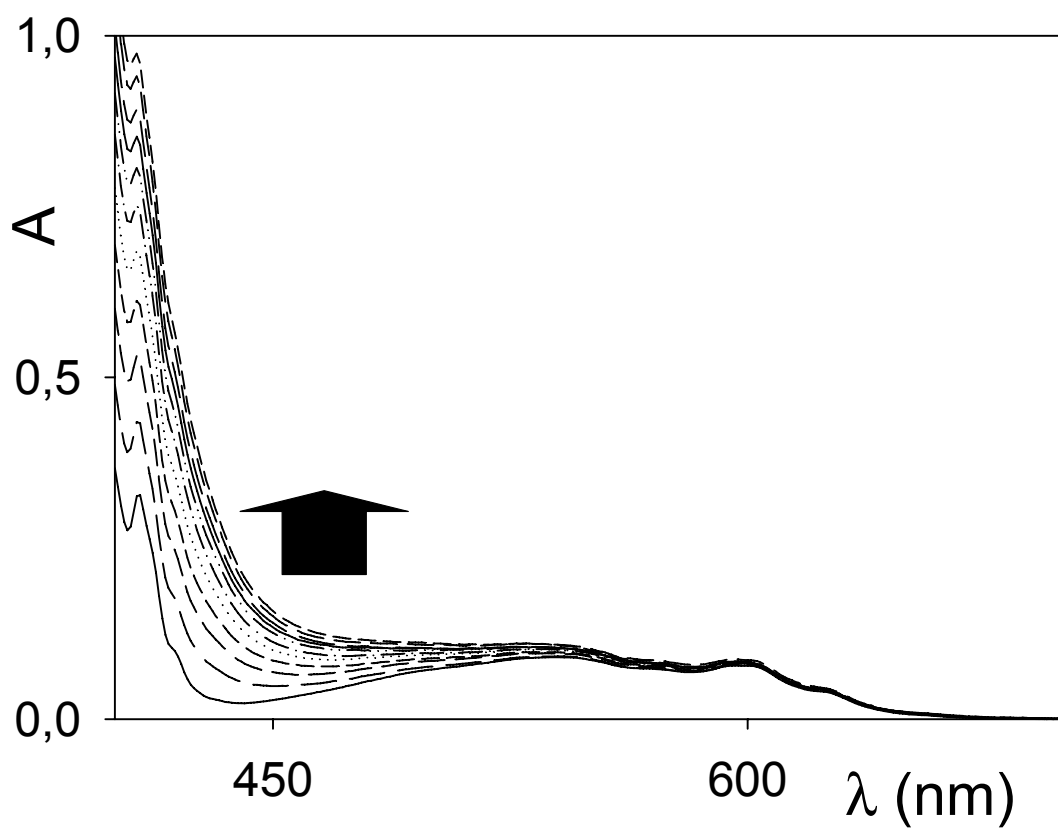


Figure S5. Calculated curves for the 1:1 complexes between macrocycles (*RR*)-8, (*RR*)-9 and (*RR*)-11 in toluene at 25°C and related simulated macrocycle absorbance curves.

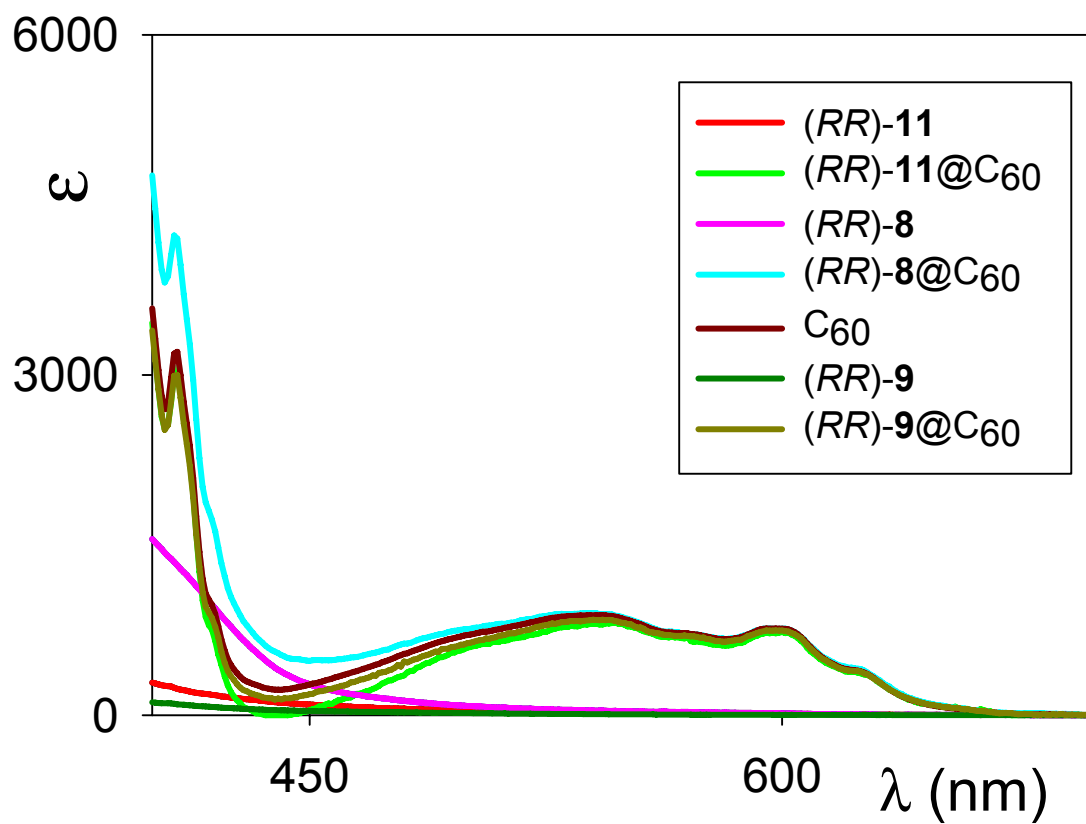
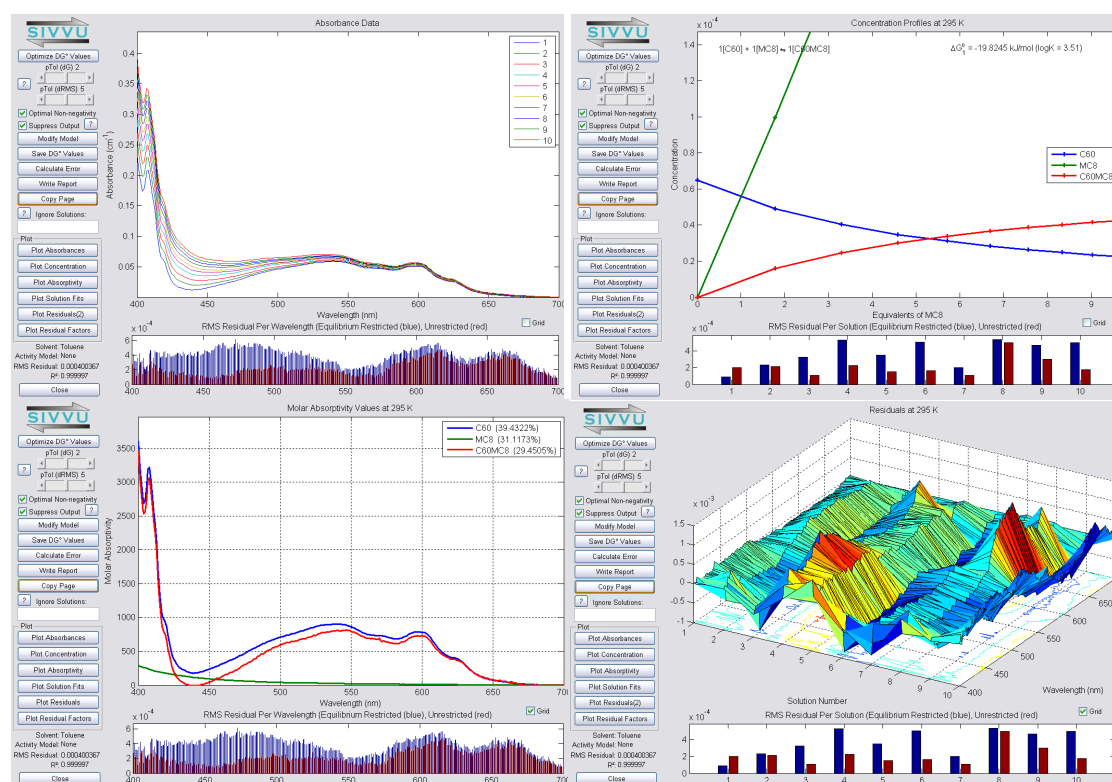


Figure S6. Spectrophotometric Titration of 65 μM C_{60} with Macrocycle (RR)-8.



Summary:

Data at 295 K

Non-negativity was enforced with optimization (not truncation).

$\text{DG1} = -19.8245 (\pm 0.0114)$; RMS Residual = 0.00040037

Unrestricted RMS Residual (3 mathematical factors): 0.0002411

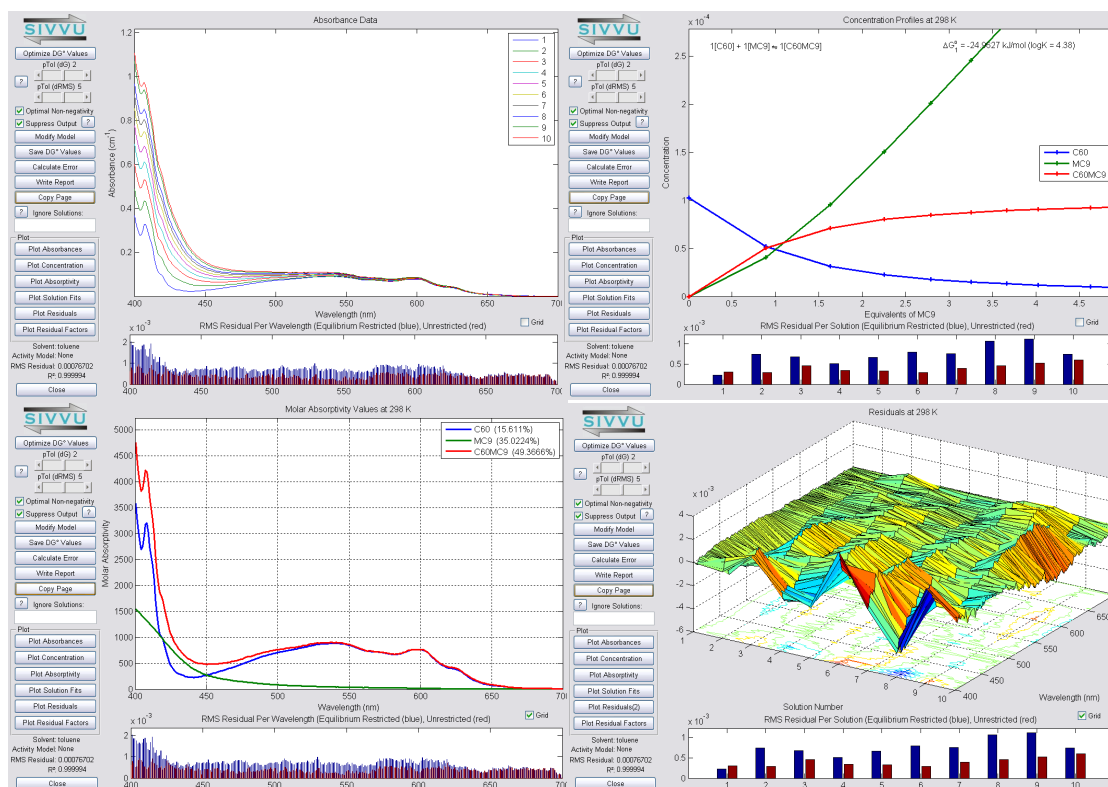
Restricted Data Reconstruction (3 chemical factors): 99.2892%

Unrestricted Data Reconstruction (3 mathematical factors): 99.3934%

Remaining Imbedded Error in Absorbance Values: 0.0002621

R^2 : 99.9997%

Figure S7. Spectrophotometric Titration of 103 μM C_{60} with Macrocycle (*RR*)-9.



Summary:

Data at 298 K

Non-negativity was enforced with optimization (not truncation).

DG1 = -24.9627 (± 0.0875); RMS Residual = 0.00076702

Unrestricted RMS Residual (3 mathematical factors): 0.00041173

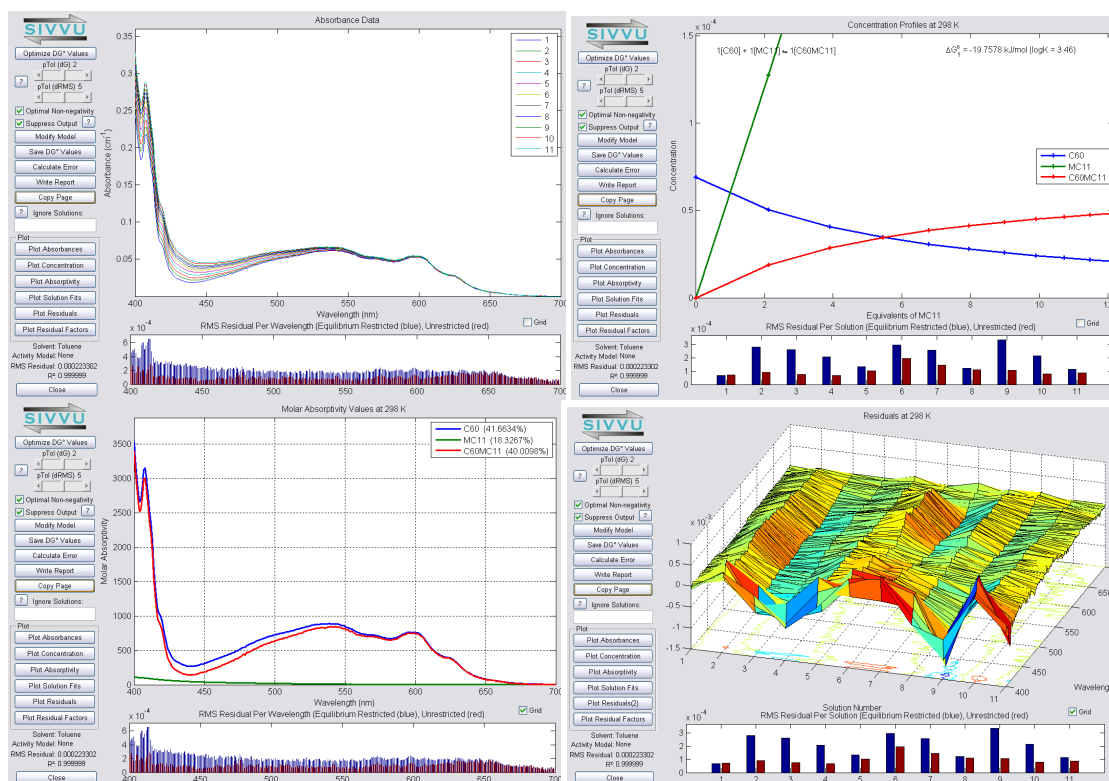
Restricted Data Reconstruction (3 chemical factors): 99.3925%

Unrestricted Data Reconstruction (3 mathematical factors): 99.5166%

Remaining Error Imbedded in Absorbance Values: 0.00050213

R²: 99.9994%

Figure S8. Spectrophotometric Titration of 69 μM C_{60} with Macrocycle (*RR*)-11.



Summary:

Data at 298 K

Non-negativity was enforced with optimization (not truncation).

$\text{DG1} = -19.7578 (\pm 0.015)$; $\text{RMS Residual} = 0.0002233$

Unrestricted RMS Residual (3 mathematical factors): 0.00010936

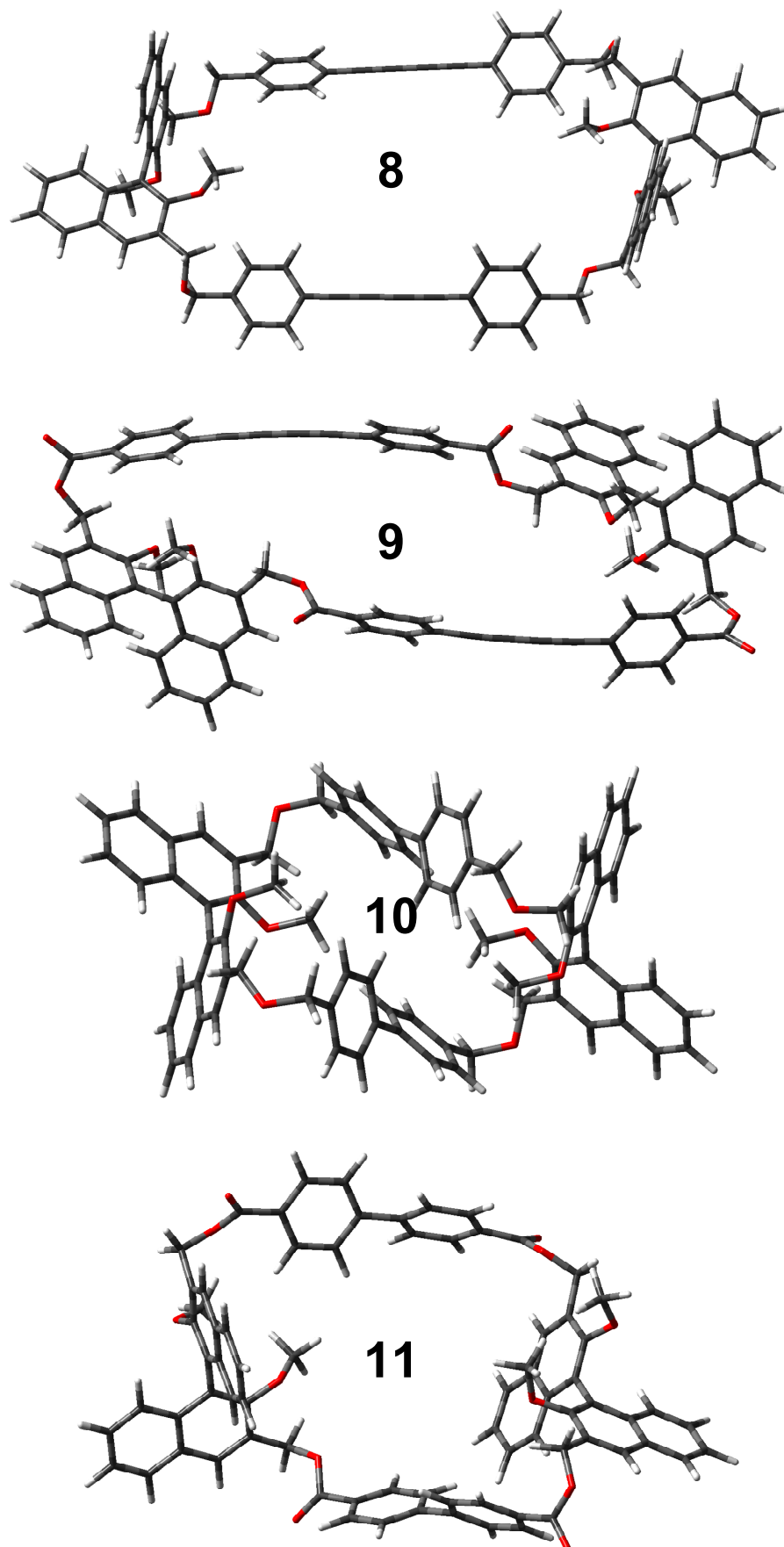
Restricted Data Reconstruction (3 chemical factors): 99.6088%

Unrestricted Data Reconstruction (3 mathematical factors): 99.629%

Remaining Imbedded Error in Absorbance Values: 0.00013674

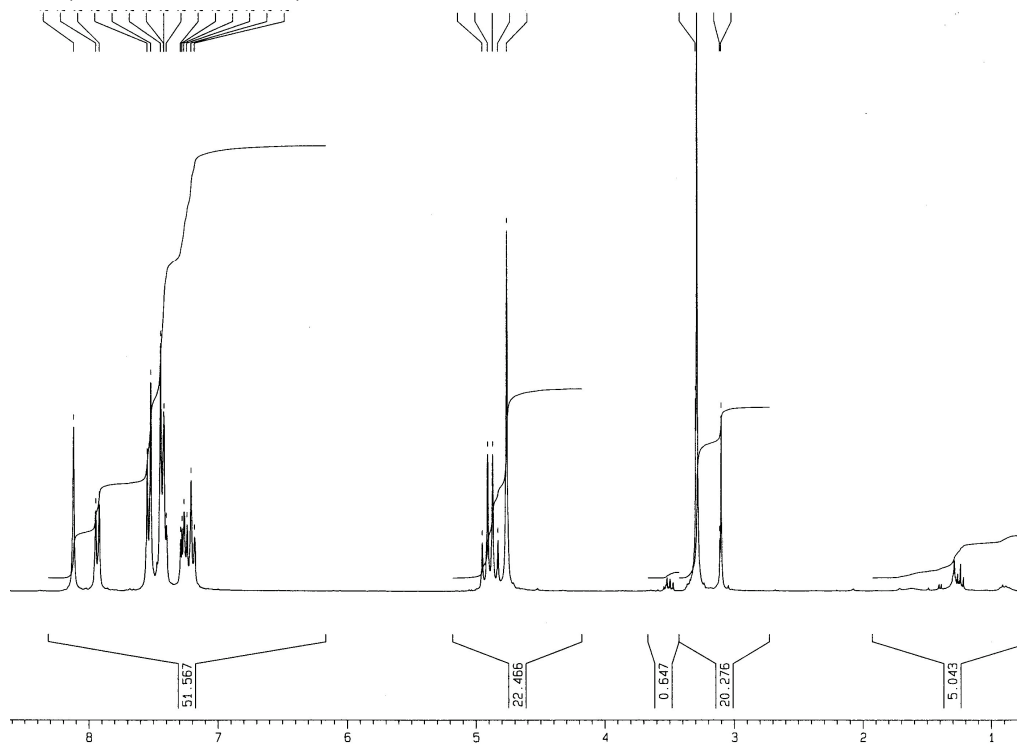
R^2 : 99.9999%

Figure S9. Minimized structures of macrocycles (*RR*)-8, (*RR*)-9, (*RR*)-10 and (*RR*)-11.

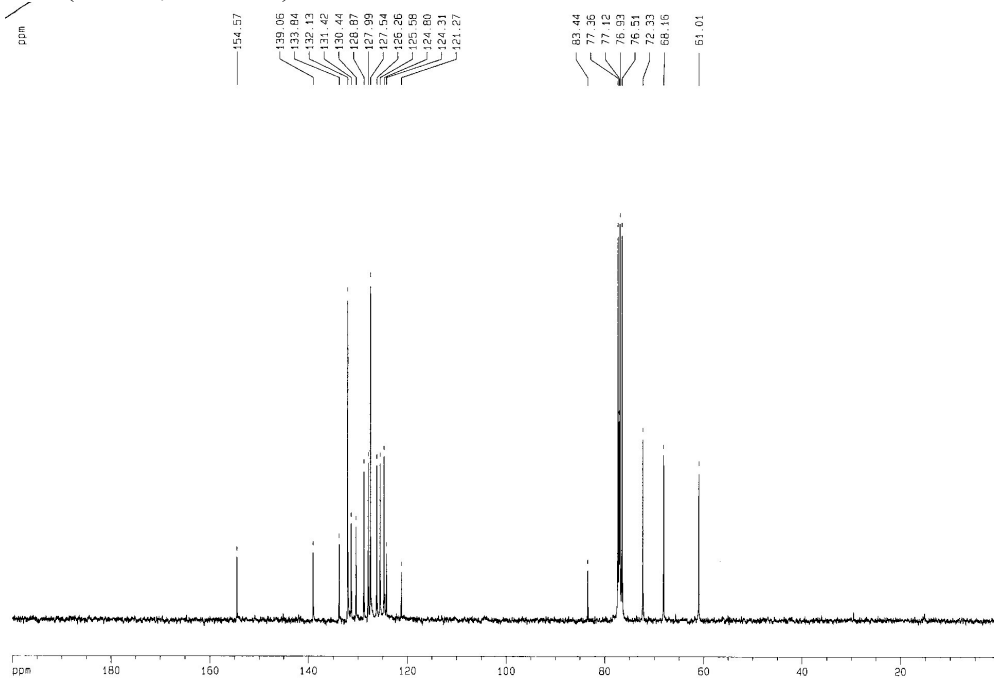


Compound (R)-4.

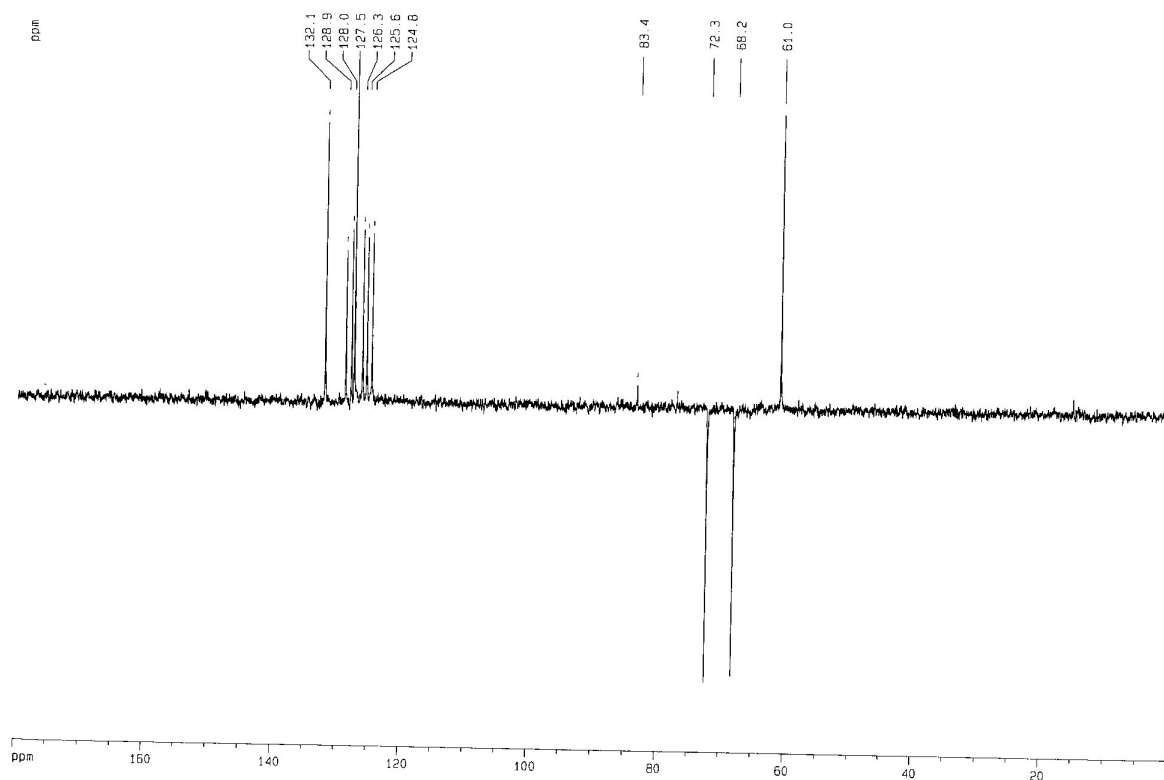
^1H NMR (CDCl_3 , 300 MHz)



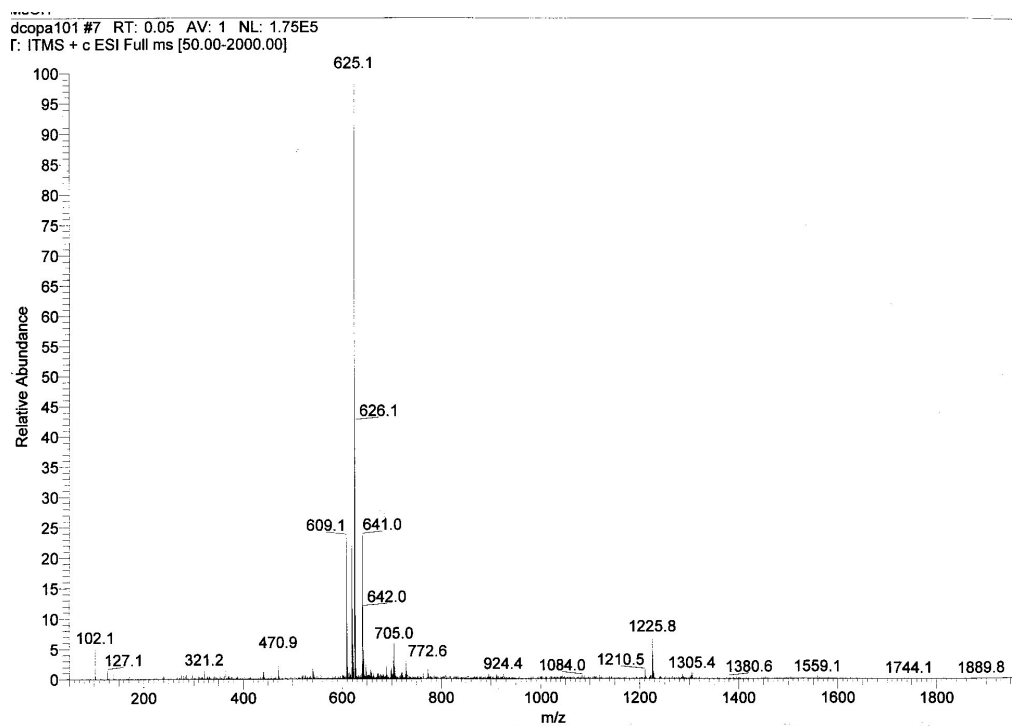
^{13}C NMR (CDCl_3 , 75 MHz)



^{13}C NMR DEPT (CDCl₃, 75 MHz)

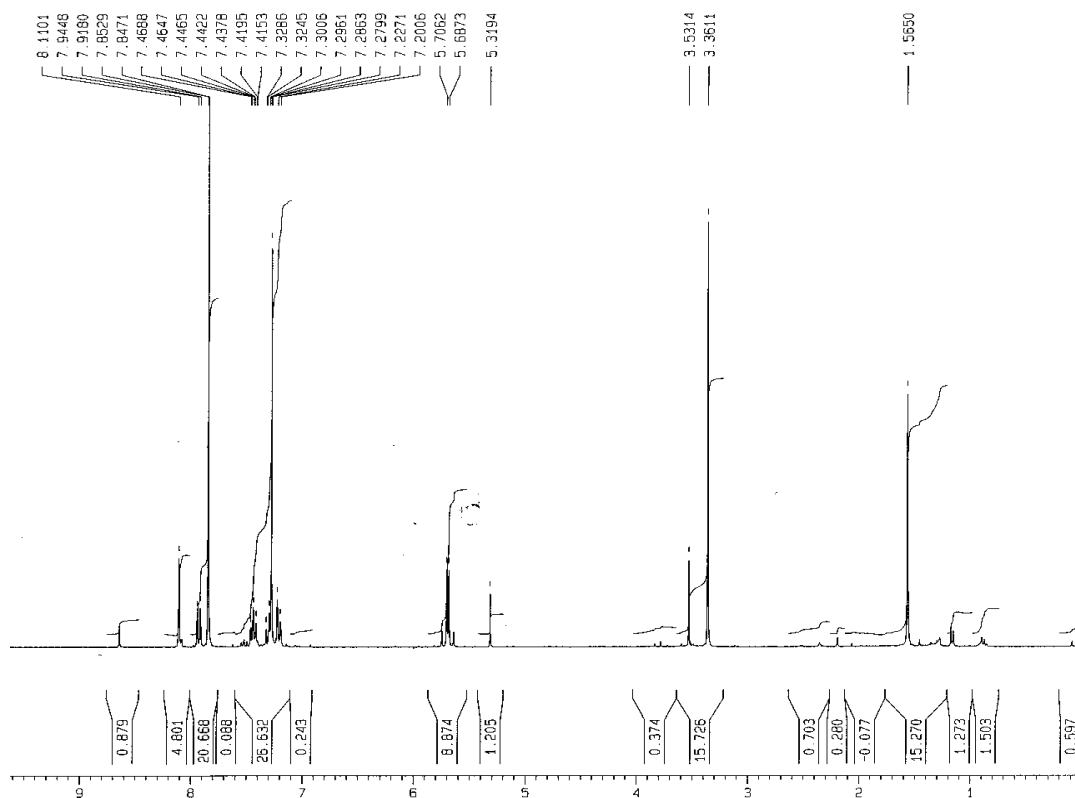


ESI MS

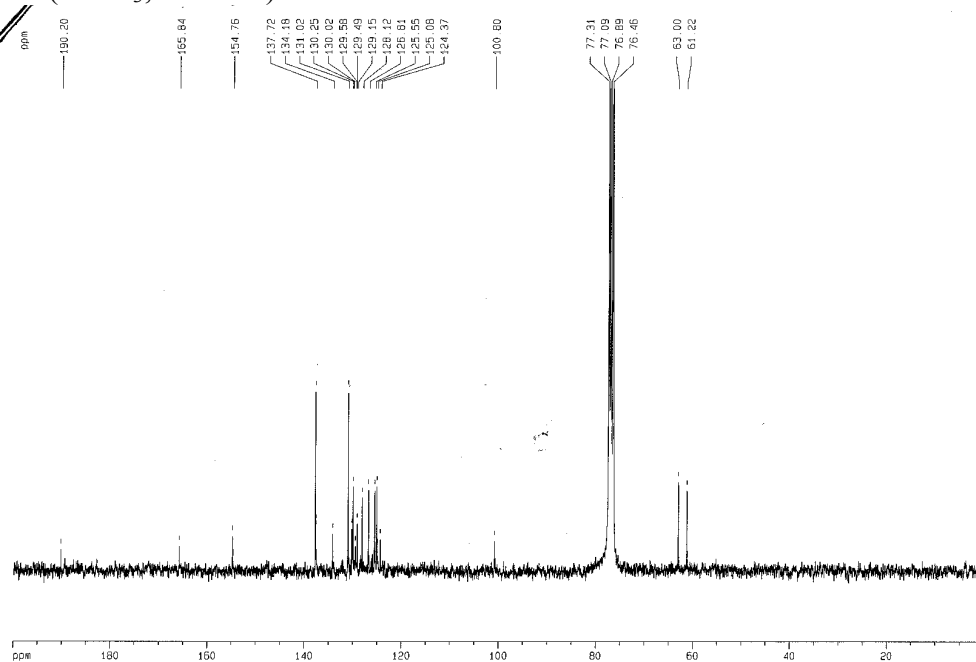


Compound (R)-5.

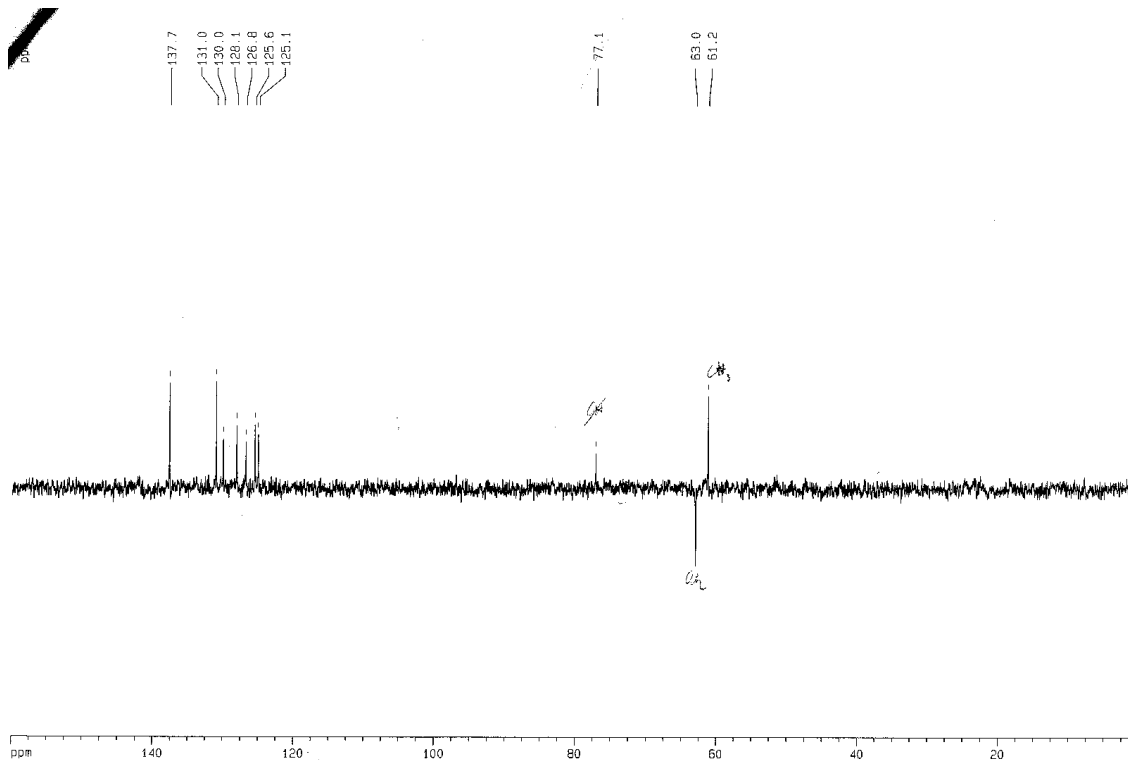
^1H NMR (CDCl_3 , 300 MHz)



^{13}C NMR (CDCl_3 , 75 MHz)

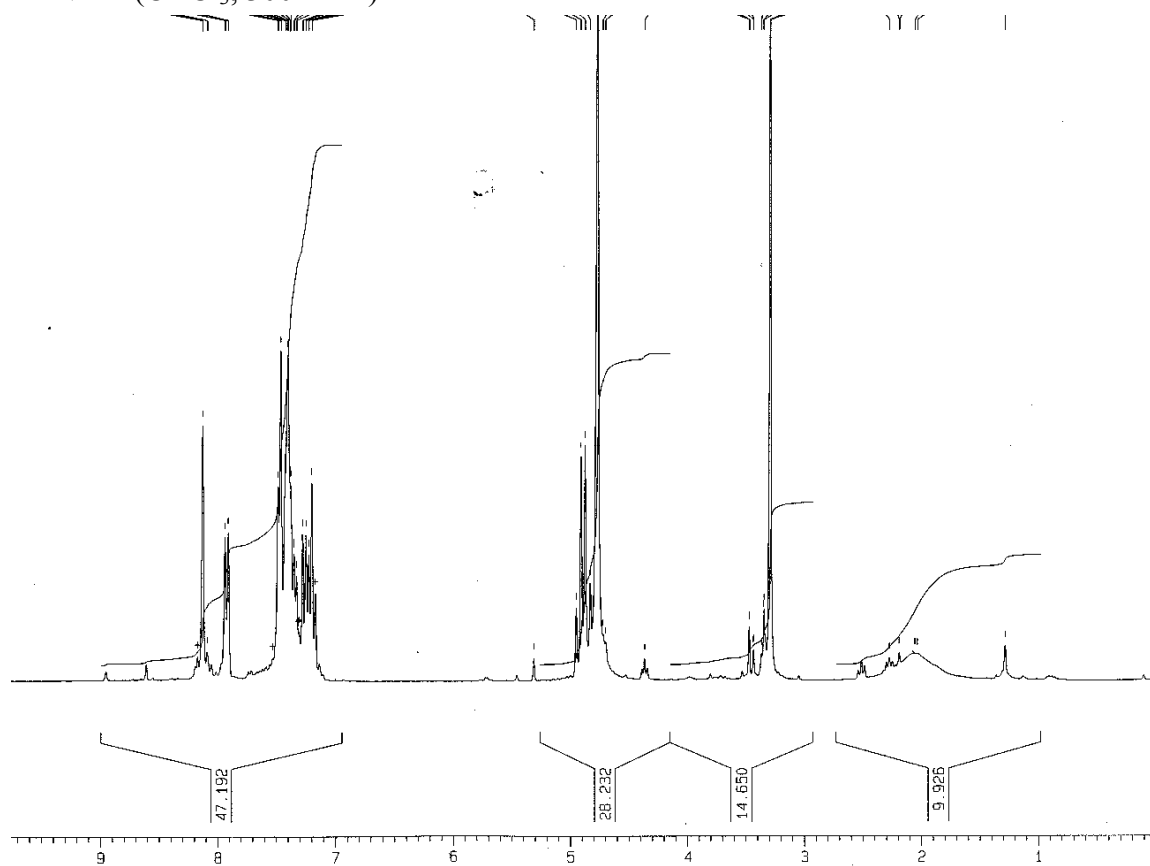


^{13}C NMR DEPT (CDCl_3 , 75 MHz)

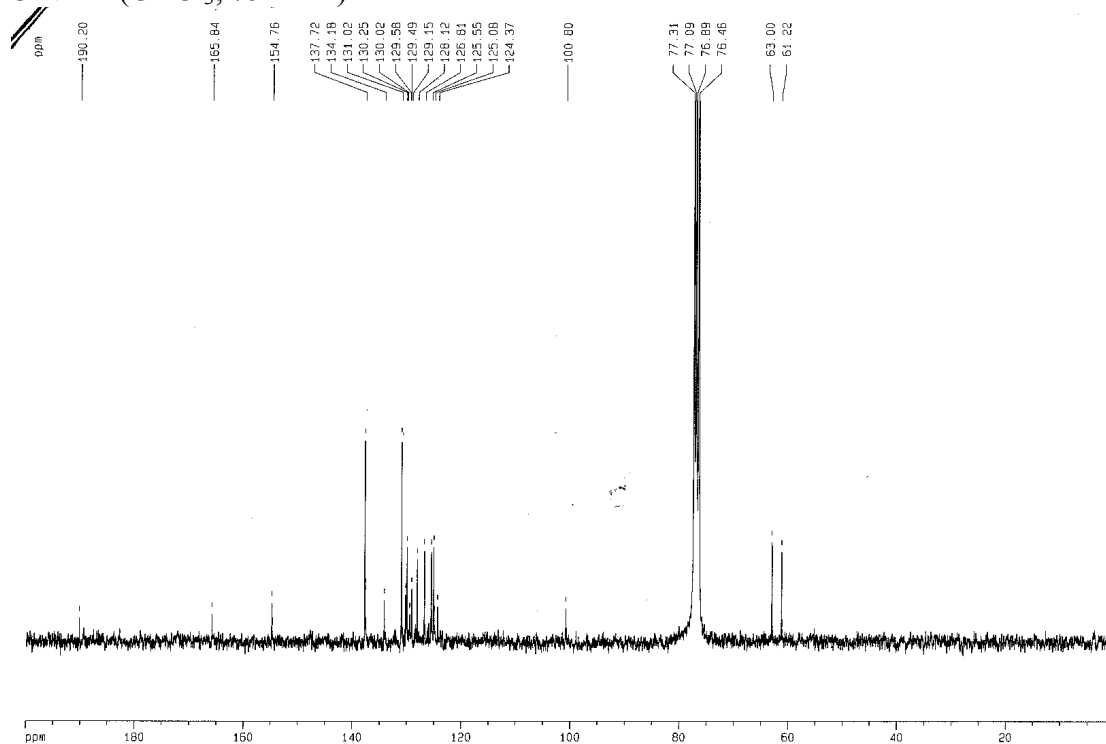


Compound (R)-6.

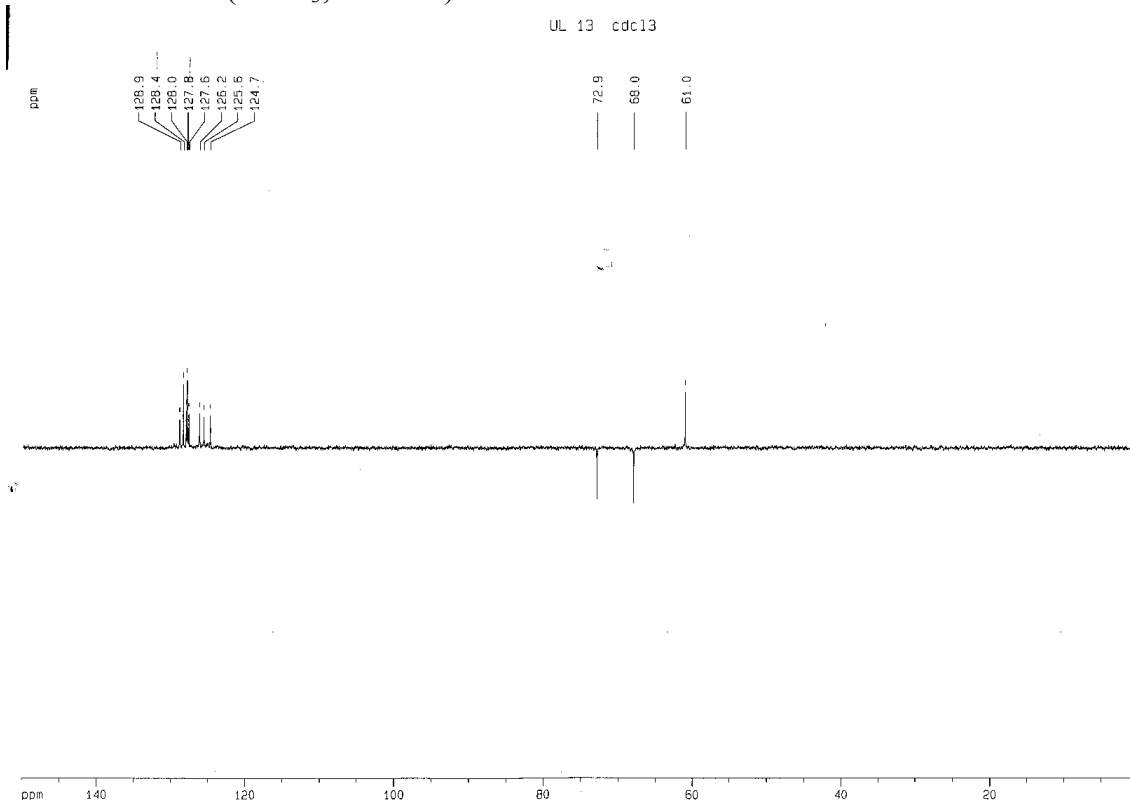
^1H NMR (CDCl_3 , 300 MHz)



^{13}C NMR (CDCl_3 , 75 MHz)

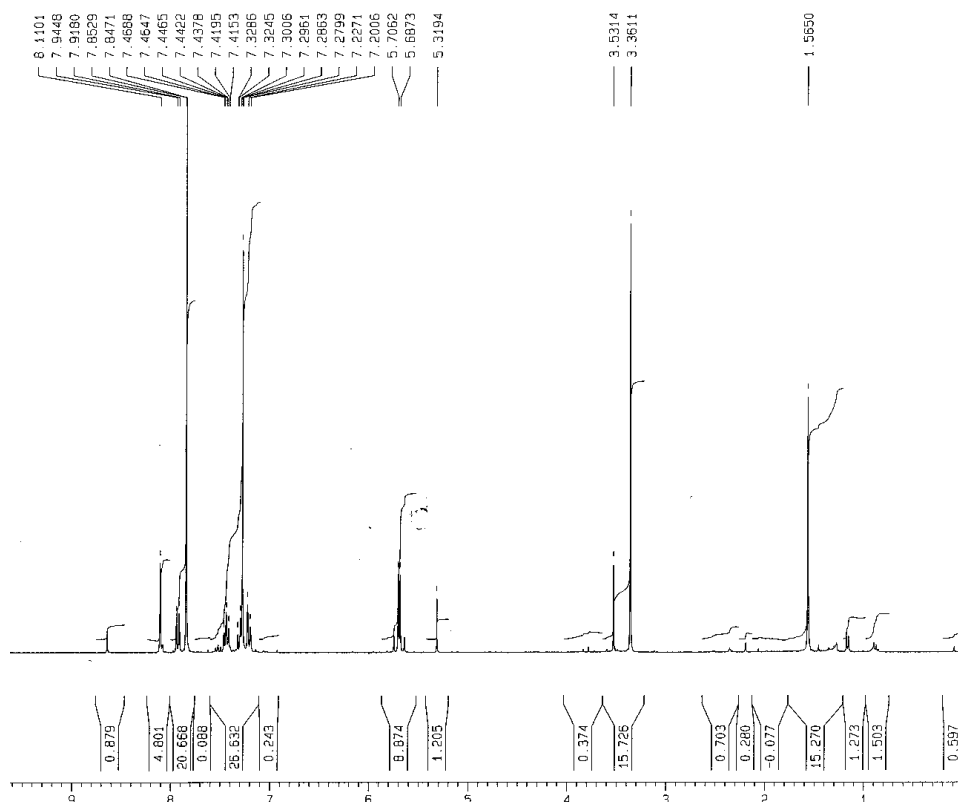


^{13}C NMR DEPT (CDCl_3 , 75 MHz)

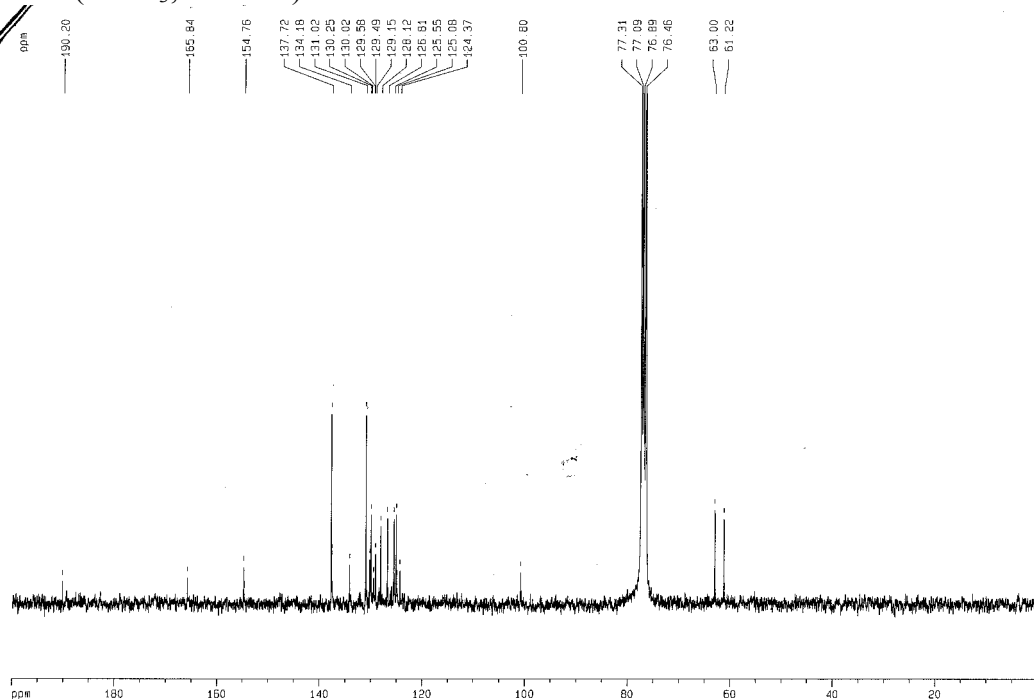


Compound (R)-7.

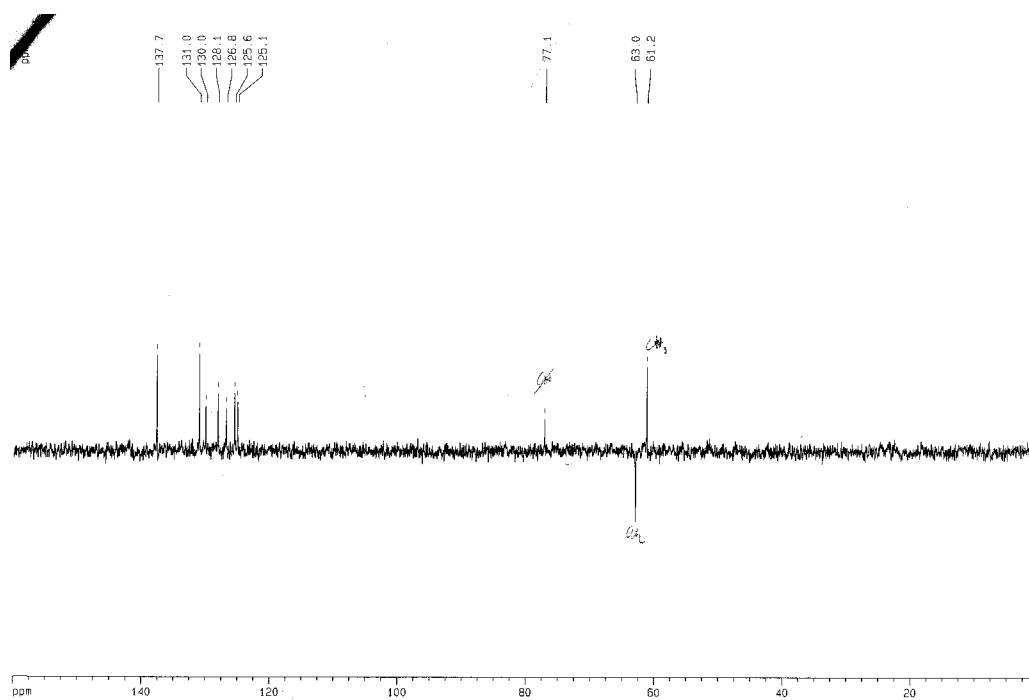
^1H NMR (CDCl_3 , 300 MHz)



^{13}C NMR (CDCl_3 , 75 MHz)

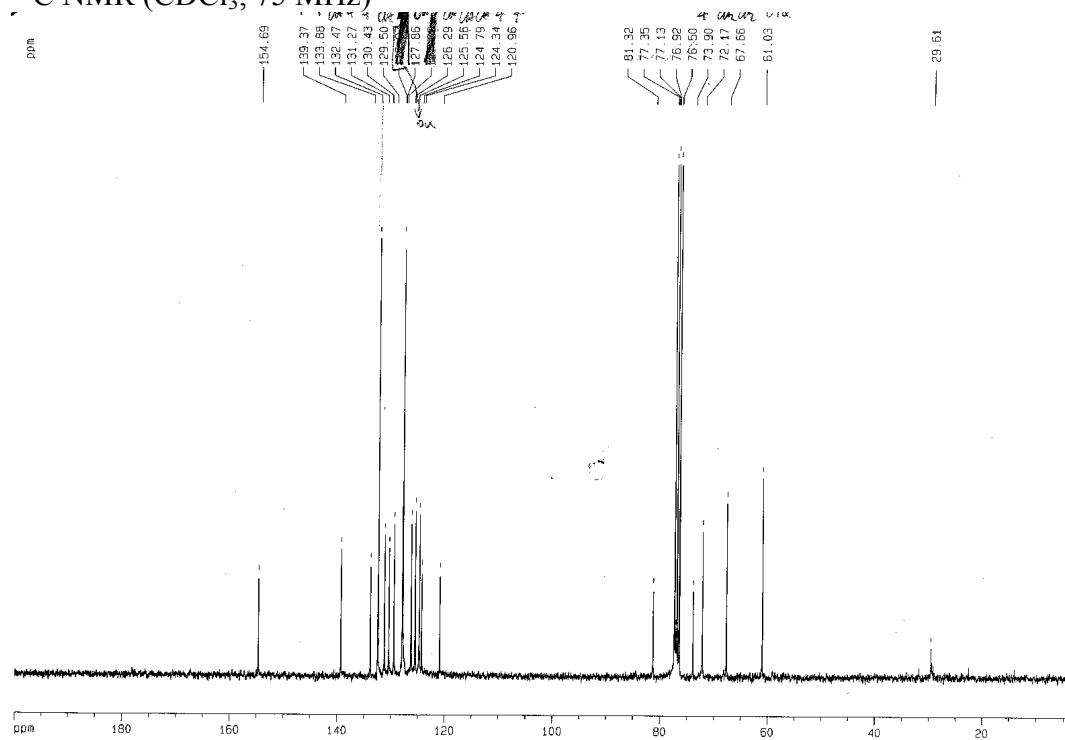


^{13}C NMR DEPT (CDCl_3 , 75 MHz)

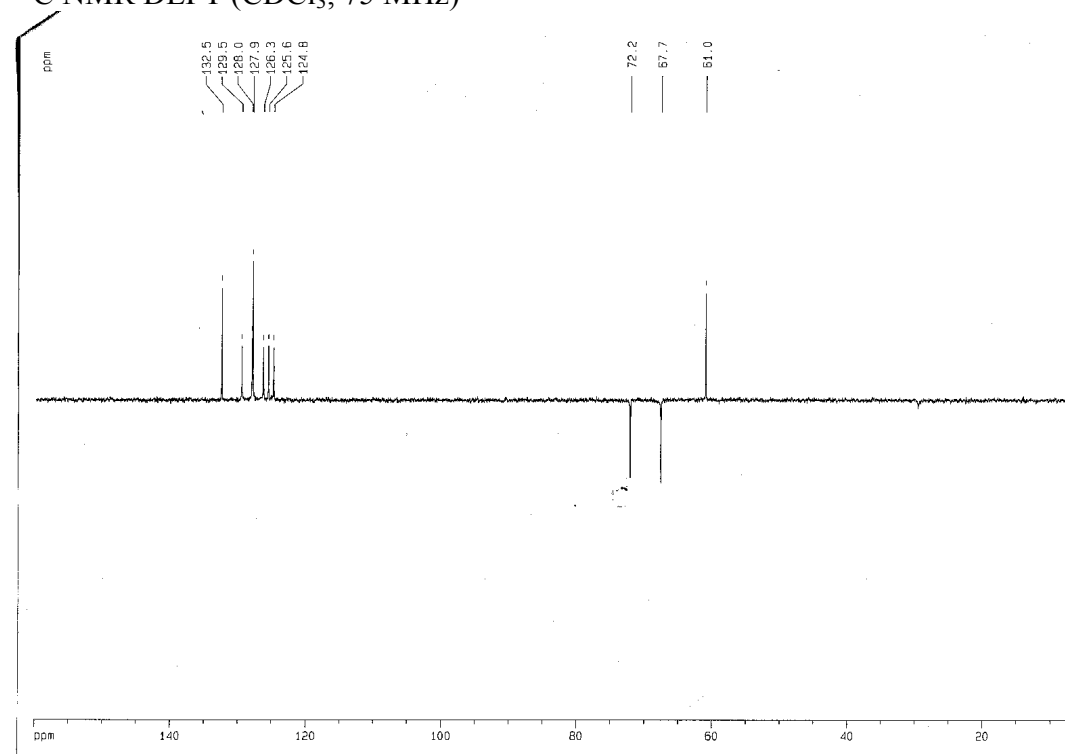


Macrocycle (RR)-8.

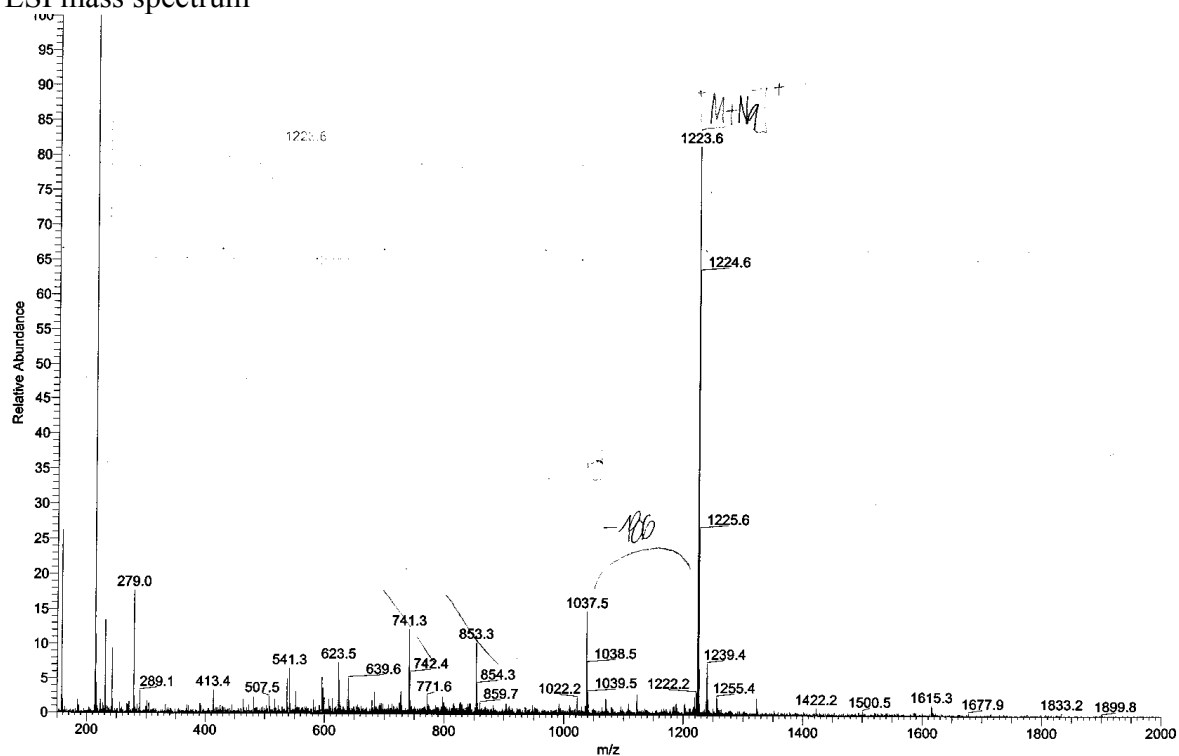
^{13}C NMR (CDCl_3 , 75 MHz)



^{13}C NMR DEPT (CDCl_3 , 75 MHz)

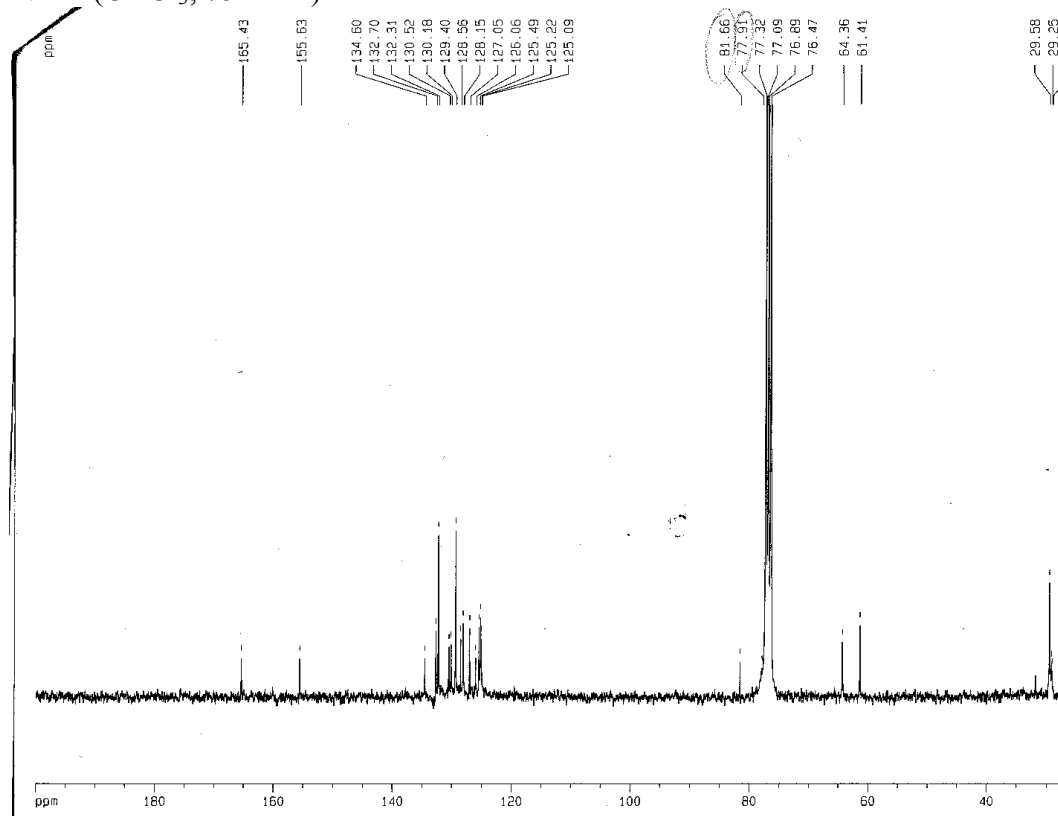


ESI mass spectrum

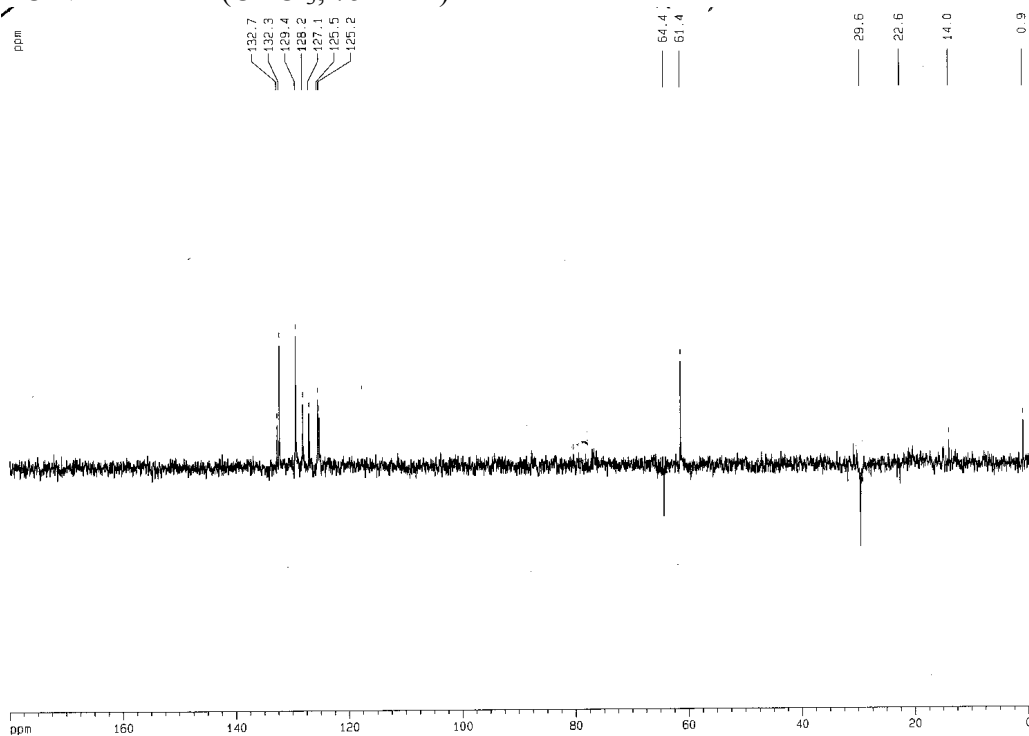


Macrocycle (RR)-9.

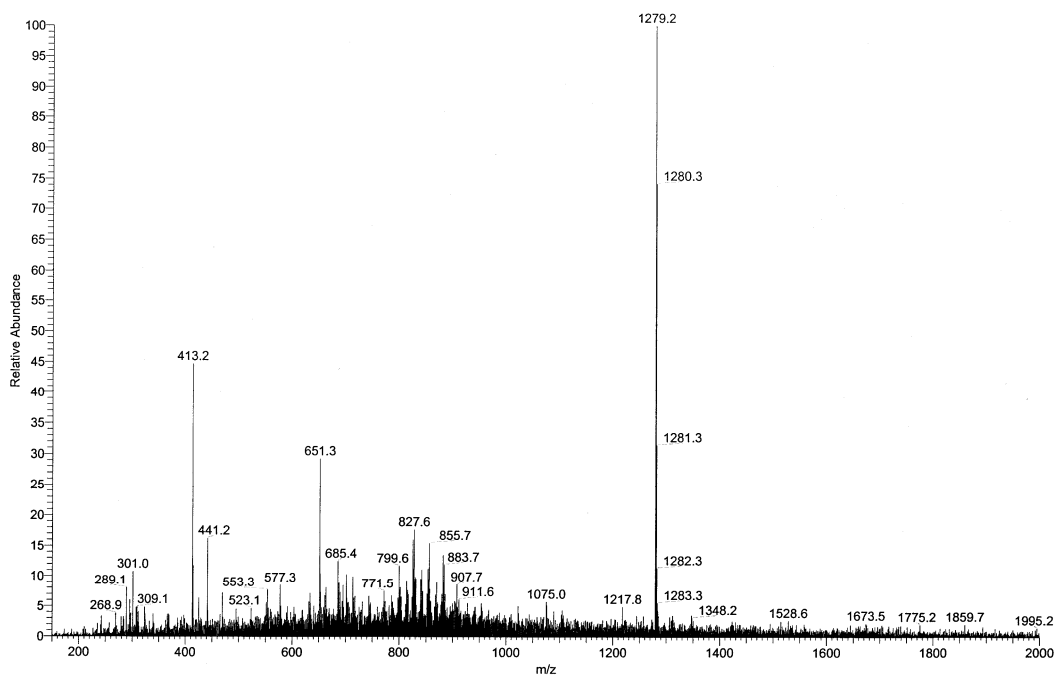
^{13}C NMR (CDCl_3 , 75 MHz)



^{13}C NMR DEPT (CDCl_3 , 75 MHz)

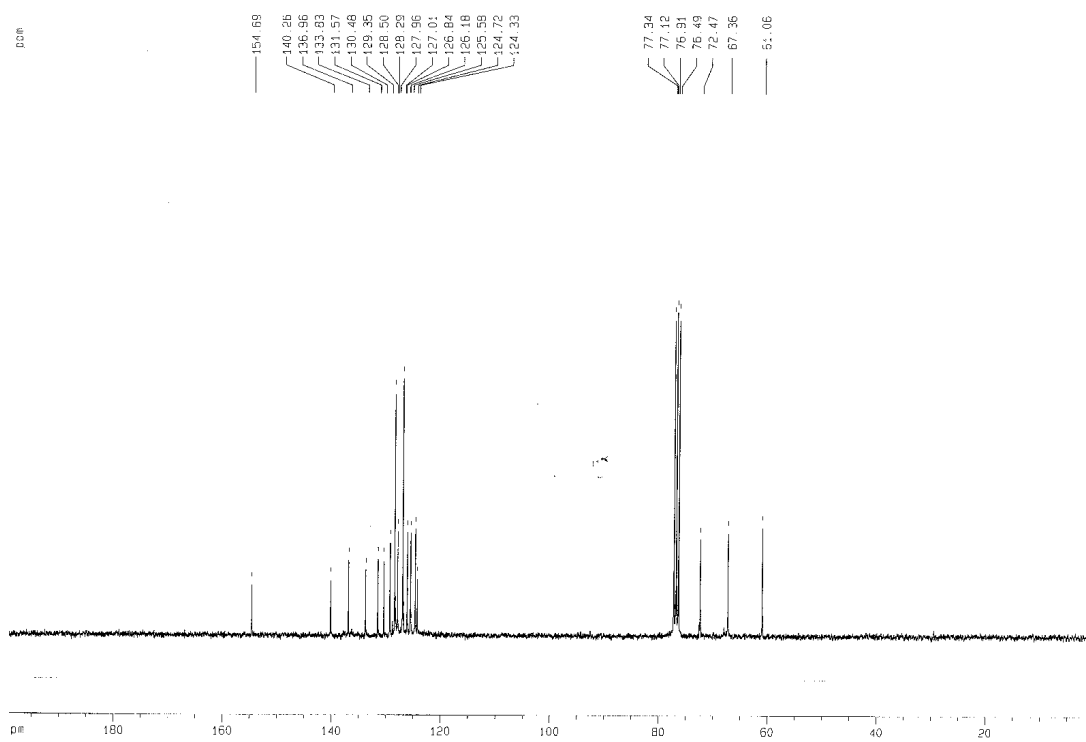


ESI mass spectrum

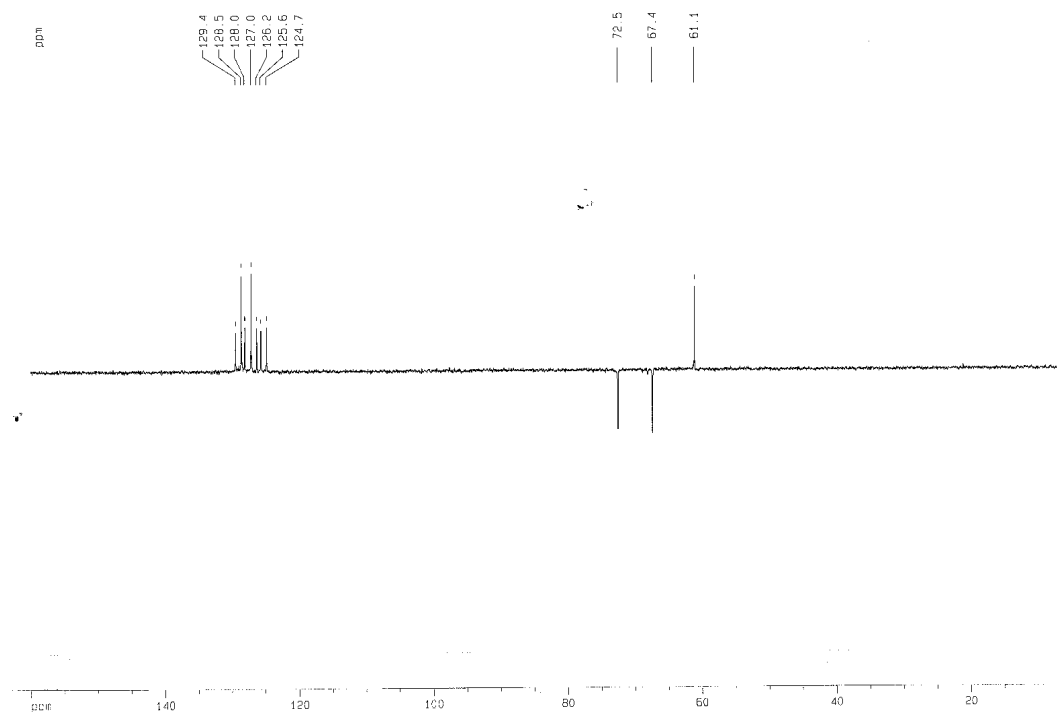


Macrocycle (RR)-10.

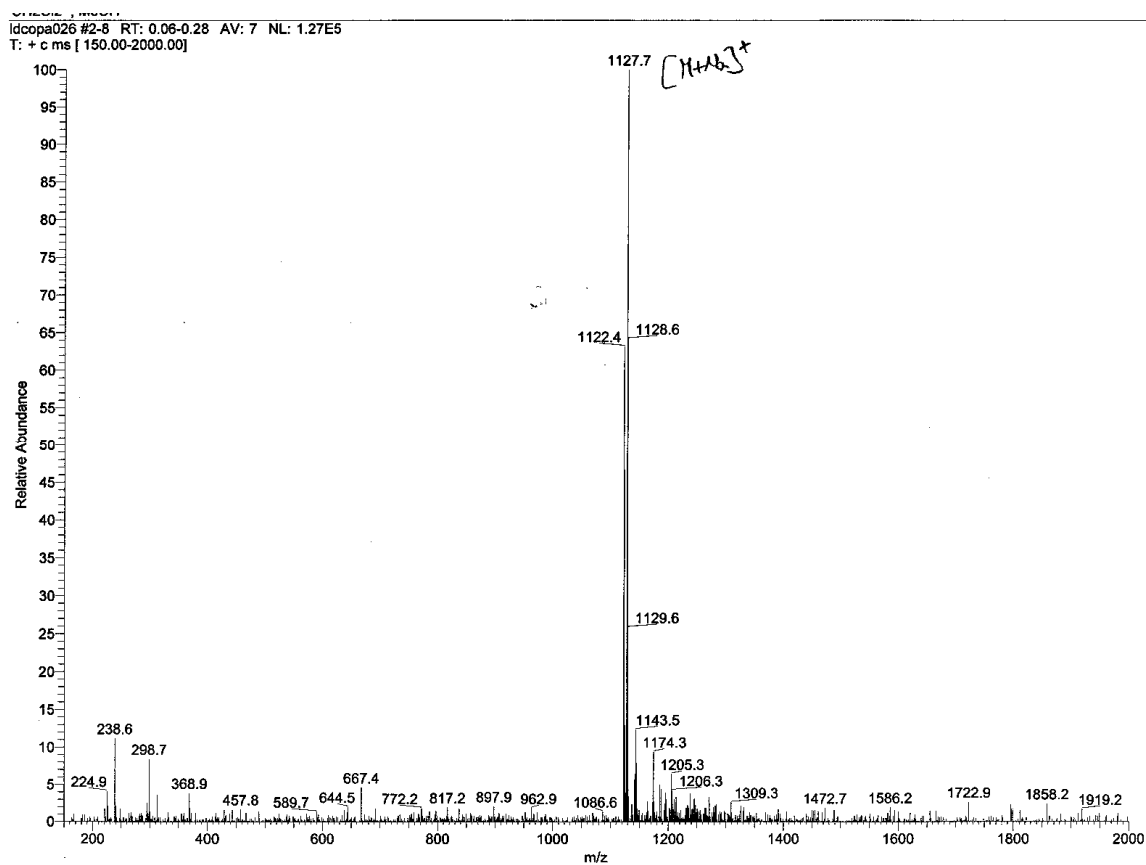
^{13}C NMR (CDCl_3 , 75 MHz)



^{13}C NMR DEPT (CDCl_3 , 75 MHz)

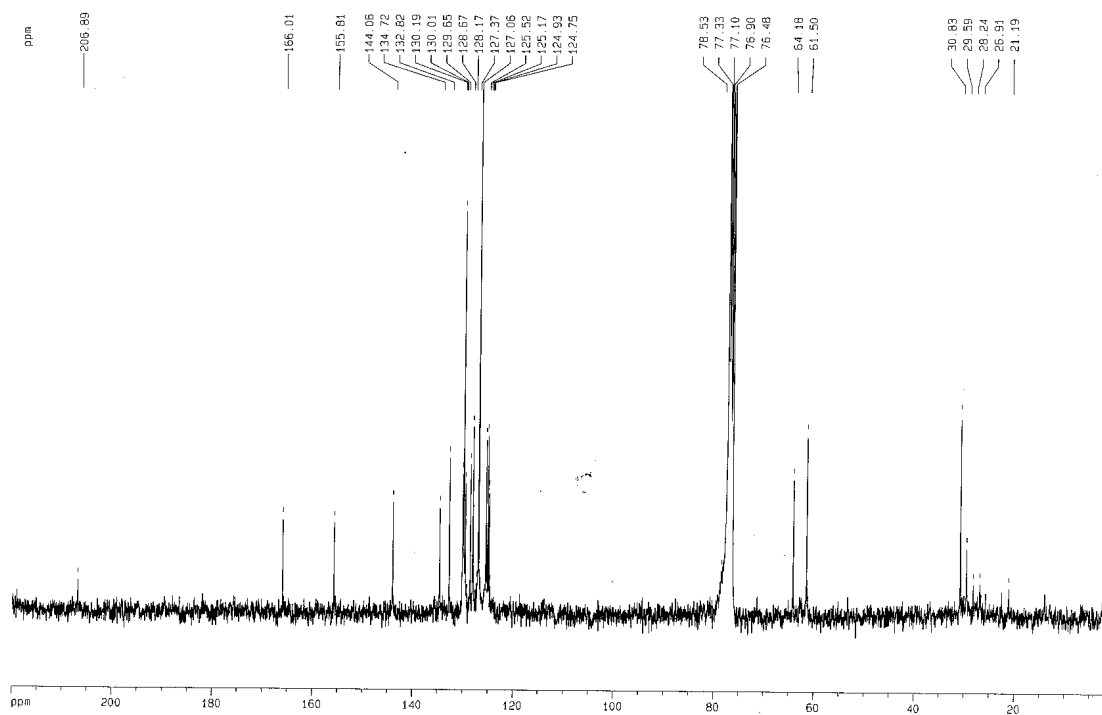


ESI mass spectrum

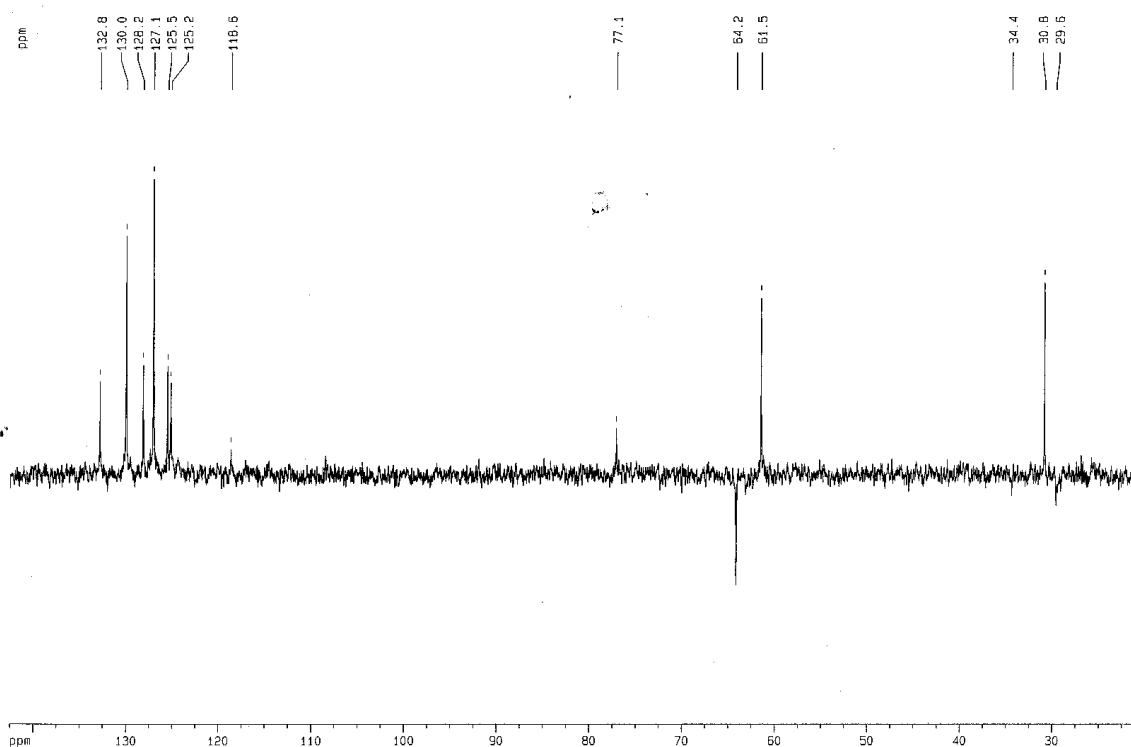


Macrocycle (RR)-11.

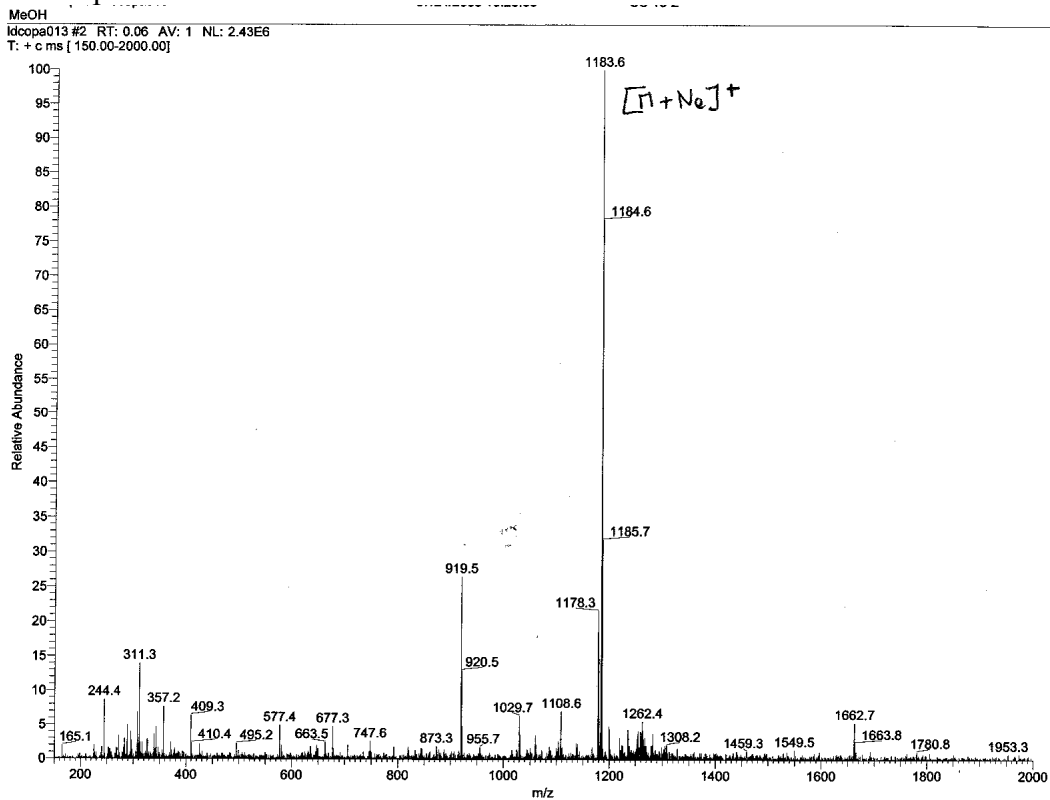
^{13}C NMR (CDCl_3 , 75 MHz)



^{13}C NMR DEPT (CDCl_3 , 75 MHz)



ESI mass spectrum



Details on calculations.

Optimizations were carried out at the PM3 level of theory as implemented by the Gaussian 2003 package.^{S4}

Atomic Coordinates and Energies for the reported molecules

Below are listed coordinates in cartesian format (units are in Å) and energies (in parentheses, units are in Hartrees) for the most stable conformers of the reported molecules. The calculated energy for C₆₀, used in this paper, was 1.29212107 Ha.

(RR) -8 (0.29613092 Ha)

C	10.095490	2.286756	4.187483
C	10.139838	1.431024	3.120872
C	-9.789137	1.878419	1.816152
C	-9.393643	3.220607	1.645605
C	-9.354326	4.090807	2.769379
C	-9.697758	3.632277	4.011466
H	10.368680	1.938931	5.189268
H	10.453137	0.387521	3.252338
C	-9.824274	1.010753	0.681003
C	-9.034134	3.688878	0.356567
H	-9.043836	5.131419	2.621316
H	-9.669168	4.298357	4.879998
C	-9.069813	2.863208	-0.738906
C	-9.478628	1.503951	-0.567307
H	-8.700479	4.733240	0.243380
C	10.215940	-0.401910	0.864888
C	11.600006	-0.756742	0.827173
C	-9.264331	-1.389032	1.063875
C	12.623736	0.213088	0.636126
C	11.969465	-2.107923	0.985565
C	-9.638635	-2.760764	1.209838
C	13.940316	-0.158218	0.607953
H	12.335864	1.265513	0.519559
C	13.344210	-2.469329	0.951742
C	10.968815	-3.095875	1.173849
C	14.306335	-1.514725	0.766654
H	14.725045	0.591753	0.463538
H	13.615794	-3.524037	1.075735
H	11.274170	-4.144773	1.283981
H	15.366181	-1.788207	0.739995
O	-7.908876	-1.063669	1.017153
O	-9.420404	0.644955	-1.663981
C	-8.683738	3.406119	-2.091674
H	-9.288034	4.307345	-2.317971
C	-8.613282	-3.846371	1.414451
H	-7.576365	-3.457765	1.391973
H	-8.776097	-4.349381	2.384164
H	-8.666021	-3.717979	-1.199978
C	-8.266336	-4.671649	-0.803840
H	-8.719872	-5.504072	-1.370079
O	-8.754513	-4.919619	0.502980
C	-6.765193	-4.706626	-0.886531
C	-6.035923	-3.517168	-0.912317
C	-6.097712	-5.930402	-0.948204
C	-4.649767	-3.547478	-1.001719
H	-6.558872	-2.552952	-0.859531
C	-4.712083	-5.970327	-1.036146
H	-6.671092	-6.864274	-0.924614

C	-3.983388	-4.776121	-1.063710
H	-4.190586	-6.932120	-1.084156
H	-8.846084	2.673898	-2.902933
H	-4.080303	-2.612040	-1.024817
C	-2.572057	-4.809603	-1.153896
C	-1.377656	-4.833500	-1.229816
O	-7.299586	3.652956	-2.226327
C	-0.015013	-4.855310	-1.316437
C	1.179522	-4.869840	-1.392463
C	2.591074	-4.881403	-1.483014
C	3.230043	-5.779475	-2.344572
C	3.347825	-3.990868	-0.713220
C	4.616371	-5.782643	-2.434094
H	2.637864	-6.474097	-2.949755
C	4.733569	-4.004542	-0.804489
H	2.847586	-3.283996	-0.042679
C	5.373503	-4.899235	-1.663867
H	5.114398	-6.480821	-3.116856
H	5.329676	-3.303820	-0.208395
C	6.871043	-4.924551	-1.749246
H	7.230401	-5.706258	-2.447603
H	7.308656	-5.147382	-0.749816
C	-7.366268	-0.736329	2.279140
H	-7.888857	0.109980	2.743875
H	-7.377505	-1.594614	2.961214
H	-6.337556	-0.461723	2.033841
C	10.644133	0.536020	-2.359805
H	11.457432	0.183363	-1.711850
H	10.933228	1.485119	-2.826426
H	10.418198	-0.207911	-3.127485
C	10.215882	0.401888	0.864889
C	9.824292	-1.010791	0.680960
C	11.599924	0.756806	0.827123
C	9.264223	1.388944	1.063953
C	9.789216	-1.878496	1.816083
C	9.478610	-1.503956	-0.567352
C	12.623706	-0.212953	0.635991
C	11.969309	2.108000	0.985577
C	9.638450	2.760691	1.209969
O	7.908787	1.063496	1.017263
C	10.139915	-1.431126	3.120812
C	9.393780	-3.220696	1.645499
C	9.069830	-2.863219	-0.738982
O	9.420322	-0.644920	-1.663991
C	13.940262	0.158434	0.607791
H	12.335895	-1.265394	0.519412
C	13.344028	2.469493	0.951702
C	10.968608	3.095883	1.173945
C	8.613025	3.846208	1.414692
C	7.366228	0.736146	2.279269
C	10.095619	-2.286894	4.187397
H	10.453142	-0.387606	3.252314
C	9.354528	-4.090936	2.769244
C	9.034227	-3.688930	0.356460
C	8.683706	-3.406093	-2.091748
C	10.644023	-0.535922	-2.359853
C	14.306205	1.514955	0.766541
H	14.725032	-0.591483	0.463310
H	13.615554	3.524208	1.075763
H	11.273909	4.144791	1.284133
H	7.576128	3.457563	1.391961
H	8.775675	4.348983	2.384554
O	8.754326	4.919687	0.503507

H	7.888875	-0.110127	2.744002
H	7.377435	1.594442	2.961329
H	6.337524	0.461479	2.034000
C	9.697966	-3.632432	4.011340
H	10.368830	-1.939094	5.189185
H	9.044095	-5.131561	2.621152
H	8.700615	-4.733303	0.243245
H	9.288041	-4.307275	-2.318118
H	8.845968	-2.673824	-2.902981
O	7.299556	-3.652996	-2.226325
H	11.457353	-0.183330	-1.711903
H	10.933090	-1.484980	-2.826575
H	10.418060	0.208081	-3.127456
H	15.366032	1.788506	0.739838
C	8.266378	4.671989	-0.803450
H	9.669421	-4.298543	4.879849
H	8.666199	3.718441	-1.199746
H	8.719946	5.504578	-1.369418
C	6.765248	4.706876	-0.886372
C	6.036062	3.517374	-0.912486
C	6.097695	5.930619	-0.947929
C	4.649918	3.547607	-1.002109
H	6.559067	2.553183	-0.859794
C	4.712077	5.970467	-1.036078
H	6.671008	6.864526	-0.924065
C	3.983468	4.776217	-1.063975
H	4.080520	2.612135	-1.025464
H	4.190524	6.932233	-1.084008
C	2.572149	4.809628	-1.154356
C	1.377739	4.833491	-1.230148
C	0.015092	4.855246	-1.316709
C	-1.179444	4.869734	-1.392718
C	-2.591002	4.881277	-1.483189
C	-3.230081	5.780179	-2.343809
C	-3.347651	3.989913	-0.714259
C	-4.616410	5.783348	-2.433247
H	-2.637977	6.475466	-2.948300
C	-4.733406	4.003588	-0.805439
H	-2.847337	3.282391	-0.044462
C	-5.373445	4.899109	-1.663871
H	-5.114522	6.482177	-3.115283
H	-5.329429	3.302221	-0.210021
C	-6.870987	4.924445	-1.749148
H	-7.230393	5.706241	-2.447383
H	-7.308501	5.147177	-0.749652

(RR) -9 (0.05863044)

C	-8.357097	4.381667	3.160884
C	-8.726161	3.353164	2.336668
C	-7.816036	2.831463	1.376377
C	-6.524850	3.390249	1.291927
C	-6.165074	4.457833	2.158642
C	-7.062329	4.941316	3.071735
H	-9.062066	4.783316	3.896306
H	-9.732678	2.920234	2.397353
C	-8.171196	1.758474	0.500231
C	-5.590732	2.881923	0.350197
H	-5.159213	4.886231	2.080652
H	-6.789411	5.764765	3.739804
C	-5.929716	1.862924	-0.500172
C	-7.246966	1.303967	-0.423655
H	-4.586266	3.325918	0.325137

C	-9.507844	1.138860	0.609520
C	10.606190	1.696585	-0.115857
C	-9.709706	0.013108	1.390216
C	10.466662	2.864660	-0.916110
C	11.870063	1.077446	-0.035049
C	10.983693	-0.635259	1.442811
C	11.539992	3.379161	-1.591366
H	-9.483306	3.348620	-0.973873
C	12.969921	1.630399	-0.746335
C	12.035663	-0.095295	0.747254
C	12.806247	2.755940	-1.506741
H	11.429290	4.280385	-2.203726
H	13.946894	1.138269	-0.674002
H	13.025477	-0.570475	0.780172
H	13.650488	3.185654	-2.055953
O	-8.630352	-0.566469	2.057932
O	-7.530315	0.197103	-1.223535
C	-4.971410	1.276012	-1.498313
H	-5.365707	1.402324	-2.526812
C	11.178210	-1.883586	2.260370
H	10.215717	-2.360070	2.532475
H	11.727144	-1.648808	3.190511
C	11.532473	-3.725809	0.744576
O	12.039434	-2.826807	1.643885
C	10.085716	-3.831814	0.415761
C	-9.598657	-3.233393	-0.745549
C	-9.231098	-4.544165	1.257685
C	-8.244811	-3.313208	-1.048705
H	10.277248	-2.687772	-1.411228
C	-7.878055	-4.631794	0.955098
H	-9.624224	-5.030747	2.157401
C	-7.379458	-4.001415	-0.190961
H	-7.201321	-5.182948	1.616954
H	-4.830805	0.195557	-1.304884
H	-7.854931	-2.815891	-1.944831
C	-5.991949	-4.026104	-0.466318
C	-4.815491	-4.001251	-0.686012
O	-3.635957	1.735770	-1.378564
C	-3.473322	-3.925291	-0.926516
C	-2.298680	-3.816339	-1.129624
C	-0.915673	-3.635136	-1.364417
C	-0.433543	-3.555659	-2.675846
C	-0.037197	-3.502027	-0.282684
C	0.915525	-3.313008	-2.902647
H	-1.119721	-3.677373	-3.521123
C	1.310021	-3.255052	-0.513609
H	-0.413958	-3.580679	0.742940
C	1.782564	-3.144222	-1.822222
H	1.297397	-3.250403	-3.928412
H	2.000297	-3.136563	0.330607
C	3.215696	-2.835495	-2.080503
C	-8.495988	-0.115929	3.389661
H	-8.377381	0.974028	3.445637
H	-9.346942	-0.426511	4.007670
H	-7.583604	-0.616216	3.722696
C	-8.194220	0.516884	-2.427945
H	-9.131094	1.062029	-2.253563
H	-7.552923	1.094496	-3.104093
H	-8.399801	-0.470721	-2.850810
C	9.507825	-1.138740	0.609592
C	8.171297	-1.758589	0.500164
C	10.606350	-1.696368	-0.115591
C	9.709430	-0.012919	1.390258

C	7.816209	-2.831584	1.376333
C	7.247153	-1.304379	-0.423952
C	10.467095	-2.864515	-0.915784
C	11.870127	-1.077051	-0.034649
C	10.983322	0.635631	1.442978
O	8.629896	0.566527	2.057798
C	8.726239	-3.352949	2.336899
C	6.525166	-3.390668	1.291678
C	5.930066	-1.863685	-0.500729
O	7.530412	-0.197471	-1.223801
C	11.540588	-3.378912	-1.590861
H	9.483811	-3.348608	-0.973665
C	12.970159	-1.629897	-0.745748
C	12.035458	0.095766	0.747600
C	11.177539	1.884031	2.260498
C	8.495554	0.116210	3.389606
C	8.357233	-4.381441	3.161155
H	9.732641	-2.919775	2.397758
C	6.165446	-4.458231	2.158444
C	5.591150	-2.882697	0.349656
C	4.971876	-1.277207	-1.499247
C	8.194477	-0.517151	-2.428146
C	12.806752	-2.755530	-1.506076
H	11.430104	-4.280215	-2.203144
H	13.947067	-1.137658	-0.673271
H	13.025209	0.571071	0.780630
H	10.214941	2.360505	2.532243
H	11.726171	1.649341	3.190840
O	12.038934	2.827224	1.644213
H	8.377112	-0.973755	3.445766
H	9.346436	0.427029	4.007597
H	7.583080	0.616415	3.722515
C	7.062615	-4.941401	3.071787
H	9.062130	-4.782833	3.896786
H	5.159705	-4.886879	2.080276
H	4.586808	-3.326960	0.324405
H	5.366194	-1.404296	-2.527644
H	4.831492	-0.196595	-1.306552
O	3.636338	-1.736646	-1.379133
H	9.131362	-1.062251	-2.253691
H	7.553281	-1.094762	-3.104392
H	8.400046	0.470487	-2.850941
H	13.651117	-3.185134	-2.055184
C	11.532186	3.726204	0.744763
H	6.789738	-5.764827	3.739902
C	10.085491	3.832226	0.415681
C	9.598520	3.233391	-0.745449
C	9.230840	4.545000	1.257215
C	8.244716	3.313219	-1.048805
H	10.277133	2.687420	-1.410819
C	7.877847	4.632641	0.954427
H	9.623908	5.031899	2.156785
C	7.379329	4.001858	-0.191446
H	7.854904	2.815589	-1.944788
H	7.201085	5.184134	1.615973
C	5.991851	4.026556	-0.466954
C	4.815408	4.001774	-0.686739
C	3.473245	3.925773	-0.927268
C	2.298605	3.816627	-1.130280
C	0.915593	3.635206	-1.364875
C	0.433260	3.555616	-2.676219
C	0.037318	3.501964	-0.282991
C	-0.915795	3.312666	-2.902790

H	1.119271	3.677451	-3.521613
C	-1.309882	3.254696	-0.513686
H	0.414235	3.580715	0.742569
C	-1.782619	3.143719	-1.822219
H	-1.297830	3.249981	-3.928490
H	-2.000001	3.136124	0.330648
C	-3.215707	2.834576	-2.080241
O	-3.976814	3.413450	-2.828234
O	12.442354	4.395510	0.307500
O	12.442539	-4.395142	0.307143
O	3.976534	-3.414748	-2.828476

(RR) -10 (-0.03838677)

C	-9.322731	1.728164	0.620554
C	-8.216339	0.929746	0.517638
C	-7.208517	1.207144	-0.447467
C	-7.376103	2.317052	-1.299838
C	-8.532514	3.134281	-1.171483
C	-9.483364	2.844593	-0.231755
C	-6.043093	0.390473	-0.585763
C	-6.397822	2.607175	-2.285609
C	-5.283355	1.820086	-2.433567
C	-5.117041	0.688104	-1.574137
C	-5.865696	-0.769818	0.312742
C	-6.169219	-2.079444	-0.175684
C	-5.429023	-0.617047	1.619634
C	-6.661754	-2.300248	-1.492206
C	-5.986020	-3.191303	0.671174
C	-5.267650	-1.743879	2.485794
C	-6.939521	-3.566035	-1.931109
C	-6.275272	-4.497870	0.190645
C	-5.534715	-2.999589	2.002104
C	-6.741122	-4.679224	-1.082528
O	-5.271876	0.659403	2.163016
O	-4.085429	-0.220920	-1.810358
C	-4.287301	2.131199	-3.518119
C	-4.897108	-1.567148	3.933940
O	-4.096616	3.541248	-3.609043
C	-2.754907	3.955020	-3.759432
C	-1.897764	3.707923	-2.548994
C	-2.200312	4.330119	-1.337427
C	-0.790735	2.862758	-2.632302
C	-1.413370	4.098442	-0.216376
C	-0.001671	2.628803	-1.512445
C	-0.313620	3.240357	-0.296044
C	0.513346	2.985234	0.890100
C	0.820582	1.677342	1.270034
C	1.006094	4.054127	1.643047
C	1.618774	1.442237	2.383078
C	1.801006	3.815468	2.756045
C	2.112513	2.507848	3.134479
C	2.930422	2.286395	4.375963
O	3.657833	1.072821	4.373024
C	-2.652563	-2.238188	4.471638
C	-1.916062	-2.466035	3.181290
O	-4.026065	-2.570240	4.426849
C	-1.612977	-3.762861	2.766050
C	-1.493111	-1.382472	2.412587
C	-0.885723	-3.973378	1.601003
C	-0.756549	-1.587984	1.252679
C	-0.450283	-2.886455	0.838958
C	0.322159	-3.107286	-0.390535
C	1.447851	-3.934689	-0.378684

C	-0.064040	-2.485814	-1.580146
C	2.189153	-4.121070	-1.539089
C	0.679665	-2.672580	-2.738636
C	1.815459	-3.482662	-2.722053
C	2.622858	-3.670991	-3.976106
O	3.968378	-3.257577	-3.868947
C	4.161817	-1.858634	-3.672802
C	5.188036	-1.635038	-2.594450
C	6.298109	-2.440228	-2.539905
C	5.053774	-0.574599	-1.642576
C	7.301688	-2.242970	-1.557014
C	6.002791	-0.373816	-0.651720
O	4.034707	0.367217	-1.786436
C	7.162287	-1.210257	-0.608482
C	8.452572	-3.077289	-1.526211
C	5.863837	0.699446	0.355074
C	8.192411	-1.027681	0.355822
C	9.425586	-2.878858	-0.585500
C	6.196204	2.042726	-0.006153
C	5.452099	0.426273	1.650800
C	9.292868	-1.840751	0.364862
C	6.649222	2.384026	-1.311197
C	6.082934	3.066024	0.957157
C	5.369665	1.459823	2.634917
O	5.251069	-0.892321	2.059404
C	6.955878	3.679247	-1.627916
C	6.402237	4.405484	0.603161
C	5.670525	2.749396	2.276605
C	5.036006	1.158949	4.071680
C	6.828433	4.703617	-0.661849
C	2.773121	-0.055378	-1.321526
C	3.918156	-1.336519	1.938337
C	-2.824838	0.189415	-1.332311
C	-3.979194	1.199854	2.010389
H	10.095344	1.511195	1.365498
H	-8.085187	0.066558	1.182282
H	-8.646529	3.996448	-1.838516
H	10.375692	3.470592	-0.129427
H	-6.554854	3.478026	-2.935368
H	-6.807712	-1.435604	-2.151728
H	-7.317321	-3.730362	-2.945576
H	-6.119603	-5.352449	0.858968
H	-5.410463	-3.878570	2.648205
H	-6.965647	-5.683131	-1.457078
H	-3.323476	1.603338	-3.349402
H	-4.687179	1.807094	-4.497049
H	-4.502024	-0.554213	4.145814
H	-5.798084	-1.717984	4.557155
H	-2.882185	5.036775	-3.941783
H	-2.309793	3.499468	-4.665849
H	-3.068447	4.996488	-1.272296
H	-0.539264	2.381113	-3.584767
H	-1.653855	4.588063	0.734394
H	0.874451	1.963148	-1.579670
H	0.426822	0.822110	0.694460
H	0.767175	5.082458	1.348333
H	1.881507	0.406881	2.657577
H	2.187622	4.660706	3.337188
H	2.251724	2.154616	5.238995
H	3.581263	3.160703	4.579004
H	-2.502680	-1.200418	4.832151
H	-2.288215	-2.930446	5.252250
H	-1.952736	-4.617555	3.362401

H	-1.758947	-0.356567	2.715607
H	-0.650951	-4.993554	1.276173
H	-0.408544	-0.719275	0.668262
H	1.746443	-4.434093	0.550369
H	-0.962124	-1.848384	-1.596839
H	3.078240	-4.762453	-1.526894
H	0.369551	-2.181244	-3.668591
H	2.139344	-3.176337	-4.841461
H	2.745448	-4.742639	-4.213114
H	3.204518	-1.344942	-3.437584
H	4.536005	-1.460668	-4.634349
H	6.431437	-3.255319	-3.263287
H	8.543987	-3.878605	-2.268394
H	8.084210	-0.226233	1.097296
H	10.313709	-3.518418	-0.557560
H	10.082194	-1.696682	1.109941
H	6.739952	1.588291	-2.061372
H	7.302049	3.936560	-2.634384
H	6.301764	5.190732	1.360895
H	5.606190	3.558897	3.016019
H	5.374379	0.149339	4.367105
H	5.529730	1.893853	4.739307
H	7.075403	5.733439	-0.939495
H	2.166413	0.858538	-1.382869
H	2.348085	-0.836407	-1.973569
H	2.802318	-0.418880	-0.282946
H	3.601934	-1.388918	0.885306
H	3.959484	-2.338656	2.371361
H	3.204698	-0.706215	2.494119
H	-2.414546	1.007829	-1.946806
H	-2.847545	0.497527	-0.276066
H	-2.211256	-0.713644	-1.446120
H	-3.203529	0.589964	2.503751
H	-4.065070	2.172085	2.501285
H	-3.708058	1.329278	0.951671

(RR) -11 (-0.26817776)

C	-9.487029	-3.699121	-0.399529
C	-8.561525	-2.744719	-0.075779
C	-7.354719	-2.623562	-0.819487
C	-7.131730	-3.507111	-1.894836
C	-8.107938	-4.490813	-2.212261
C	-9.259160	-4.583160	-1.479188
C	-6.364023	-1.642783	-0.503719
C	-5.933497	-3.413153	-2.647934
C	-4.978868	-2.473161	-2.349517
C	-5.199497	-1.579104	-1.255233
C	-6.586944	-0.739457	0.644457
C	-6.015969	-1.083993	1.910320
C	-7.339848	0.418491	0.531004
C	-5.267552	-2.279026	2.100228
C	-6.211904	-0.228328	3.013331
C	-7.480754	1.316831	1.634959
C	-4.754095	-2.593015	3.329135
C	-5.669076	-0.575512	4.280533
C	-6.937817	0.979242	2.848800
C	-4.957125	-1.733601	4.433097
O	-8.098497	0.651708	-0.614668
O	-4.185081	-0.719606	-0.834273
C	-3.748665	-2.402895	-3.212195
C	-8.182986	2.641548	1.494265
O	-2.549256	-2.746156	-2.534674
C	-2.174646	-4.055439	-2.410901

C	-0.865686	-4.197652	-1.715345
C	0.243770	-3.471341	-2.148850
C	-0.753493	-5.062705	-0.626788
C	1.454233	-3.589676	-1.478579
C	0.455836	-5.169421	0.050135
C	1.562843	-4.420951	-0.360339
C	2.824879	-4.478100	0.390009
C	4.049917	-4.530736	-0.280622
C	2.806364	-4.450285	1.788124
C	5.241953	-4.542187	0.434584
C	3.995800	-4.457432	2.505290
C	5.214579	-4.493791	1.827431
C	6.488960	-4.529992	2.593682
O	7.007982	-3.457561	3.267402
C	-6.406550	4.229120	1.889291
C	-5.103955	4.616729	1.284423
O	-7.275223	3.627781	1.010053
C	-4.464611	5.786293	1.698461
C	-4.485282	3.773681	0.358681
C	-3.198748	6.094819	1.213374
C	-3.219495	4.081442	-0.121079
C	-2.561972	5.235512	0.314947
C	-1.194129	5.505114	-0.147579
C	-0.196237	5.835199	0.773074
C	-0.871877	5.387957	-1.502328
C	1.120452	5.987493	0.355001
C	0.441559	5.548519	-1.923549
C	1.446655	5.818491	-0.991305
C	2.855385	5.871278	-1.467816
O	3.754922	5.387426	-0.552818
C	5.042000	4.947337	-0.976934
C	5.034513	3.453938	-1.177133
C	4.208897	2.921565	-2.135668
C	5.857188	2.575108	-0.404287
C	4.111884	1.520987	-2.329354
C	5.788241	1.199644	-0.571161
O	6.853819	3.088154	0.423740
C	4.885400	0.650978	-1.535243
C	3.222036	0.988040	-3.302122
C	6.644815	0.273563	0.199335
C	4.727846	-0.751757	-1.713991
C	3.086201	-0.365275	-3.445050
C	7.999401	0.075703	-0.216356
C	6.156138	-0.438024	1.283101
C	3.838532	-1.241956	-2.630366
C	8.554382	0.756040	-1.335515
C	8.815189	-0.823675	0.499415
C	6.973643	-1.382100	1.982199
O	4.804578	-0.329762	1.614590
C	9.856741	0.550355	-1.702033
C	10.166707	-1.017414	0.103187
C	8.281218	-1.542507	1.600194
C	6.414584	-2.177457	3.130850
C	10.674321	-0.343914	-0.974030
O	3.252098	6.285271	-2.539262
O	-6.759071	4.413227	3.036712
O	-2.878936	-4.939667	-2.854550
O	7.217172	-5.483393	2.763515
C	6.400130	3.621066	1.647567
C	4.548826	0.496618	2.727943
C	-4.003821	0.421701	-1.640134
C	-7.467560	1.433233	-1.601954
H	10.415351	-3.787836	0.174526

H	-8.737749	-2.053963	0.758303
H	-7.918684	-5.172123	-3.049807
H	10.013938	-5.339278	-1.718752
H	-5.776030	-4.120355	-3.474214
H	-5.107055	-2.942497	1.241065
H	-4.179752	-3.514539	3.470318
H	-5.831477	0.100412	5.128054
H	-7.051644	1.648538	3.712971
H	-4.537976	-2.006585	5.406997
H	-3.873061	-2.997730	-4.138124
H	-3.525870	-1.353301	-3.497570
H	-8.944674	2.641521	0.694838
H	-8.671971	2.944262	2.440199
H	0.163084	-2.798285	-3.010174
H	-1.618217	-5.653791	-0.303334
H	2.327956	-3.011285	-1.826149
H	0.539574	-5.843087	0.911160
H	4.073668	-4.559529	-1.377049
H	1.848865	-4.413070	2.321356
H	6.199912	-4.588415	-0.096084
H	3.974525	-4.436667	3.600938
H	-4.954118	6.452363	2.419208
H	-4.987973	2.858070	0.015129
H	-2.693449	7.009175	1.545786
H	-2.728344	3.404224	-0.831485
H	-0.451101	5.955682	1.832740
H	-1.656816	5.159534	-2.232738
H	1.899099	6.225426	1.088911
H	0.691816	5.454100	-2.987333
H	5.663407	5.263837	-0.115575
H	5.413221	5.461090	-1.884458
H	3.596638	3.580972	-2.765673
H	2.644558	1.679841	-3.925952
H	5.313997	-1.435327	-1.085837
H	2.393707	-0.784093	-4.182597
H	3.678890	-2.327194	-2.721814
H	7.920808	1.455792	-1.894763
H	10.279869	1.078431	-2.563027
H	10.789932	-1.715546	0.674117
H	8.936452	-2.244338	2.134136
H	6.681809	-1.699219	4.091317
H	5.311029	-2.264616	3.075750
H	11.714403	-0.489782	-1.283579
H	7.331590	3.801061	2.189888
H	5.862876	4.567718	1.491660
H	5.762666	2.921288	2.206194
H	4.855393	1.537226	2.547877
H	3.462251	0.435103	2.826856
H	5.035056	0.128286	3.639538
H	-4.919786	1.027158	-1.716851
H	-3.230705	0.978821	-1.102955
H	-3.653666	0.162053	-2.650202
H	-8.254035	1.550696	-2.351464
H	-6.601655	0.913618	-2.037977
H	-7.147424	2.412758	-1.226472

C₆₀: (RR) -8 (1.58650426)

C	10.106431	-2.513493	2.581774
C	10.194027	-1.586688	1.579097
C	9.789899	-1.910967	0.253677
C	9.296309	-3.205638	-0.004986
C	9.214075	-4.151473	1.053450
C	9.610388	-3.811040	2.317615

H	10.420670	-2.260534	3.599831
H	10.583566	-0.580340	1.778737
C	9.868544	-0.967151	-0.816628
C	8.882420	-3.551681	-1.316309
H	8.827496	-5.154033	0.837496
H	9.548796	-4.535739	3.136055
C	8.954998	-2.651569	-2.349355
C	9.464577	-1.340972	-2.088478
H	8.479527	-4.561627	-1.495809
C	10.368220	0.395797	-0.541580
C	11.773585	0.651379	-0.593106
C	9.497535	1.431529	-0.244286
C	12.717743	-0.373022	-0.883143
C	12.245845	1.956680	-0.347367
C	9.975878	2.758187	-0.009871
C	14.057289	-0.096890	-0.921665
H	12.349927	-1.390274	-1.067481
C	13.642469	2.219169	-0.393875
C	11.326046	2.997728	-0.058937
C	14.526552	1.213923	-0.675211
H	14.780636	-0.888831	-1.142349
H	13.994446	3.239204	-0.201055
H	11.711382	4.010314	0.119340
H	15.602884	1.411235	-0.711941
O	8.121217	1.207558	-0.275858
O	9.451769	-0.399195	-3.116852
C	8.510906	-3.059527	-3.731423
H	9.110961	-3.927138	-4.071954
C	9.035882	3.893310	0.304933
H	7.972523	3.591996	0.231255
H	9.221539	4.272135	1.325664
H	9.177335	4.062795	-2.314930
C	8.801475	4.976709	-1.815256
H	9.297085	5.853306	-2.268138
O	9.270146	5.047125	-0.480008
C	7.304782	5.075453	-1.922057
C	6.537965	3.922684	-2.097501
C	6.679020	6.320670	-1.854460
C	5.155746	4.010949	-2.203955
H	7.027504	2.940922	-2.147100
C	5.297159	6.418364	-1.958513
H	7.281961	7.225360	-1.715049
C	4.530862	5.260918	-2.132630
H	4.808207	7.396733	-1.903725
H	8.635407	-2.247488	-4.470478
H	4.556835	3.104319	-2.342874
C	3.122382	5.347311	-2.231648
C	1.929286	5.404011	-2.310228
O	7.122743	-3.300325	-3.832710
C	0.567034	5.447480	-2.394241
C	-0.627836	5.466737	-2.463332
C	-2.040121	5.468470	-2.543202
C	-2.692377	6.314489	-3.446244
C	-2.783597	4.612553	-1.722769
C	-4.079176	6.296863	-3.530143
H	-2.110381	6.983499	-4.088990
C	-4.169391	4.604718	-1.809834
H	-2.273098	3.944913	-1.015044
C	-4.822539	5.443971	-2.713856
H	-4.588333	6.952811	-4.245738
H	-4.754586	3.928985	-1.175270
C	-6.320230	5.431605	-2.801590
H	-6.700692	6.245576	-3.450307

H	-6.769536	5.574143	-1.793262
C	7.583293	0.843880	0.978134
H	8.050567	-0.066111	1.376726
H	7.674707	1.655058	1.710095
H	6.531426	0.661954	0.744667
C	10.660968	-0.343804	-3.843745
H	11.519067	-0.110775	-3.199550
H	10.852984	-1.277067	-4.386242
H	10.480507	0.471510	-4.548365
C	-9.953793	-0.067983	-0.822489
C	-9.468631	1.327365	-0.846066
C	11.351132	-0.325105	-0.981606
C	-9.079654	-1.130024	-0.660005
C	-9.438433	2.077611	0.369771
C	-9.036199	1.916457	-2.023757
C	12.300335	0.724333	-1.131847
C	11.810425	-1.657713	-0.984429
C	-9.543692	-2.482620	-0.684678
O	-7.708634	-0.886514	-0.570112
C	-9.873086	1.528055	1.608442
C	-8.963326	3.404504	0.348416
C	-8.551682	3.261792	-2.045247
O	-8.969476	1.160417	-3.193601
C	13.632206	0.445541	-1.275673
H	11.943346	1.761901	-1.121578
C	13.198995	-1.922447	-1.136868
C	10.885484	-2.723738	-0.838334
C	-8.592266	-3.640360	-0.526930
C	-7.248056	-0.797636	0.762148
C	-9.829882	2.272502	2.755566
H	10.249741	0.497381	1.623285
C	-8.926931	4.158018	1.553659
C	-8.524200	3.974816	-0.873212
C	-8.087317	3.909039	-3.325630
C	10.151679	1.207667	-3.964080
C	14.088227	-0.892730	-1.279530
H	14.359550	1.256425	-1.387641
H	13.540758	-2.963952	-1.137758
H	11.261125	-3.755393	-0.856302
H	-7.533050	-3.323882	-0.600661
H	-8.744147	-4.128871	0.451978
O	-8.842998	-4.703345	-1.426484
H	-7.735505	0.020865	1.307692
H	-7.391789	-1.738754	1.306673
H	-6.179134	-0.592236	0.642301
C	-9.350512	3.602565	2.729693
H	10.167227	1.846467	3.706280
H	-8.553386	5.187901	1.521982
H	-8.139165	5.007451	-0.868557
H	-8.690860	4.818027	-3.521027
H	-8.188640	3.238181	-4.197829
O	-6.700822	4.175884	-3.355752
H	11.024430	0.850038	-3.401918
H	10.350462	2.216205	-4.345607
H	-9.926575	0.529644	-4.790774
H	15.158487	-1.091655	-1.396743
C	-8.411023	-4.483569	-2.758173
H	-9.324053	4.178513	3.660499
H	-8.812620	-3.527759	-3.147163
H	-8.906822	-5.314725	-3.289614
C	-6.916460	-4.545445	-2.910918
C	-6.169379	-3.368060	-2.969836
C	-6.272678	-5.780222	-2.997494

C	-4.788097	-3.421929	-3.106619
H	-6.673081	-2.394896	-2.901369
C	-4.891489	-5.843719	-3.132565
H	-6.860483	-6.704323	-2.952785
C	-4.144310	-4.662075	-3.182450
H	-4.204348	-2.496042	-3.151523
H	-4.387987	-6.814152	-3.196258
C	-2.734888	-4.714410	-3.291507
C	-1.540203	-4.741833	-3.361235
C	-0.175778	-4.751458	-3.415753
C	1.020875	-4.741888	-3.443849
C	2.435053	-4.715860	-3.464898
C	3.134293	-5.372894	-4.482674
C	3.132930	-4.026232	-2.466692
C	4.523061	-5.336745	-4.500103
H	2.587554	-5.909612	-5.265265
C	4.521241	-3.999183	-2.489485
H	2.584176	-3.505864	-1.669719
C	5.221578	-4.653418	-3.504338
H	5.069437	-5.844536	-5.303367
H	5.071682	-3.454466	-1.713720
C	6.721747	-4.630399	-3.518596
H	7.134864	-5.325722	-4.276456
H	7.124920	-4.942080	-2.529123
C	0.781248	-3.307768	0.982330
C	1.423963	-3.452211	2.282355
C	-0.591290	-3.445279	0.870947
C	1.470371	-2.249697	0.253173
C	2.508788	-2.482049	2.358622
C	0.662361	-3.728352	3.404534
C	-1.349251	-2.530942	0.026280
C	-1.393558	-3.736163	2.052471
C	2.536763	-1.737994	1.105727
C	0.748876	-1.379632	-0.546336
C	2.777416	-1.836975	3.553282
C	0.945121	-3.048829	4.662443
C	-0.782984	-3.874182	3.286631
C	-0.696568	-1.525072	-0.664228
C	-2.620121	-2.256906	0.685160
C	-2.647317	-3.001605	1.937648
C	2.830845	-0.385615	1.111171
C	1.059000	0.044467	-0.541213
C	1.975382	-2.127634	4.734939
C	3.087603	-0.412991	3.558743
C	-0.325429	-2.774563	5.321908
C	-1.393527	-3.284601	4.471537
C	-1.279910	-0.191139	-0.732224
C	-3.174557	-0.990601	0.620096
C	-3.227232	-2.442115	3.062693
C	3.113561	0.293905	2.369253
C	2.073275	0.528751	0.266053
C	-0.194843	0.778905	-0.655948
C	1.789807	-0.883242	5.470693
C	2.477292	0.176510	4.743762
C	-0.501615	-1.592945	6.020520
C	-2.583923	-2.587145	4.362444
C	-2.486473	0.069149	-0.106436
C	-3.786788	-0.401138	1.804660
C	-3.810259	-1.108073	2.994768
C	2.530489	1.628074	2.301634
C	1.887586	1.773199	1.001774
C	-0.371027	1.960620	0.042203
C	0.583395	-0.622808	6.096848

C	1.923574	1.443210	4.679430
C	-1.755228	-0.858492	5.905627
C	-2.769400	-1.342738	5.097949
C	-2.671752	1.313249	0.629494
C	-3.474289	1.022844	1.810818
C	-3.527204	-0.428681	4.252693
C	1.950998	2.187900	3.426860
C	0.696957	2.470166	0.893059
C	-1.642544	2.236602	0.700245
C	0.000309	0.711221	6.029213
C	0.653037	1.717498	5.338830
C	-1.445048	0.565568	5.911012
C	-3.205434	1.667967	3.005304
C	-3.232721	0.923531	4.257926
C	0.697380	2.922378	3.312093
C	0.086542	3.059633	2.077864
C	-1.358822	2.914125	1.959637
C	-0.104834	2.631619	4.493668
C	-2.164670	1.433529	5.108456
C	-2.120500	2.638137	3.081596
C	-1.477260	2.493266	4.381407

C₆₀: (RR) -9 (1.34900475)

C	8.798097	2.332308	3.828862
C	9.282734	1.384450	2.968640
C	8.540045	0.201486	2.700352
C	7.294502	0.024225	3.335366
C	6.811787	1.023163	4.223993
C	7.548442	2.151098	4.463906
H	9.374856	3.239775	4.036253
H	10.256046	1.517111	2.479471
C	9.018668	-0.808871	1.808740
C	6.528828	-1.144787	3.082125
H	5.842968	0.871836	4.713826
H	7.181067	2.921884	5.149333
C	6.990236	-2.124637	2.243034
C	8.263224	-1.950908	1.608639
H	5.552876	-1.241190	3.576875
C	10.298472	-0.607249	1.098941
C	11.520838	-1.017592	1.715525
C	10.329424	-0.042447	-0.165399
C	11.556044	-1.576439	3.023595
C	12.732866	-0.861251	1.012735
C	11.555915	0.090201	-0.888317
C	12.743816	-1.954309	3.588355
H	10.612751	-1.689905	3.572997
C	13.954028	-1.263392	1.619898
C	12.726701	-0.309789	-0.294888
C	13.957028	-1.797907	2.879231
H	12.767137	-2.380950	4.596746
H	14.888410	-1.137897	1.060380
H	13.680290	-0.214347	-0.831588
H	14.894951	-2.108931	3.351008
O	9.135099	0.308007	-0.795655
O	8.671506	-2.911509	0.682610
C	6.208752	-3.374350	1.944654
H	6.704418	-4.251145	2.407926
C	11.583290	0.673095	-2.275593
H	10.569439	0.786394	-2.707492
H	12.068788	1.665877	-2.262104
C	11.919362	-1.104510	-3.871917
O	12.425401	-0.053750	-3.156038
C	10.478640	-1.474574	-3.885766

C	10.032642	-2.542373	-3.108094
C	9.589590	-0.769580	-4.698036
C	8.686839	-2.889421	-3.117788
H	10.736789	-3.099725	-2.479655
C	8.244523	-1.116232	-4.714384
H	9.950248	0.055997	-5.321841
C	7.788558	-2.169838	-3.913618
H	7.541660	-0.562835	-5.346426
H	6.143336	-3.542373	0.852920
H	8.329066	-3.712934	-2.489486
C	6.412124	-2.496175	-3.886623
C	5.246930	-2.764553	-3.830909
O	4.832038	-3.292107	2.273248
C	3.918974	-3.068241	-3.733607
C	2.757456	-3.333704	-3.618727
C	1.389741	-3.651360	-3.448192
C	0.938713	-4.955044	-3.684742
C	0.492471	-2.666484	-3.021181
C	-0.397089	-5.272991	-3.475713
H	1.638868	-5.723702	-4.030006
C	-0.841645	-2.989855	-2.808825
H	0.836239	-1.638665	-2.843556
C	-1.287431	-4.294995	-3.025002
H	-0.753724	-6.293093	-3.663982
H	-1.533769	-2.209724	-2.461190
C	-2.705463	-4.674153	-2.782422
C	8.770426	1.656362	-0.587840
H	8.661233	1.893758	0.478499
H	9.489856	2.345106	-1.046510
H	7.804840	1.725335	-1.094415
C	9.506042	-3.908943	1.233284
H	10.405591	-3.485113	1.698678
H	8.971152	-4.527920	1.963302
H	9.774947	-4.504268	0.357049
C	-9.035149	-2.056072	-0.815551
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References:

S1: E. A. Johnson, *J. Chem. Soc.* **1957**, 4155-4156.

S2: B. Williamson, W. H. Rodebush, *J. Am. Chem. Soc.* **1941**, *63*, 3018–3025.

S3: A. S. Batsanov, J. C. Collings, I. J. S. Fairlamb, J. P. Holland, J. A. K. Howard, Z. Lin, T. B. Marder, A. C. Parsons, R. M. Ward, J. Zhu, *J. Org. Chem.* **2005**, *70*, 703-706.

S4: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, *Gaussian 03, Revision B.02*, Gaussian, Inc., Pittsburgh PA, 2003.