Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

Structurally-Variable, Rigid and Optically-Active D_2 and D_3 Macrocycles Possessing Recognition Properties towards C_{60}

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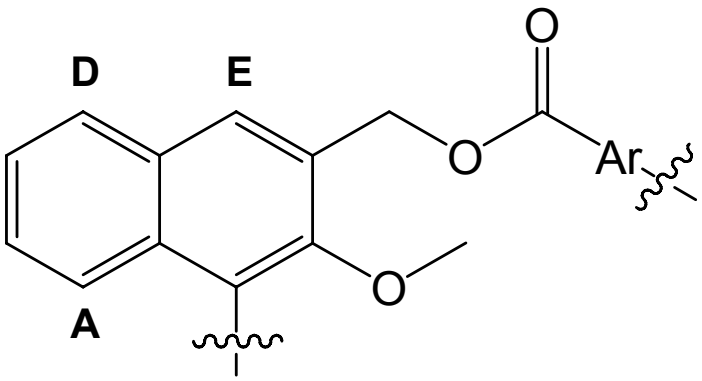
Contents:

Table S1. Crystal data for investigated crystals.

	3b	**3c**
Formula	$C_{70}H_{60}O_{14}$	$C_{70}H_{60}O_{14}$
M	1125.18	1125.18
Colour	colorless	colorless
Dimension [mm]	0.43 x 0.36 x 0.15	0.86 x 0.58 x 0.43
Crystal system	monoclinic	monoclinic
Space group	$P\,2_1$ (no.4)	$P\,2_1$ (no.4)
a [Å]	10.423(2)	11.414 (2)
b [Å]	10.230(3)	20.620(3)
c [Å]	27.358(6)	12.643(4)
β [°]	93.50(2)	91.47(2)
V [Å³]	2911.7(12)	2974.7(11)
Z	2	2
ρ_{calcd} [g cm^{-3}]	1.283	1.256
μ $Mo_{K\alpha}$ [mm^{-1}]	0.089	0.087
Scan type	ω scans	ω scans
θ range [°]	1.5 - 25.1	1.5 - 25.1
Measured reflections	5970	6900
Unique reflections	5506	5419
R_{int}	0.038	0.015
Strong data [$I_O>2\sigma(I_O)$]	2935	3884
Refined parameters	754	757
R1, wR2 (strong data)	0.0689, 0.1588	0.0482, 0.1202
R1, wR2 (all data)	0.1470, 0.1980	0.0760, 0.1371
GOF	1.045	1.031
Max / min residuals [eÅ^{-3}]	0.20 / -0.24	0.22 / -0.13

Table S2. Selected ^{1}H NMR chemical shifts for precursor **1** and macrocycles **3** and **4** in $CDCl_3$ at room temperature.[a]



Compound	BINOL-A	BINOL-D	BINOL-E	CH_2	OMe
1[b]	7.15(d)	7.89 (d)	8.03 (s)	4.98 (dd)	3.30 (s)
3a[b]	7.02 (d)	7.95 (d)	8.03 (s)	5.63 (dd)	2.88 (s)
3b	7.08 (d)	7.83 (d)	8.04 (s)	5.62 (dd)	3.24 (s)
3c[b]	7.10 (d)	7.95 (d)	8.19 (s)	5.63 (dd)	3.48 (s)
3d	N.D.[c]	7.94 (d)	8.00 (s)	5.64 (dd)	3.14 (s)
4a[b]	7.06 (d)	N.D.[c]	8.08 (d)	5.49(cdd)	3.07 (s)
4b	7.19 (d)	7.79 (d)	8.08 (s)	5.67(cdd)	3.30 (s)
4c[b]	7.10 (d)	7.93 (d)	8.13 (d)	5.68 (cdd)	3.34 (s)

[a] Spectra taken either at 200 MHz or 300 MHz with 5-10 mM sample concentration in $CDCl_3$. Peak multiplicity as follows: s singlet, bs broad singlet, d doublet, dd double doublet (AB system), cdd collapsed double doublet. [b] Data taken from reference 11. [c] Not unequivocally assigned.

Figure S1. ^{1}H NMR spectra ($CDCl_3$, 300 MHz, room temperature) of macrocycles a) **3c**; b) **3a**; c) **3b**; d) **3d**.

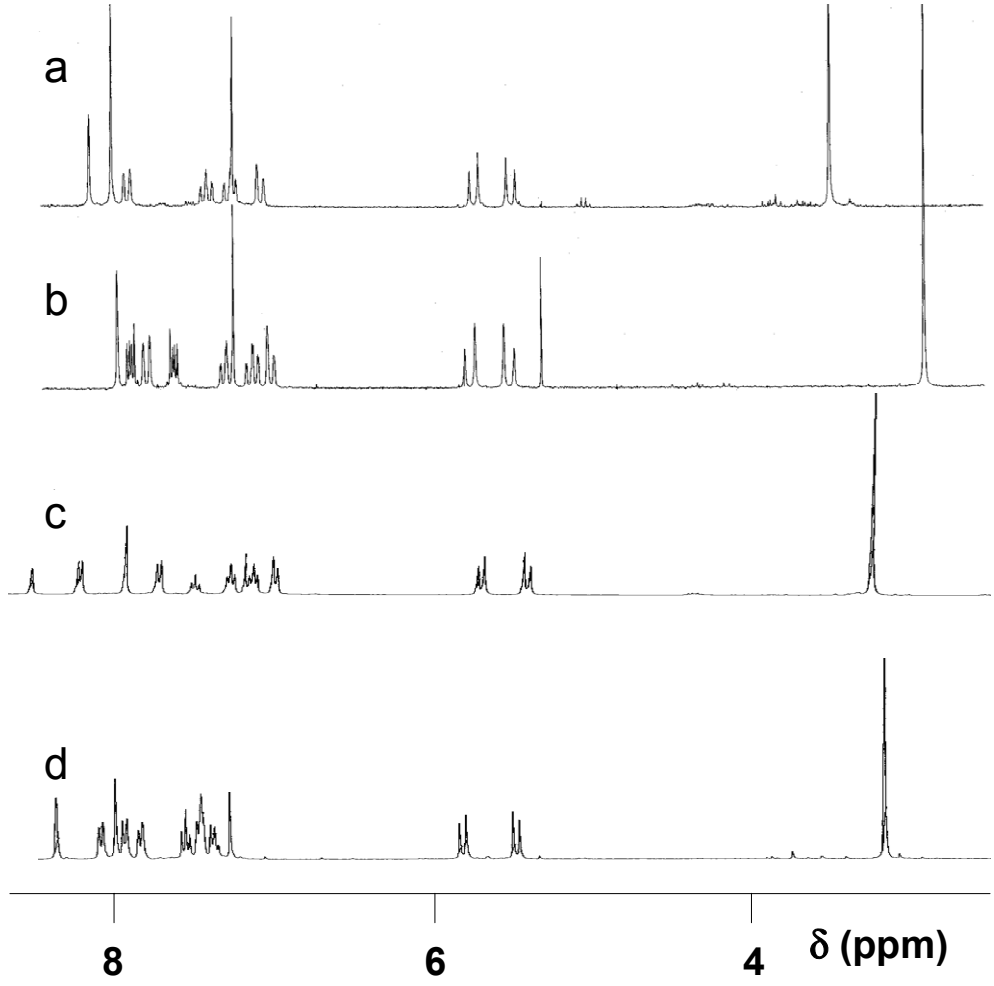


Figure S2. ^{1}H NMR spectra (toluene-d_8, 300 MHz, room temperature) of **3c** (10^{-3} M) in the presence of C_{60} (a: 0; b: 3 x 10^{-4} M; c: 5.3 x 10^{-4} M; d: 1.2 x 10^{-3} M).

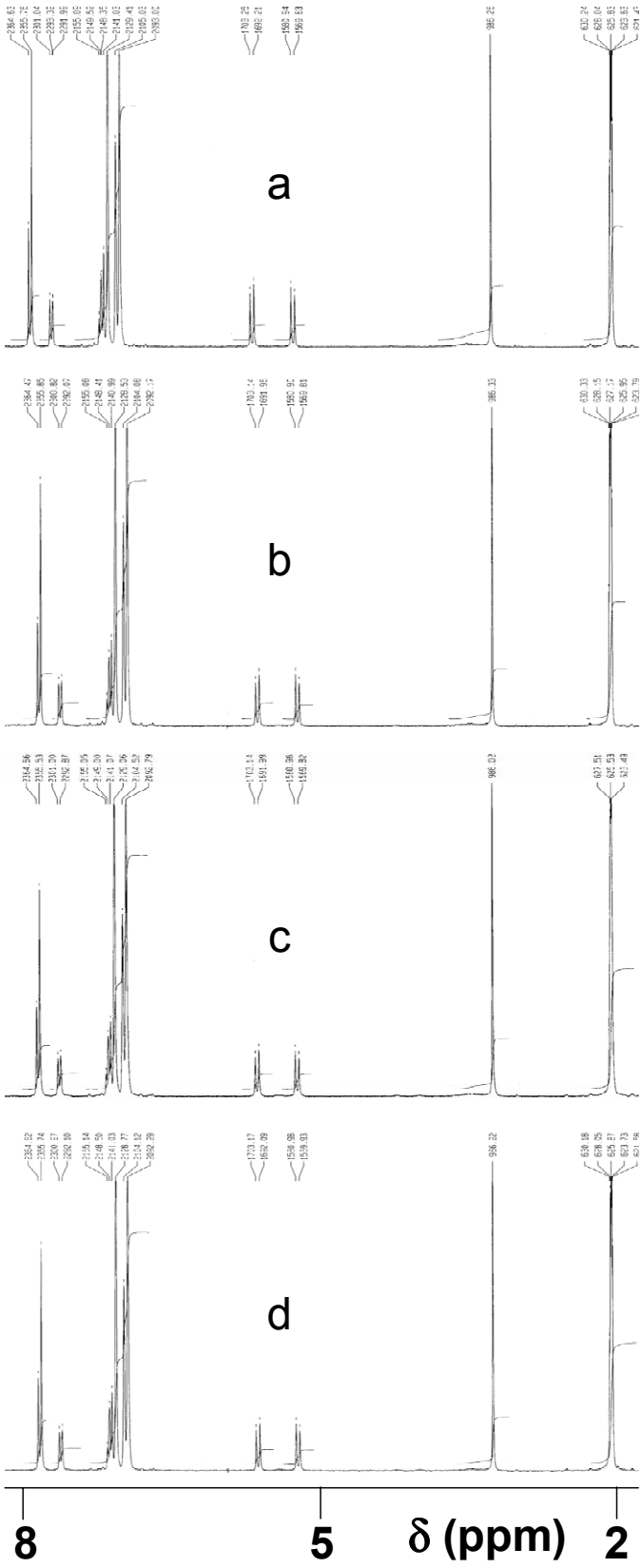

a
b
c
d
8
5
δ (ppm)
2

Figure S3. ^{1}H NMR spectra (toluene-d_8, 300 MHz, room temperature) of **4c** (10^{-3} M) in the presence of C_{60} (a: 0; b: 1.7 x 10^{-3} M; c: 3.2 x 10^{-3} M; d: 6.9 x 10^{-3} M).

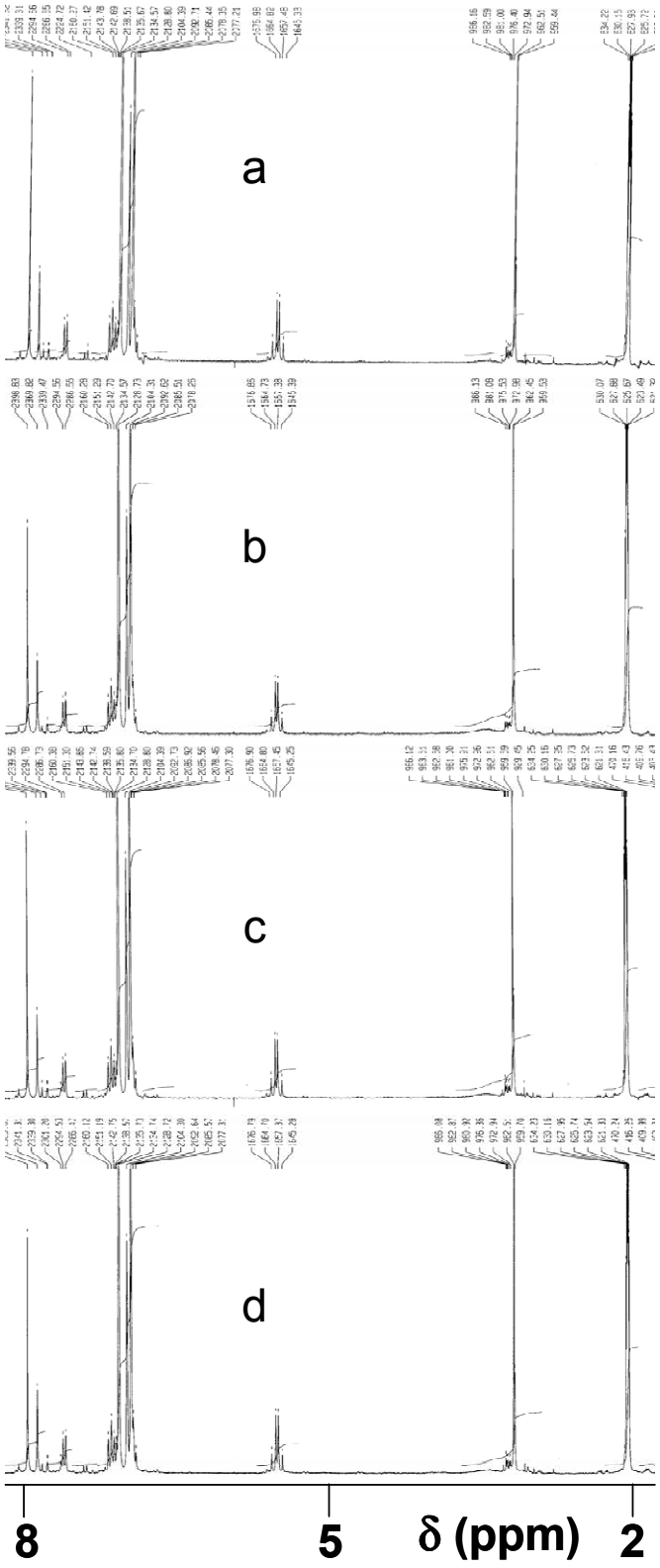
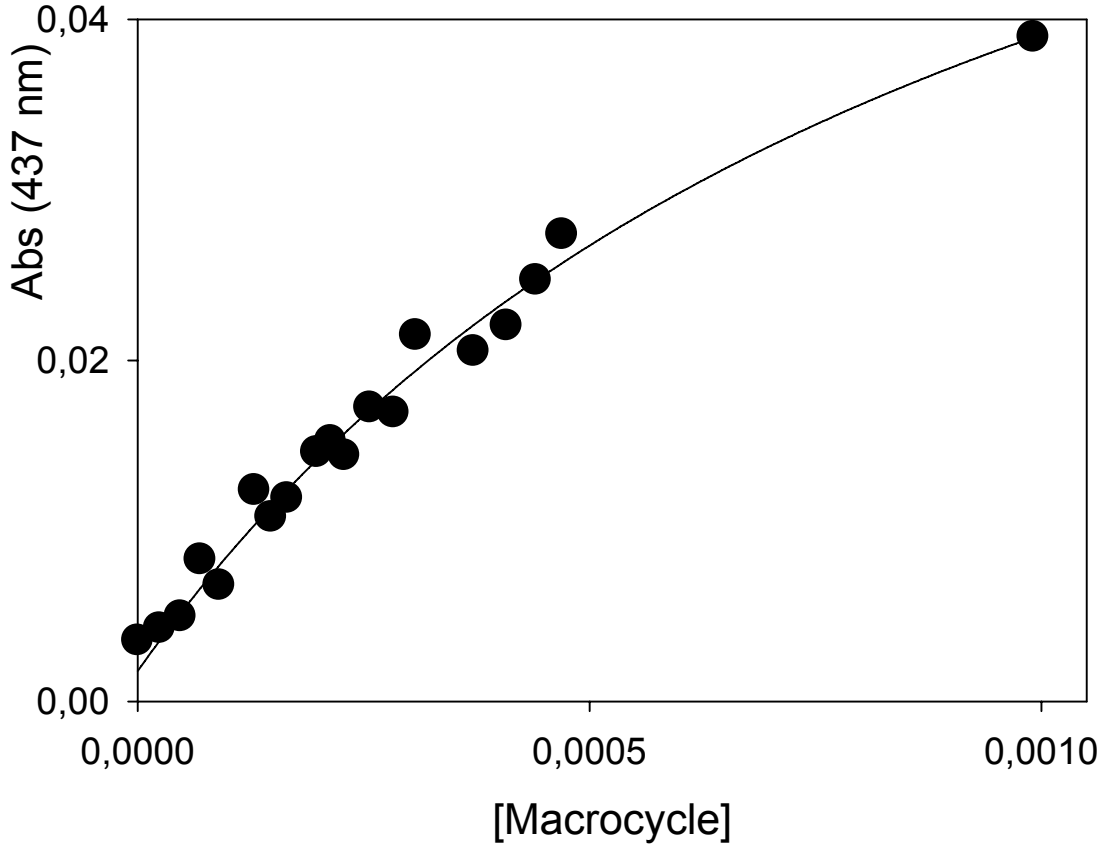


Figure S4. Best fitting and related parameters for the titration reported in Figure 5 (including titration endpoint, toluene, C_{60} constant at 5 10^{-5} M).



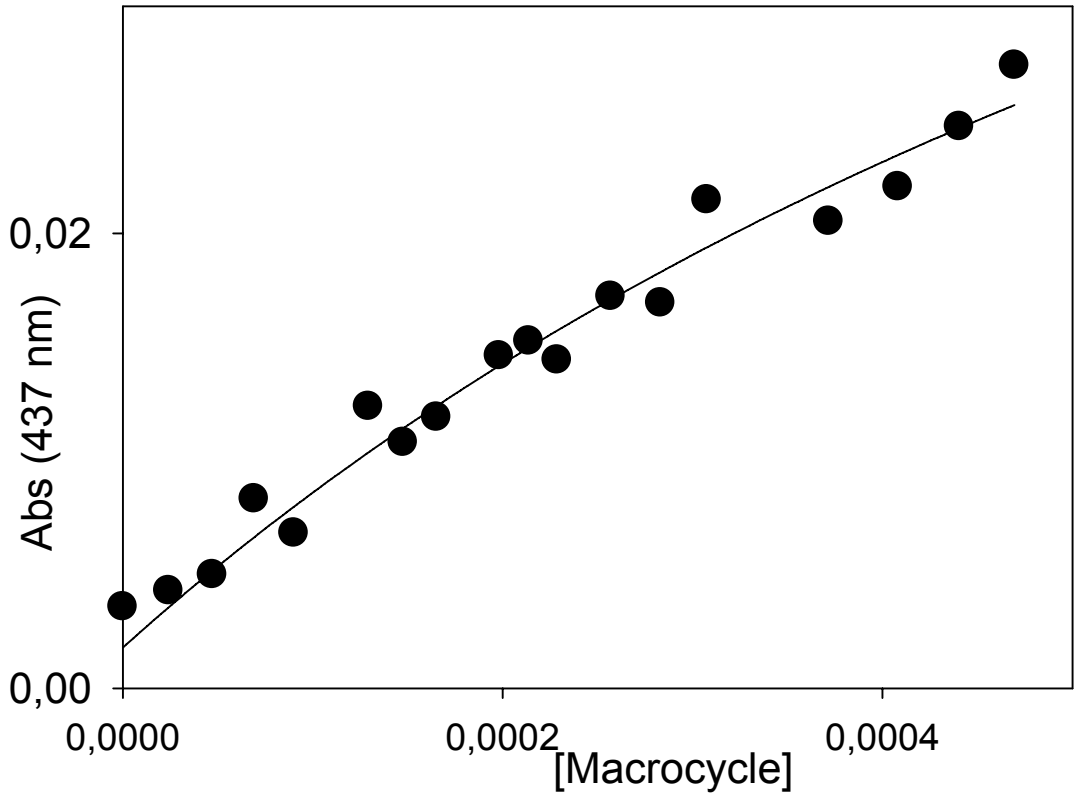
Nonlinear Regression

Data Source: Data 1 in titolazione4creplicaSIinset.JNB
Equation: User-Defined; Untitled
f=(E-15)*((k*(0,00005+x)+1)-((k*(0,00005+x)+1)^2-4*(k^2)*0,00005*x)^(0.5))/(2*k)+0,00005*15

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0,9901	0,9804	0,9792	0,0013

		Std. Error
Calcd ε	1491,9284	148,4209
Calcd K_a	1079,1666	164,4081

Figure S5. Best fitting and related parameters for the titration reported in Figure 5 (without titration endpoint, toluene, C_{60} constant at 5 x 10^{-5} M).



Nonlinear Regression

Data Source: Data 1 in titolazione4creplicaSIinset-finalpoint.JNB

Equation: User-Defined; Untitled

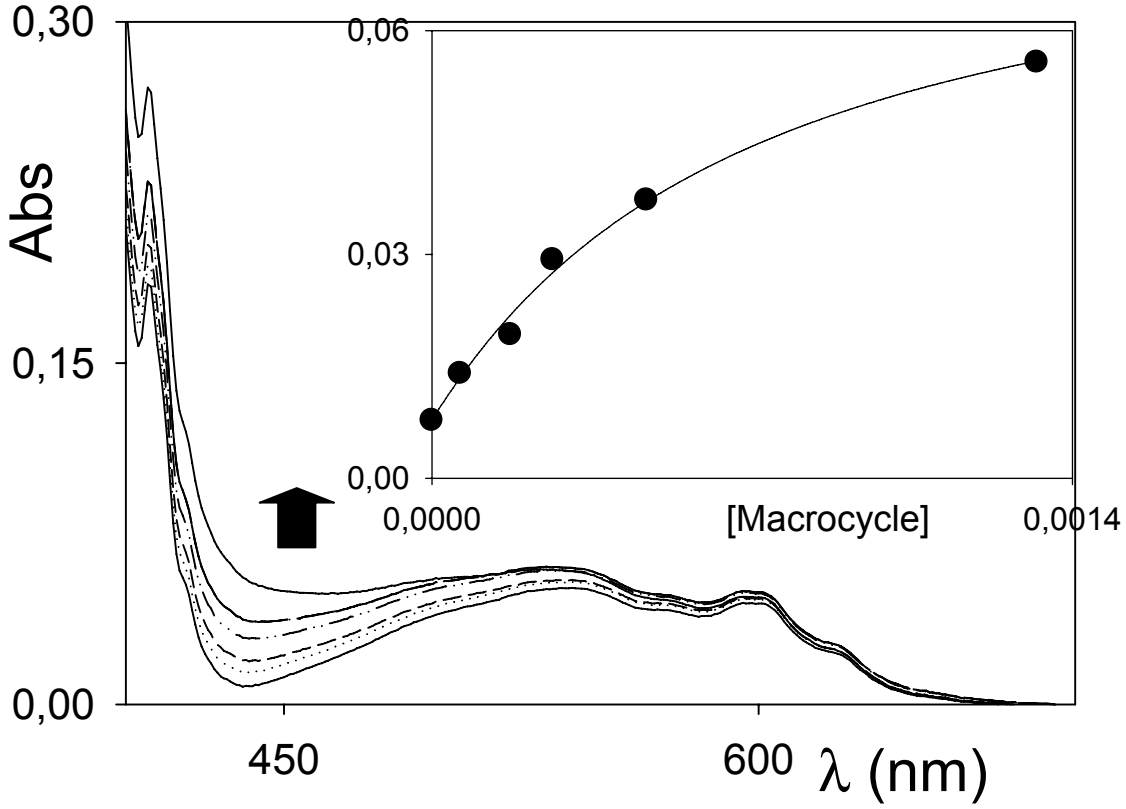
f=(E-15)*((k*(0,00005+x)+1)-((k*(0,00005+x)+1)^2-4*(k^2)*0,00005*x)^(0.5))/(2*k)+0,00005*15

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0,9835	0,9673	0,9652	0,0013

		Std. Error
Calcd ε	1466,5863	369,7897

Calcd K_a	1105,2024	395,3416

Figure S6. Replicate titration of macrocycle **4c** with C_{60} (toluene, C_{60} constant at 10^{-4} M, inset absorbance taken at 437 nm).



Nonlinear Regression

Data Source: Data 1 in titolazione4crep.JNB

Equation: User-Defined; Untitled

f = ((E-15)*((k*(0,0001+x)+1)-((k*(0,0001+x)+1)^2-4*(k^2)*0,0001*x)^(0.5))/(2*k))+0,0001*15

R = 0,99663547 Rsqr = 0,99328226 dj Rsqr = 0,99160283

Coefficient		Std. Error
Calcd ε	1103,7146	76,0135
Calcd K_a	1263,7541	354,7808

Figure S7. End point titration curve (broken line, C_{60} 10^{-4} M, macrocycle **4b** 1.02 x 10^{-3} M) vs C_{60} only (continuous line, C_{60} 10^{-4} M) for the experiment reported in Figure 6.

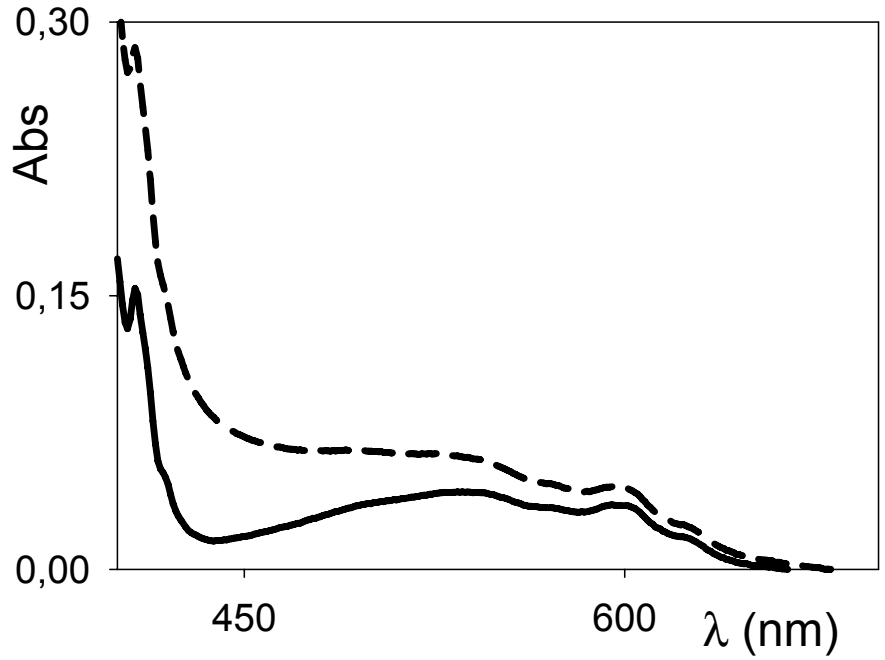
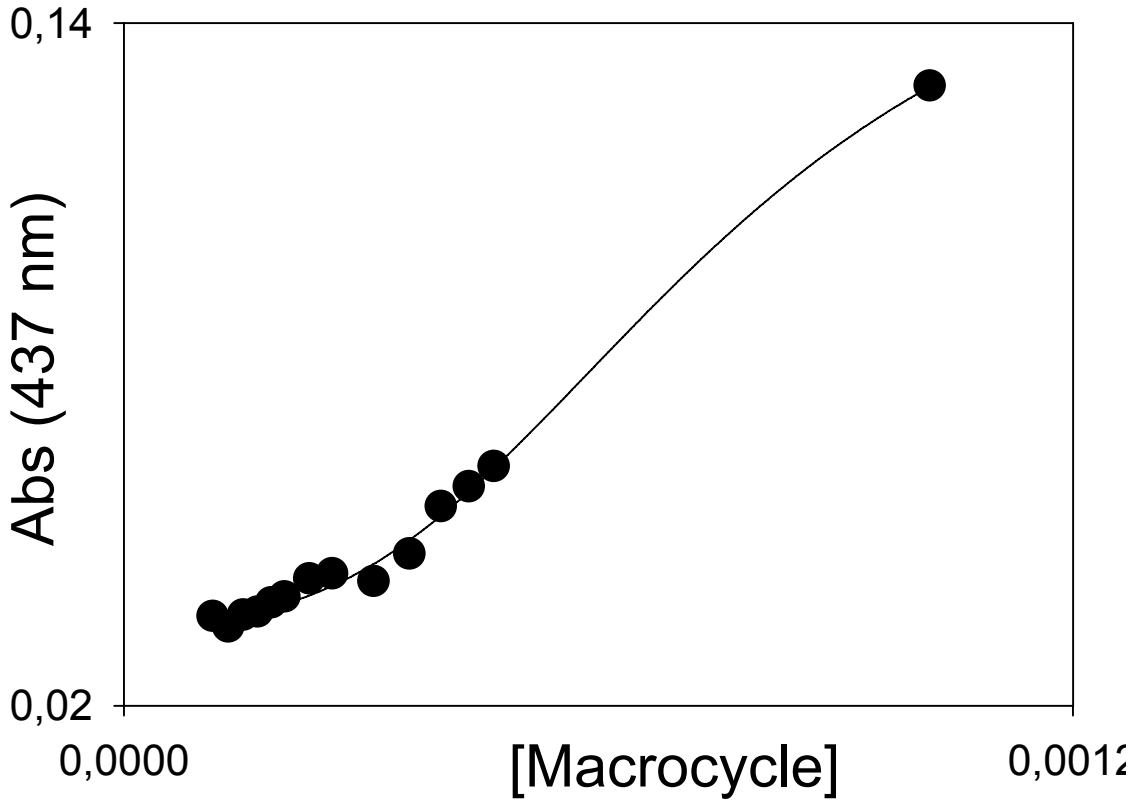


Figure S8. Best Fitting including end point titration for experiment reported in Figure 6 (fullerene 10^{-4} M, macrocycle **4b** 0-1.02 x 10^{-3} M, 0-10 equivalents).

(see experimental section for parameter explanation)



Nonlinear Regression

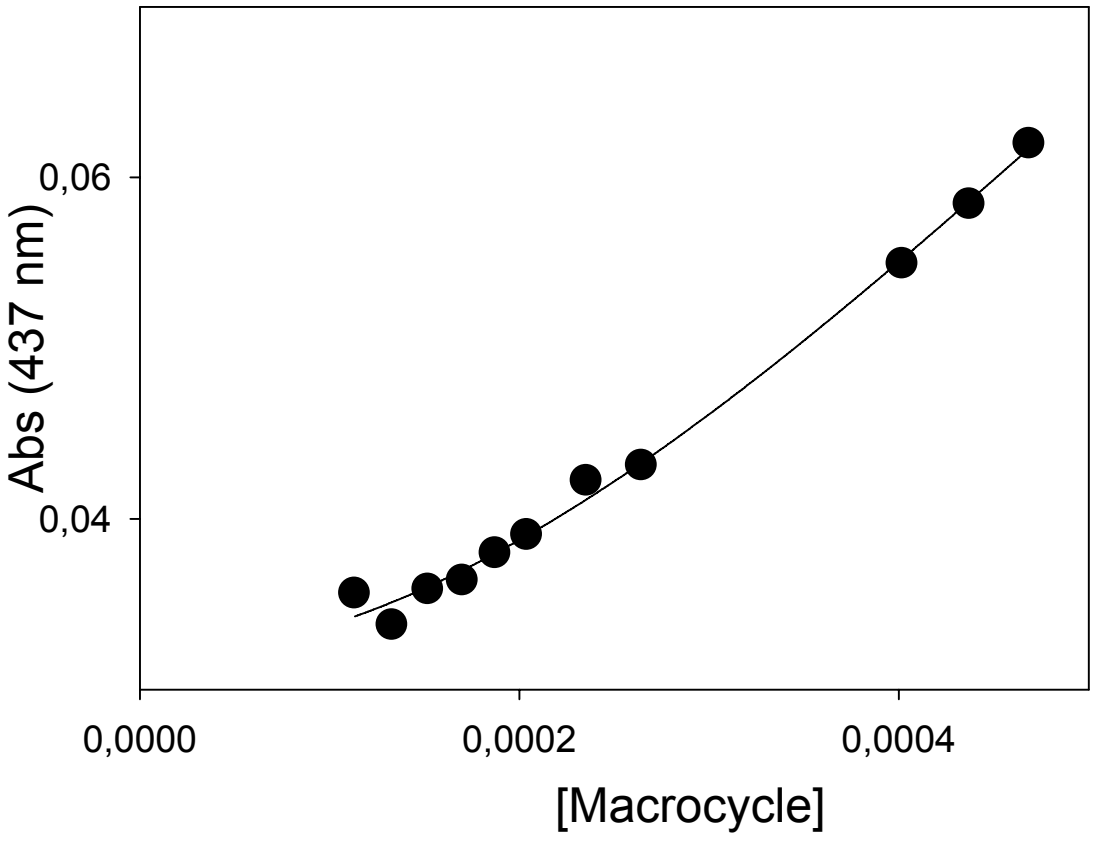
Data Source: Data 1 in titolazione4bhillfitting-2.JNB
Equation: Sigmoidal; Hill, 4 Parameter
f=y0+a*x^b/(c^b+x^b)

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0,9976	0,9951	0,9937	0,0019

	Coefficient	Std. Error
a	0,1323	0,0320
b	2,9090	0,6294
c	0,0008	0,0002
y0	0,0351	0,0014

Figure S9. Fitting for the experiment reported in Figure 6 without end point (fullerene 10^{-4} M, macrocycle **4b** 0-4.6 x 10^{-3} M, 0-4.6 equivalents).

(see experimental section for parameter explanation)



Nonlinear Regression

Data Source: Data 1 in titolazione4bhillfitting-some points-endpoint SI.JNB
Equation: Sigmoidal; Hill, 4 Parameter
f=y0+a*x^b/(c^b+x^b)

R	**Rsqr**	**Adj Rsqr**	**Standard Error of Estimate**
0,9973	0,9947	0,9924	0,0009

	Coefficient	**Std. Error**
a	0,1493	0,0949

b	1,9360	0,1498
c	0,0010	0,0002
y0	0,0319	0,0025

Figure S10. Control titration of macrocycle **3c** with C_{60} (Toluene, C_{60} constant at 2 x 10^{-4} M).

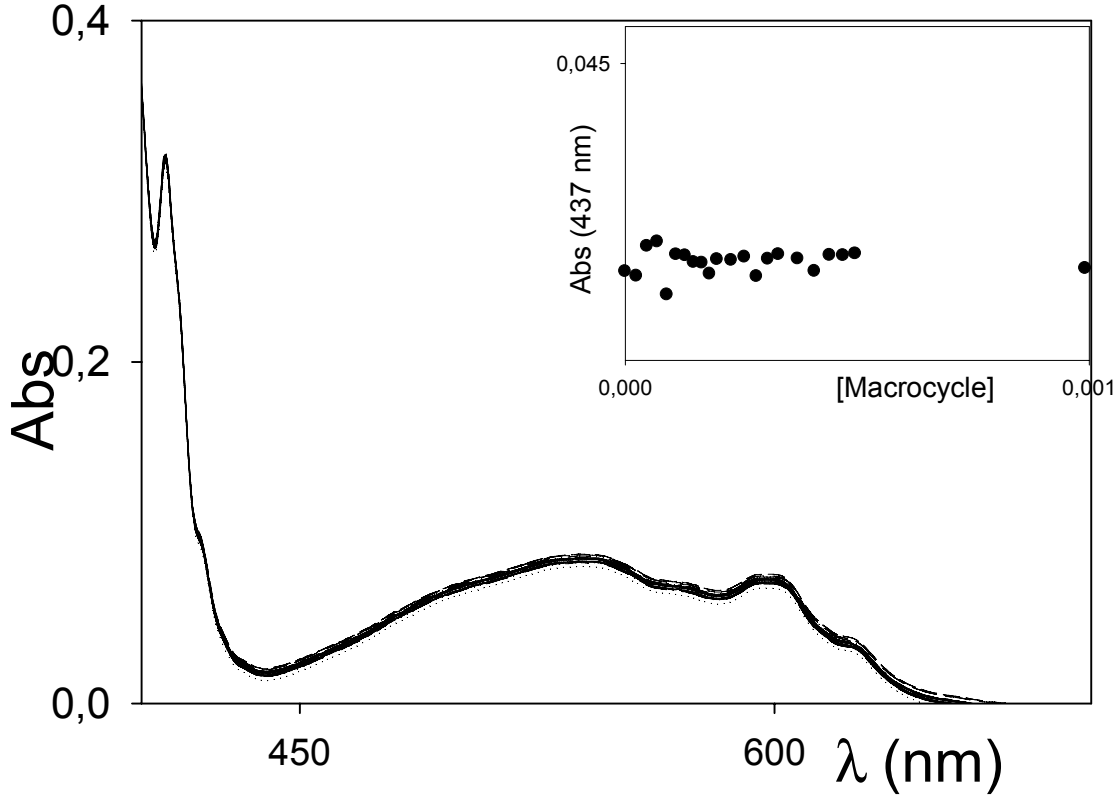


Figure S11. Control titration of terephthalic acid dimethyl ester with C_{60} (Toluene, C_{60} constant at 5 x 10^{-5} M).

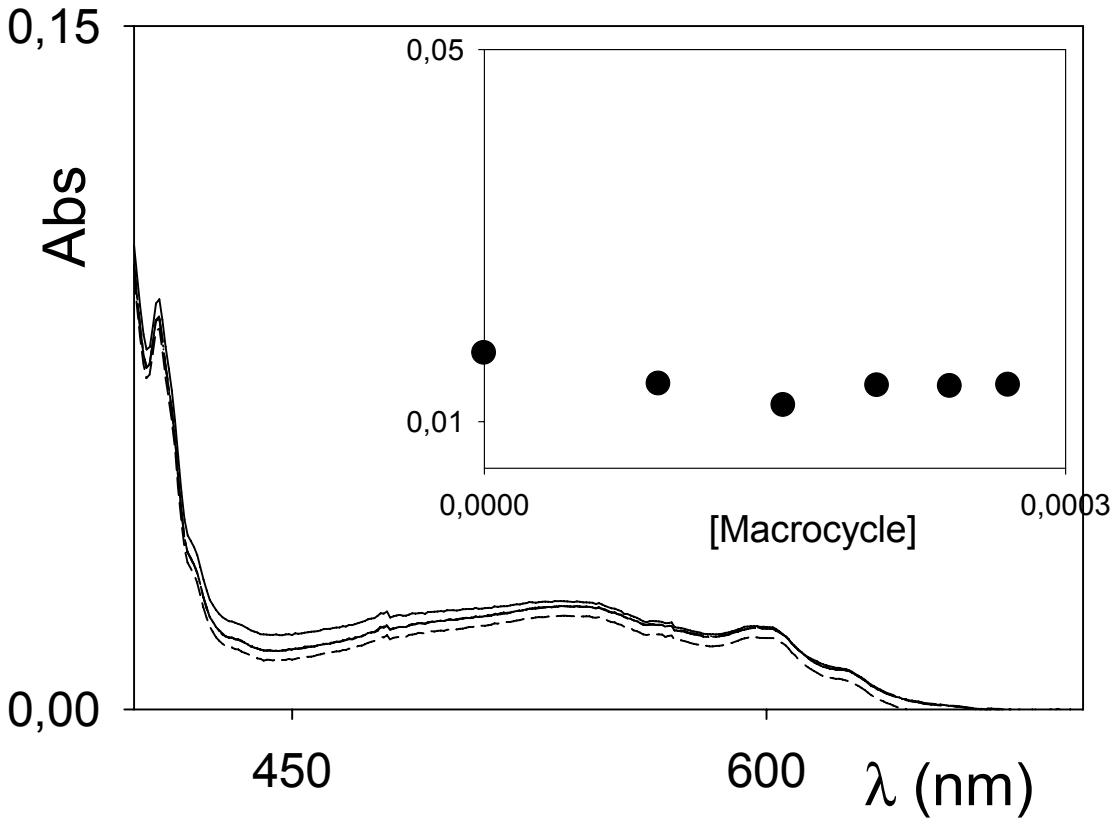


Figure S12. Control titration of 2,2'-dimethoxy-1,1'-binahpthyl with C_{60} (Toluene, C_{60} constant at 5 x 10^{-5} M).

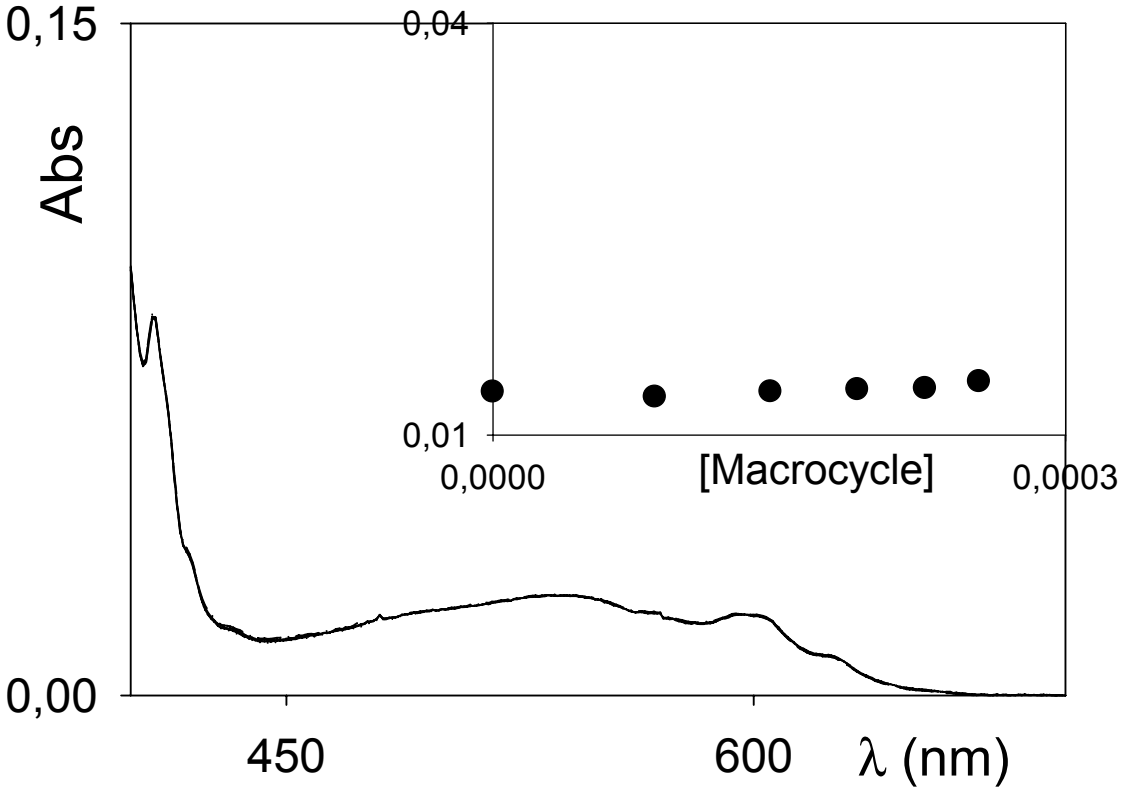
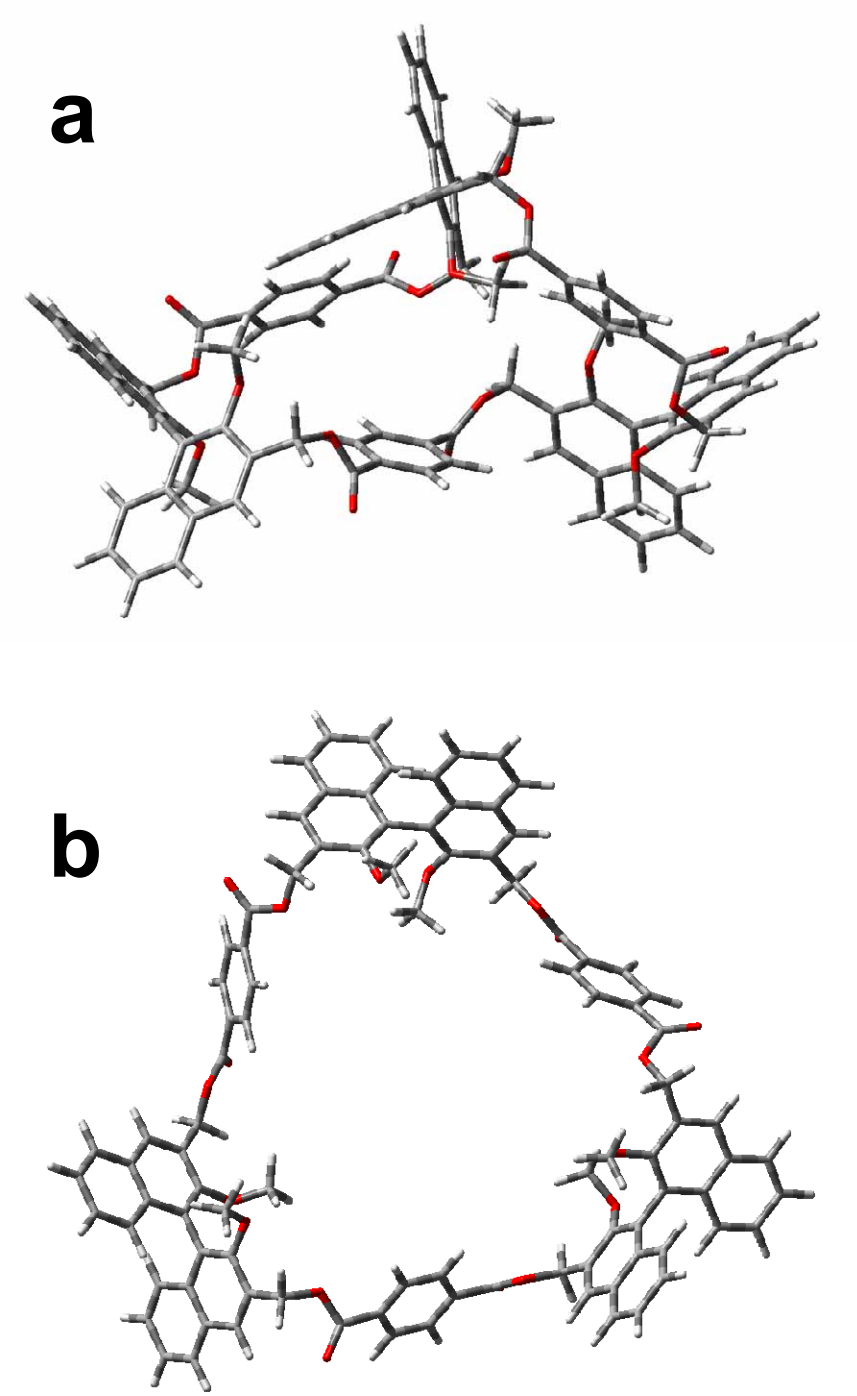
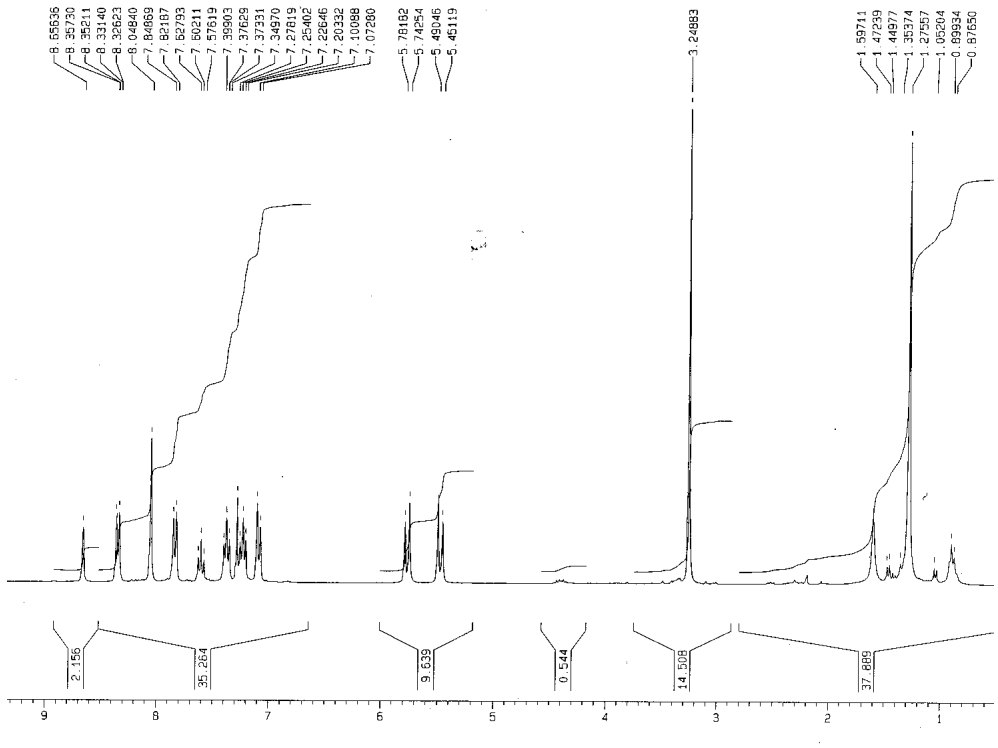


Figure S13. Optimized conformers of **4c**. a) collapsed structure; b) open structure.

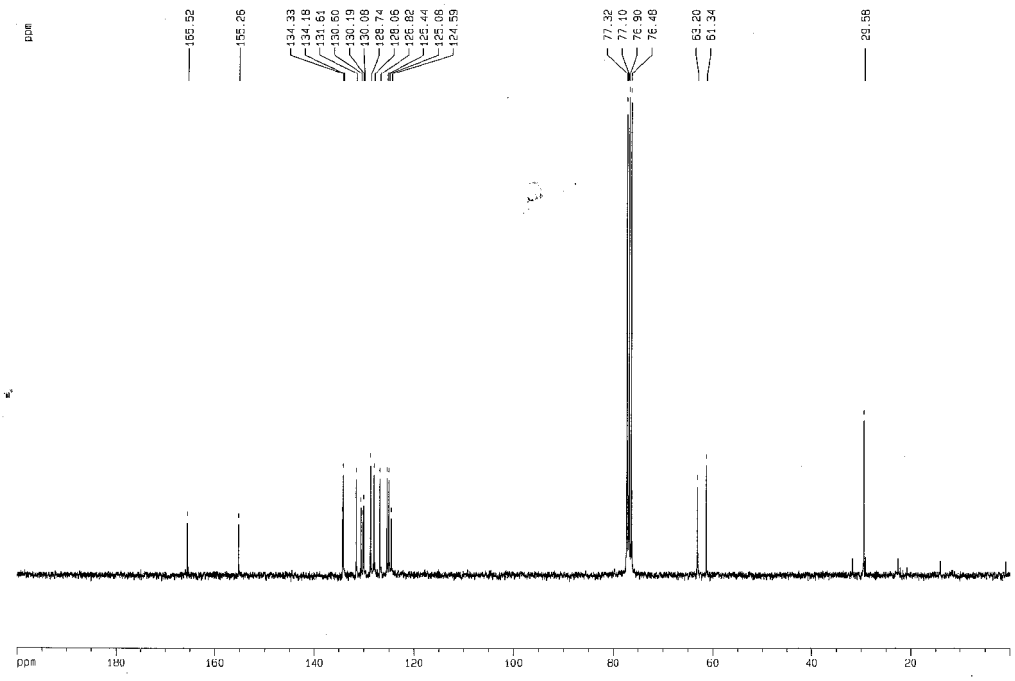


*Macrocycle **3b**.*

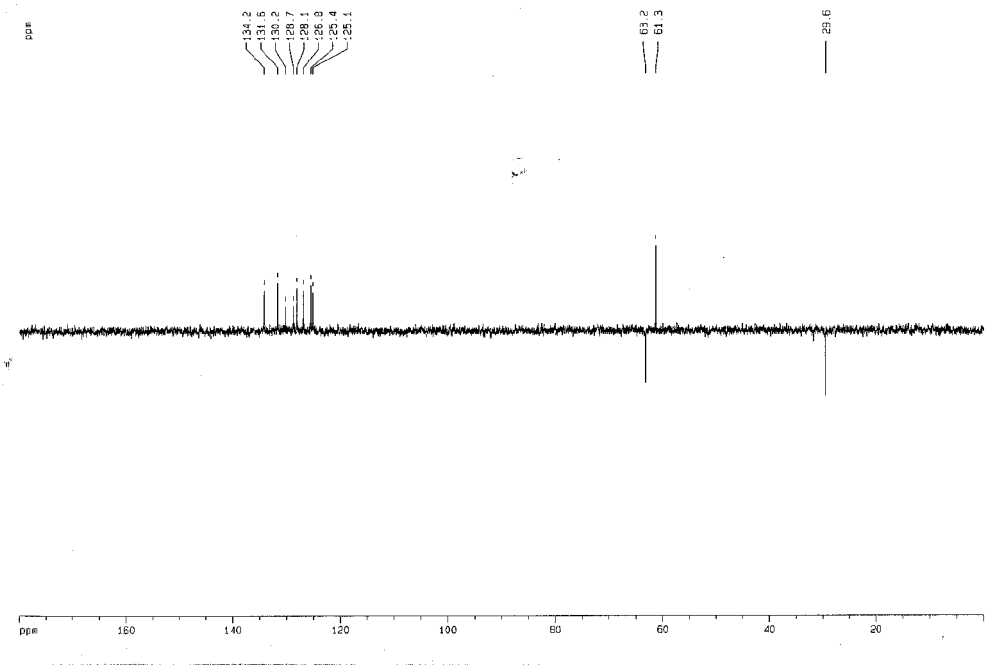
^{1}H NMR ($CDCl_3$, 300 MHz)



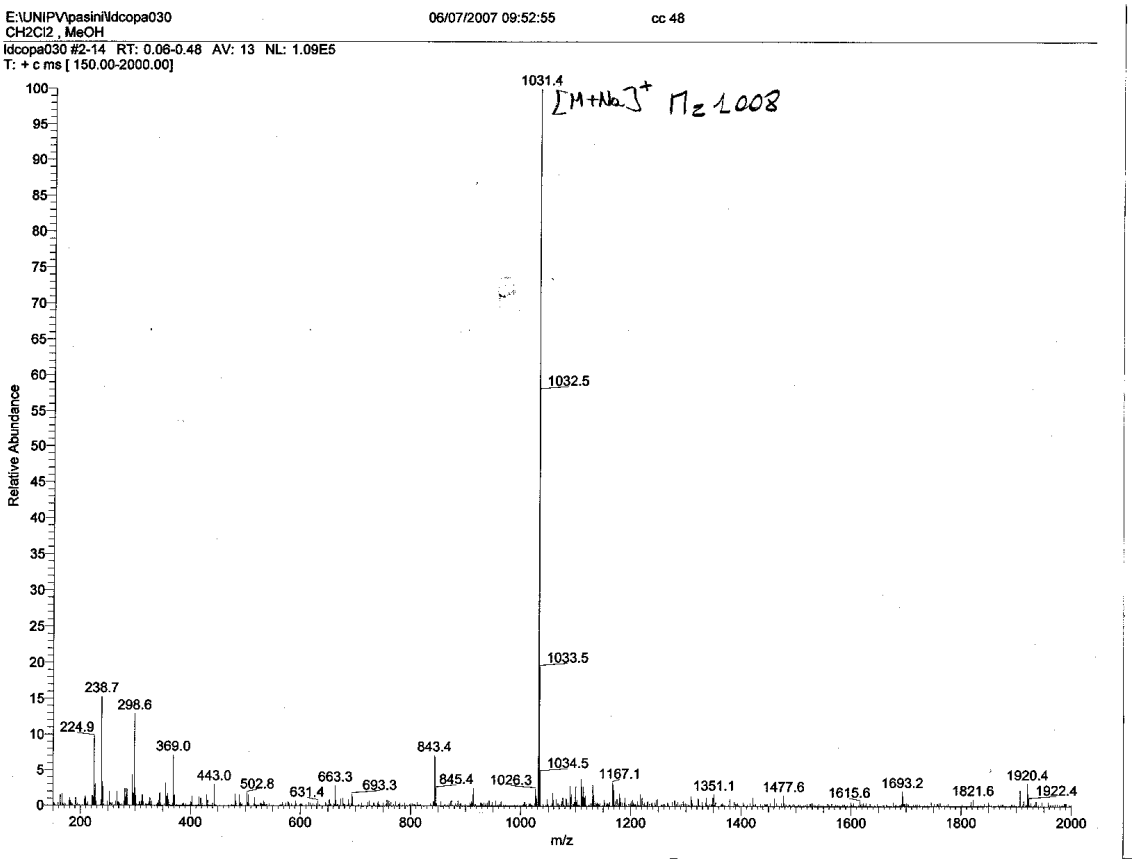
^{13}C NMR ($CDCl_3$, 75 MHz)



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

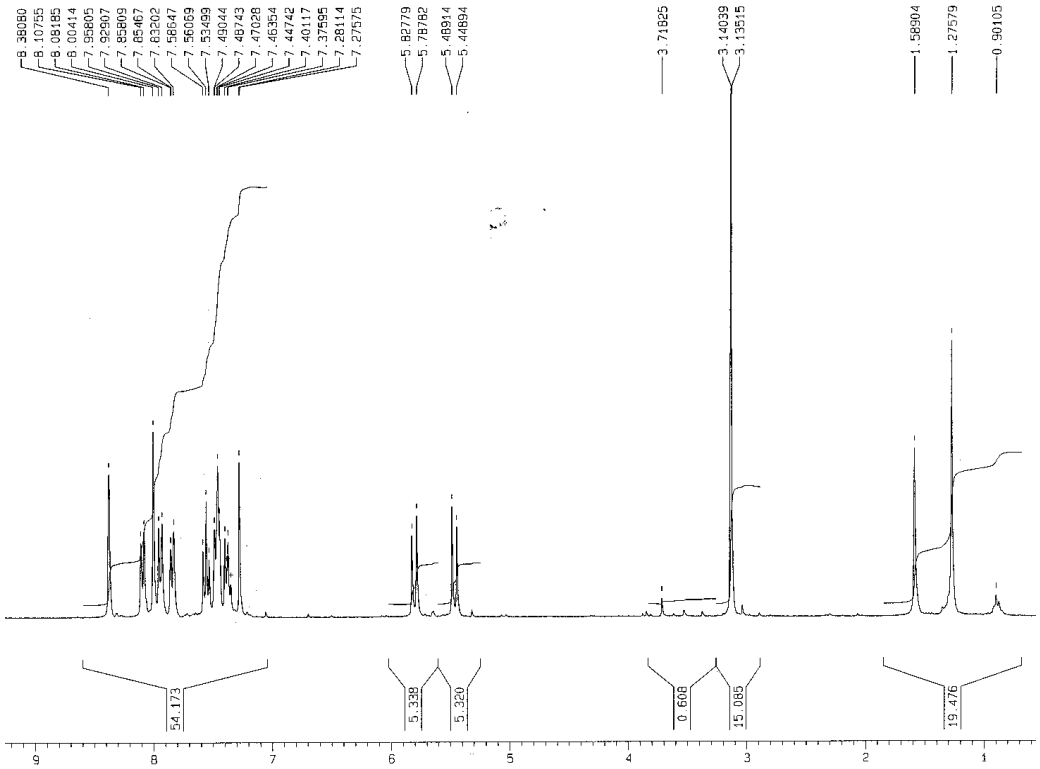


ESI mass spectrum

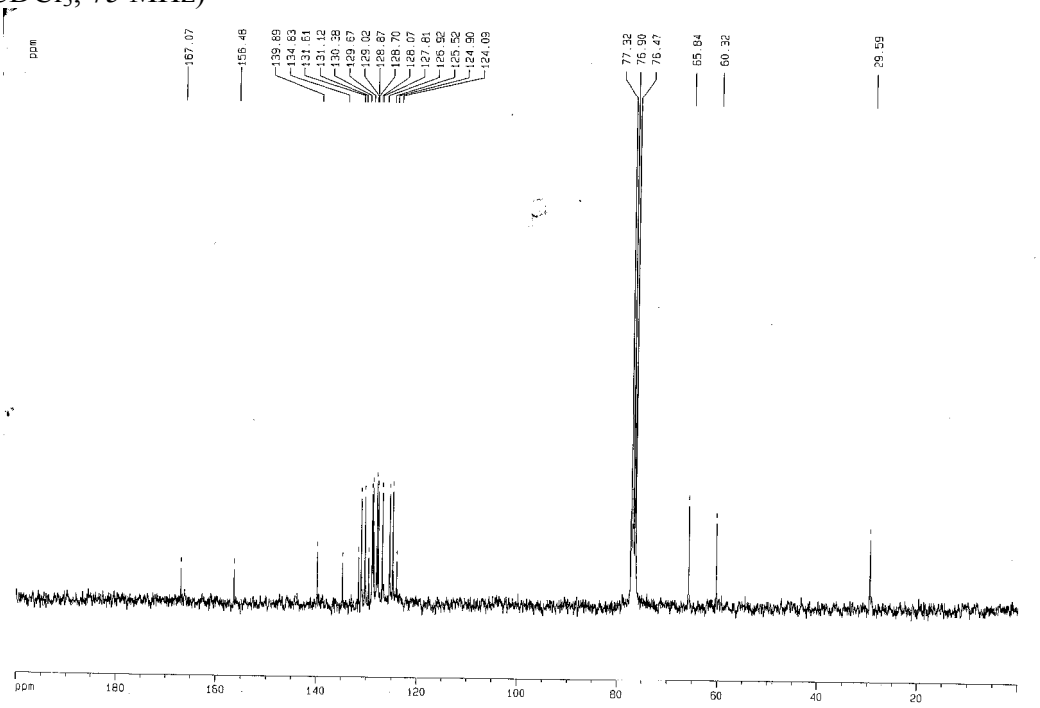


Macrocycle **3d**.

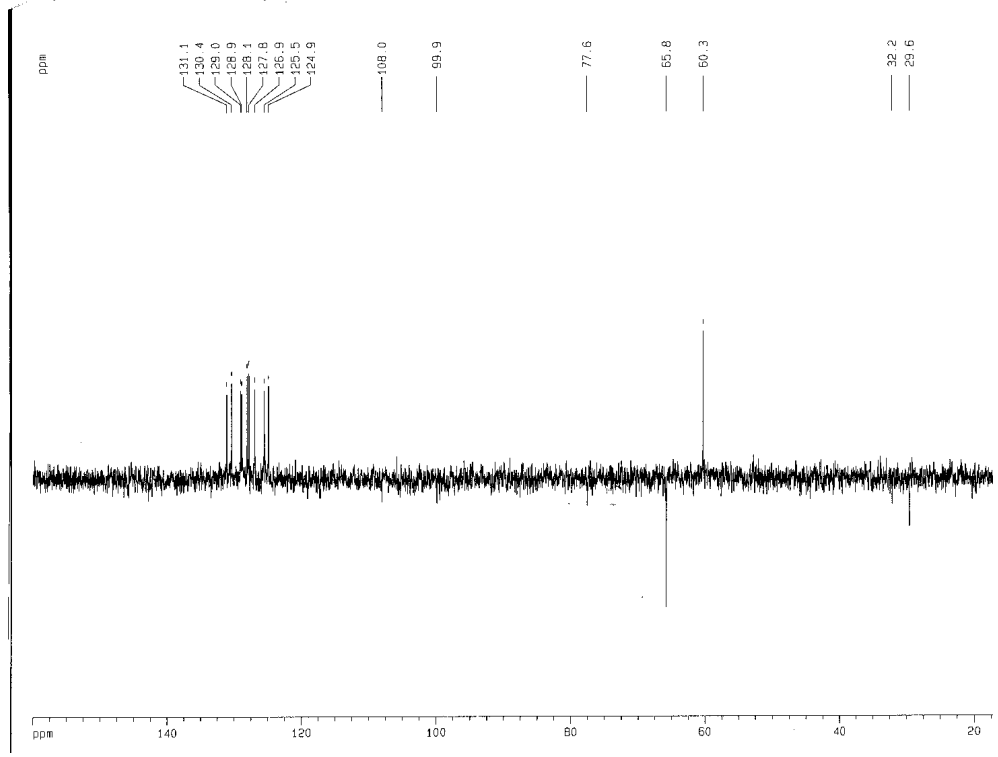
^{1}H NMR ($CDCl_3$, 300 MHz)



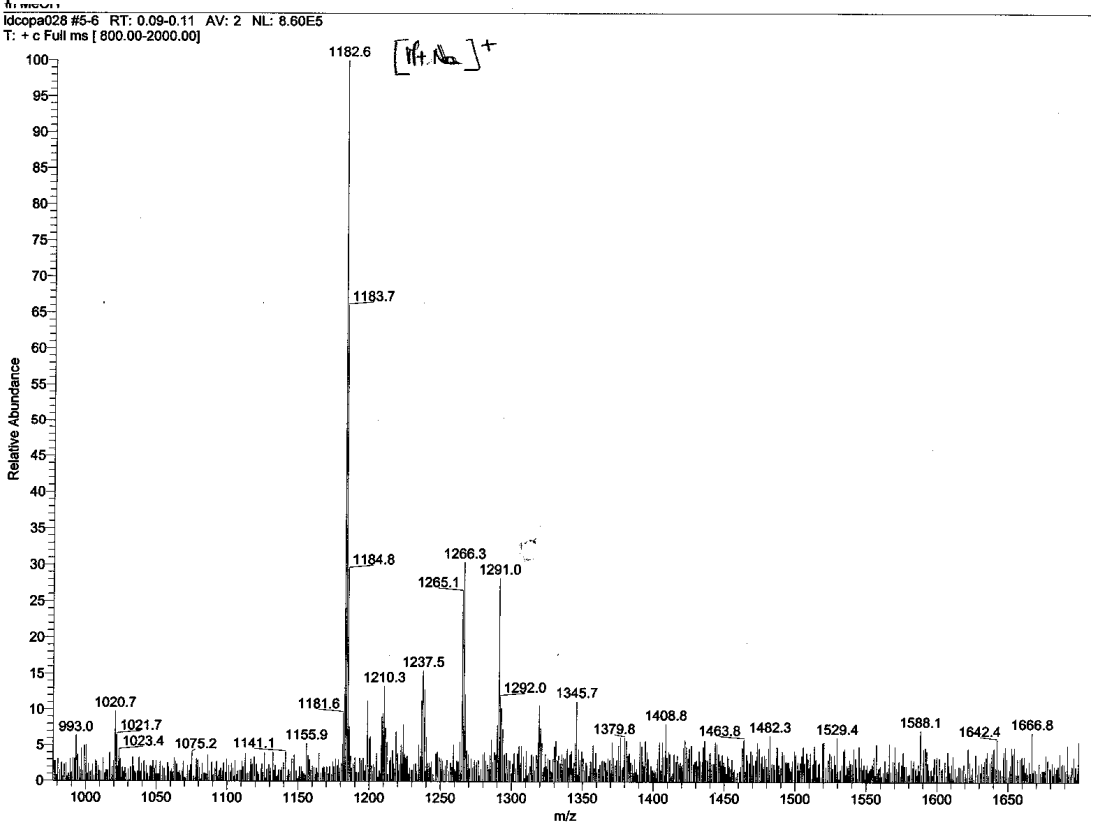
^{13}C NMR ($CDCl_3$, 75 MHz)



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

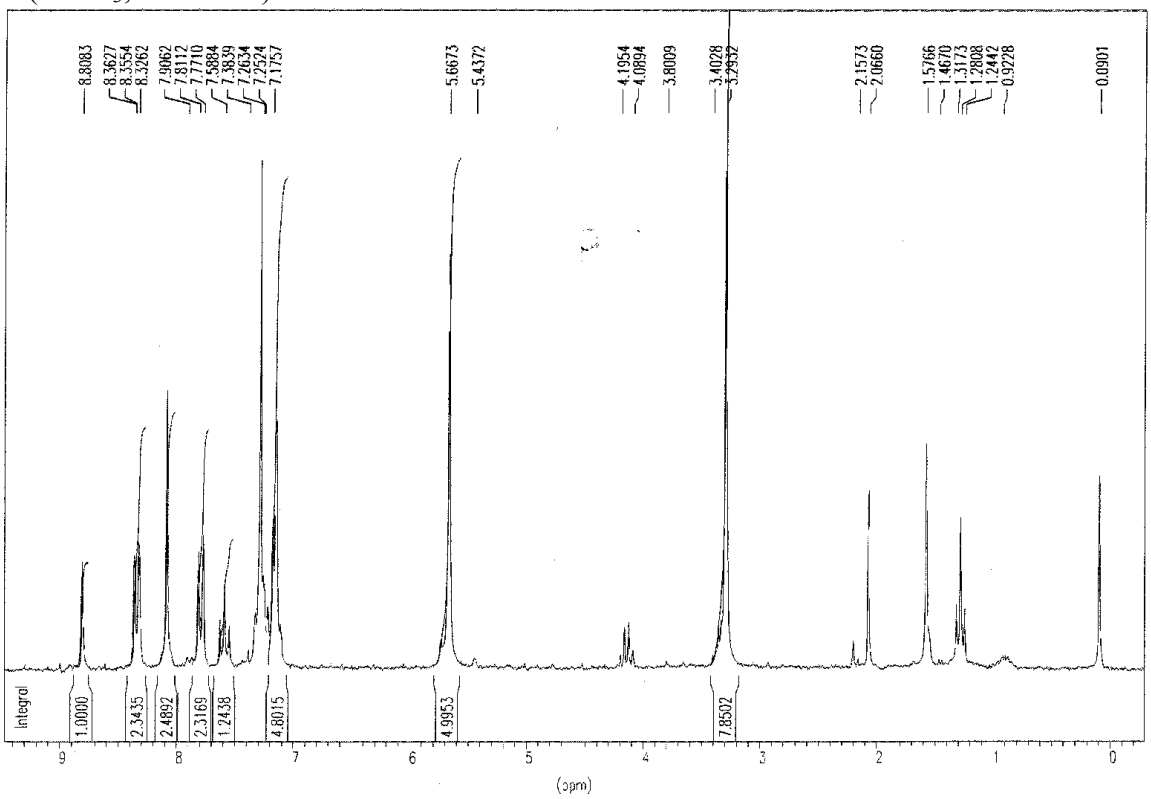


ESI mass spectrum

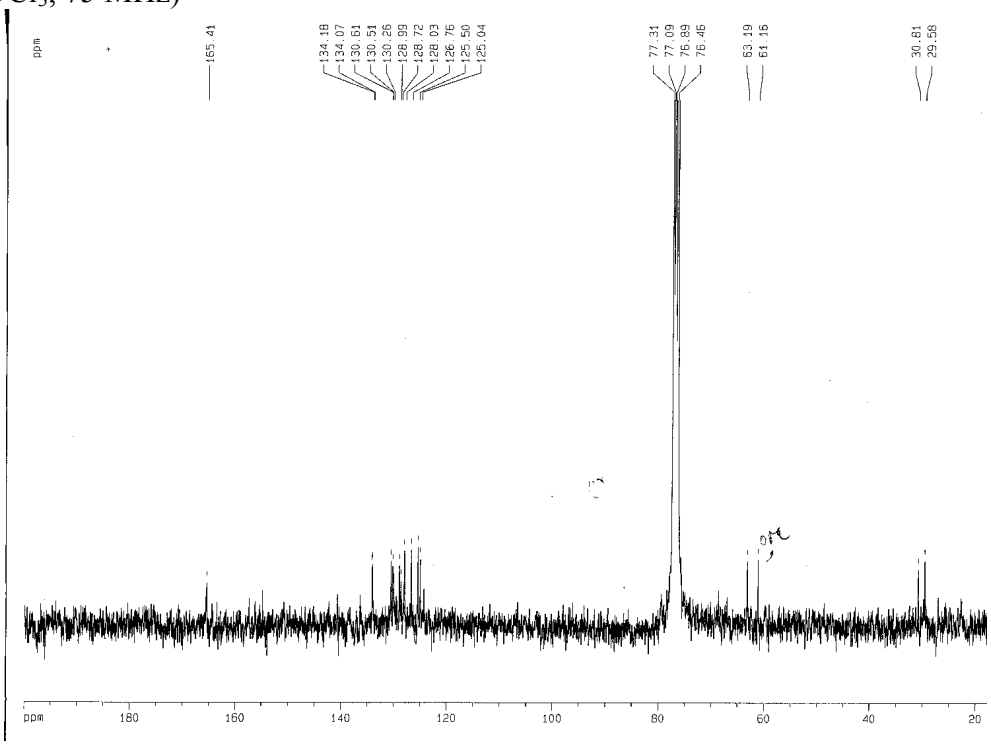


Macrocycle **4b**.

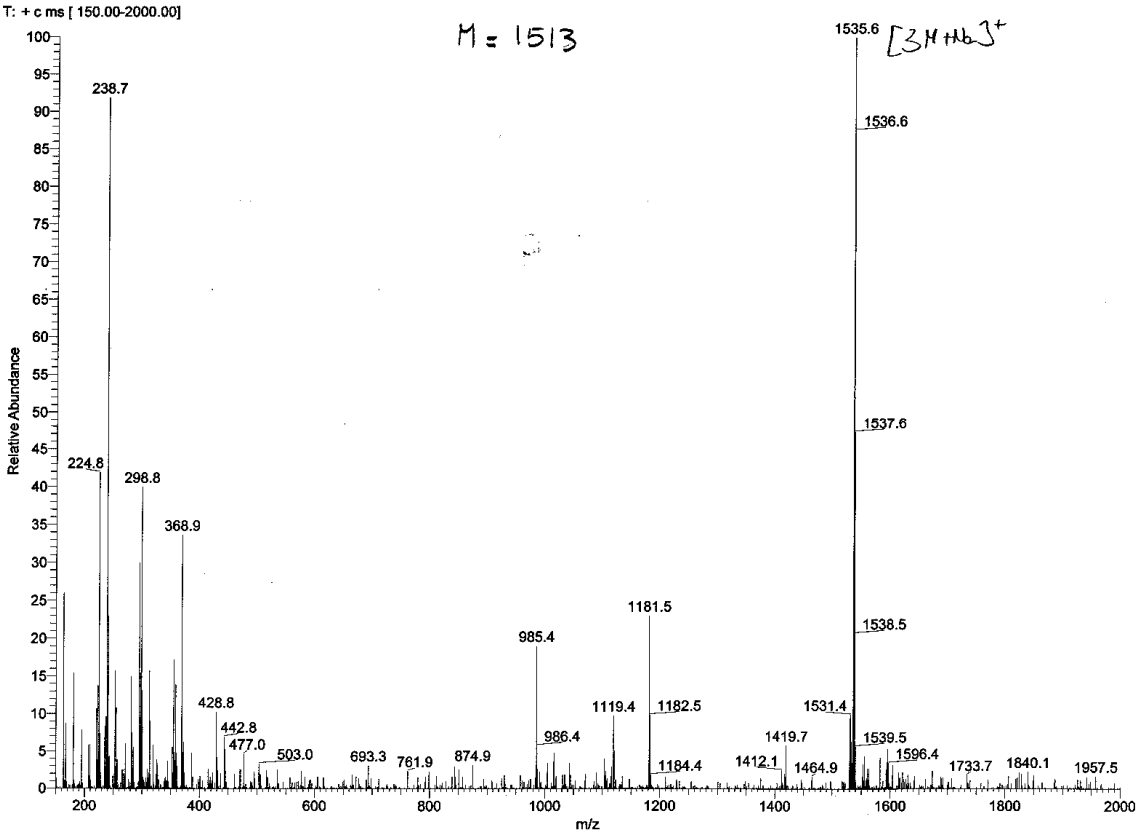
^{1}H NMR ($CDCl_3$, 200 MHz)



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



ESI mass spectrum



Details on calculations.

Geometry optimizations were carried out using the semiempirical PM3 method as implemented by the Gaussian 2003 package.[S1]

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 reported molecules. The calculated energy for C_{60}, used in this paper, was 1.29212107 Ha.

3b (E = -0.33873499 Ha)

C	8.397506	1.016337	2.816303
C	7.331641	1.178721	1.973748
C	7.068042	0.228235	0.948660
C	7.915947	-0.891987	0.826283
C	9.016654	-1.038045	1.714087
C	9.251197	-0.103186	2.685059
H	8.601001	1.752121	3.601344
H	6.666606	2.046426	2.067921
C	5.975221	0.377639	0.042130
C	7.646966	-1.878003	-0.159149
H	9.668486	-1.912844	1.607927
H	10.098019	-0.211504	3.370538
C	6.605065	-1.729380	-1.039159
C	5.794288	-0.554369	-0.967016
H	8.277937	-2.776357	-0.190433
C	4.995155	1.466328	0.226779
C	5.186890	2.739332	-0.389213
C	3.846249	1.232378	0.963534
C	6.350707	3.040786	-1.148585
C	4.190745	3.727598	-0.247233
C	2.812123	2.215465	1.062488
C	6.510064	4.274836	-1.717999
H	7.115380	2.262976	-1.266624
C	4.381301	5.002234	-0.847203
C	2.999514	3.439059	0.470141
C	5.516271	5.268475	-1.563410
H	7.408371	4.505954	-2.299759
H	3.602316	5.763912	-0.727170
H	2.215287	4.217631	0.516095
H	5.666458	6.249368	-2.025921
O	3.632176	-0.031872	1.513168
O	4.721603	-0.387451	-1.841035
C	6.317776	-2.813923	-2.040649
H	6.288367	-2.396144	-3.069678
H	7.071478	-3.622740	-1.998358
C	1.541706	1.860746	1.787238
H	1.258429	0.802370	1.612855
H	1.655354	2.022719	2.875225
C	-0.204245	2.594634	0.303322
O	0.465194	2.735002	1.495070
C	-0.998011	3.807562	-0.035046
C	-2.339916	3.673502	-0.381981
C	-0.379689	5.059087	-0.040336
C	-3.069091	4.810118	-0.738534

H	-2.811333	2.679574	-0.383813
C	-1.118086	6.185460	-0.385003
H	0.690575	5.132284	0.222382
C	-2.460003	6.065951	-0.735782
H	-0.641037	7.171187	-0.387079
H	-3.035984	6.954344	-1.021135
C	4.033283	-0.130734	2.862640
H	5.099077	0.098376	2.991857
H	3.435065	0.516952	3.514452
H	3.837117	-1.181347	3.091218
C	5.118835	-0.009204	-3.141419
H	5.680681	0.932415	-3.141444
H	5.714917	-0.798426	-3.626038
H	4.164363	0.115608	-3.657842
C	-4.479838	4.665027	-1.186496
O	-5.035038	5.271463	-2.082485
O	-5.183500	3.734144	-0.474474
O	-0.120144	1.572557	-0.341571
H	-8.433957	2.597463	0.531856
C	-7.747303	1.749578	0.408893
C	-8.051360	0.528698	1.066235
C	-6.622654	1.871376	-0.366387
C	-7.169440	-0.566228	0.958444
C	-9.238585	0.400832	1.837817
C	-5.736883	0.755209	-0.492257
C	-6.352166	3.171395	-1.073098
C	-7.503345	-1.780025	1.621618
C	-5.977594	-0.431162	0.181434
C	-9.531531	-0.777890	2.467393
H	-9.912214	1.261779	1.917738
O	-4.555313	0.887243	-1.220264
H	-6.196466	2.981399	-2.159788
H	-7.187346	3.887998	-0.962209
C	-8.654677	-1.881136	2.354239
H	-6.823222	-2.635909	1.525236
C	-5.007558	-1.544391	0.124831
H	-10.445106	-0.880928	3.061994
C	-4.745761	0.806666	-2.617366
H	-8.909983	-2.818504	2.859532
C	-5.088577	-2.498259	-0.936226
C	-3.999641	-1.659111	1.068062
H	-5.188843	-0.151490	-2.915992
H	-5.368579	1.636776	-2.986126
H	-3.727599	0.893692	-3.003833
C	-6.120178	-2.453773	-1.914675
C	-4.115312	-3.513936	-1.023443
C	-3.019783	-2.700536	0.988146
O	-3.858284	-0.672741	2.043997
C	-6.164440	-3.376414	-2.924376
H	-6.882555	-1.668051	-1.840247
C	-4.179256	-4.457498	-2.084929
C	-3.081802	-3.590986	-0.053477
C	-1.962078	-2.811844	2.055710
C	-4.465589	-0.999941	3.275093
C	-5.181701	-4.388722	-3.013411
H	-6.961653	-3.340492	-3.674164
H	-3.412188	-5.238222	-2.144319
H	-2.318623	-4.381140	-0.167645
H	-1.671761	-1.815865	2.444806
H	-2.343848	-3.418125	2.898645
O	-0.846314	-3.576364	1.628579

H	-5.543056	-1.180097	3.167620
H	-3.992324	-1.870757	3.744729
H	-4.287532	-0.104368	3.875249
H	-5.234949	-5.113775	-3.832038
C	0.271536	-2.933099	1.143053
C	1.061897	-3.761766	0.192635
O	0.539418	-1.827893	1.562330
C	2.443474	-3.575258	0.108301
C	0.426543	-4.693204	-0.633033
C	3.181351	-4.340260	-0.794928
H	2.937981	-2.820730	0.736561
C	1.174890	-5.452126	-1.525015
H	-0.669359	-4.817770	-0.582151
C	2.553297	-5.282020	-1.608004
C	4.657142	-4.139152	-0.886530
H	0.676967	-6.184572	-2.169108
H	3.139498	-5.880821	-2.313796
O	5.513510	-4.617191	-0.172389
O	5.000027	-3.336460	-1.939273

3c (E = -0.34805572 Ha)

C	-6.890309	3.007423	0.755079
C	-6.919926	1.608573	0.926271
C	-7.666205	3.837519	1.609697
C	-6.086075	3.577360	-0.265658
C	-7.734653	1.064484	1.958091
C	-6.135318	0.782153	0.063584
C	-8.439749	3.285579	2.593801
H	-7.629611	4.923736	1.466117
C	-5.326485	2.787397	-1.091318
H	-6.072633	4.670760	-0.378477
C	-8.474047	1.882900	2.767905
H	-7.761914	-0.024797	2.088062
C	-5.351333	1.368599	-0.916532
C	-6.176070	-0.683957	0.237255
H	-9.038559	3.920432	3.254956
C	-4.503927	3.435651	-2.171447
H	-9.101343	1.459828	3.559505
O	-4.502729	0.561328	-1.672116
C	-7.148797	-1.443478	-0.484100
C	-5.289027	-1.334717	1.078843
H	-4.421315	2.784373	-3.066915
H	-4.947836	4.400233	-2.486408
C	-4.988229	0.286529	-2.968841
C	-8.080914	-0.831739	-1.368049
C	-7.191802	-2.842742	-0.319259
C	-5.332656	-2.754495	1.242087
O	-4.278427	-0.596171	1.692175
H	-5.992786	-0.154345	-2.952820
H	-4.988214	1.195032	-3.590132
H	-4.261497	-0.432989	-3.352816
C	-9.000820	-1.586581	-2.043604
H	-8.050672	0.258027	-1.493181
C	-8.155766	-3.606158	-1.032913
C	-6.270668	-3.479999	0.552020
C	-4.382068	-3.472903	2.160670
C	-4.527871	-0.318605	3.053532
C	-9.039486	-2.989899	-1.875997
H	-9.717775	-1.111322	-2.721281
H	-8.173869	-4.693790	-0.896807

H	-6.311872	-4.573516	0.655554
H	-4.148944	-2.864311	3.059663
H	-4.801610	-4.441204	2.496386
O	-3.086511	-3.626743	1.596695
H	-5.487279	0.191632	3.204910
H	-4.494403	-1.238458	3.657099
H	-3.698731	0.339601	3.322873
H	-9.783231	-3.573330	-2.428452
C	-2.841041	-4.645277	0.718526
C	-1.487237	-4.586878	0.100962
O	-3.686557	-5.500597	0.534686
C	-0.869194	-5.782904	-0.272851
C	-0.849184	-3.366997	-0.130385
C	0.382083	-5.759519	-0.876618
H	-1.376592	-6.740080	-0.100164
C	0.406886	-3.343519	-0.728404
H	-1.331275	-2.423347	0.154884
C	1.019092	-4.538985	-1.102293
H	0.861547	-6.696630	-1.182253
H	0.912594	-2.385904	-0.901210
C	2.347290	-4.526830	-1.776539
O	2.628958	-5.015457	-2.853611
O	3.308436	-3.894008	-1.046688
H	-1.092870	6.765997	-0.871200
C	-0.584004	5.820895	-0.645269
C	0.757341	5.823554	-0.284355
C	-1.286368	4.615273	-0.711018
C	1.400568	4.621219	0.018509
H	1.311360	6.769223	-0.240020
C	-0.641789	3.413004	-0.417674
C	-2.730922	4.650570	-1.072188
C	2.837843	4.661052	0.407616
C	0.701357	3.415900	-0.053636
H	-1.188411	2.463051	-0.469786
O	-3.523878	5.531758	-0.798361
O	-3.135543	3.575002	-1.811293
O	3.166888	3.732550	1.354500
O	3.681540	5.435069	-0.002955
H	1.203697	2.468149	0.177276
C	4.501637	3.647966	1.834317
C	5.402308	2.828864	0.950894
H	4.338604	3.150880	2.813976
H	4.931160	4.651447	2.021636
C	5.373644	1.399402	0.968331
C	6.293637	3.471178	0.129031
C	6.243199	0.657182	0.185894
O	4.392858	0.735496	1.702938
C	7.190866	2.738987	-0.690996
H	6.317893	4.569364	0.088342
C	6.226712	-0.819562	0.208836
C	7.174945	1.329755	-0.664300
C	4.695463	0.615465	3.076283
C	8.108312	3.416643	-1.539793
C	7.039030	-1.510343	1.161082
C	5.439617	-1.545035	-0.670488
C	8.092614	0.621669	-1.489575
H	5.659108	0.119532	3.247737
H	4.688431	1.598398	3.571555
H	3.876181	-0.001947	3.451617
C	8.976591	2.708635	-2.324846
H	8.103517	4.512812	-1.554102

C	7.869878	-0.819220	2.086788
C	7.023174	-2.919715	1.189454
C	5.435190	-2.974663	-0.647569
O	4.566643	-0.864608	-1.517420
C	8.969000	1.295129	-2.296302
H	8.087560	-0.475312	-1.462306
H	9.684359	3.225659	-2.980979
C	8.634687	-1.508173	2.988258
H	7.889677	0.277691	2.059087
C	7.824823	-3.613520	2.136754
C	6.209619	-3.634502	0.272696
C	4.614242	-3.776027	-1.618286
C	5.032044	-0.760126	-2.846477
H	9.674640	0.745977	-2.928503
C	8.611540	-2.921560	3.016253
H	9.274284	-0.971964	3.697171
H	7.799422	-4.709233	2.148892
H	6.211249	-4.731618	0.313487
H	4.564885	-3.276845	-2.611690
H	5.041935	-4.786237	-1.770549
H	6.021775	-0.290154	-2.904733
H	5.056319	-1.745928	-3.335460
H	4.279391	-0.123476	-3.317111
H	9.230472	-3.451317	3.747724

4b, conformation n.1 (E = -0.51647347 Ha)

C	6.268472	8.690380	3.117461
C	5.231746	8.523686	2.240237
C	5.402259	7.761174	1.050763
C	6.660588	7.178709	0.796954
C	7.722904	7.365721	1.723326
C	7.529122	8.105239	2.857725
H	6.132586	9.279281	4.030669
H	4.253476	8.980250	2.436612
C	4.339385	7.569656	0.113398
C	6.856598	6.402862	-0.374720
H	8.694602	6.904046	1.512237
H	8.343480	8.251021	3.574922
C	5.838125	6.213354	-1.274215
C	4.565569	6.816712	-1.027617
H	7.840796	5.944152	-0.546406
C	3.020608	8.176647	0.386840
C	2.789674	9.539015	0.017971
C	2.003591	7.453030	0.988428
C	3.796487	10.334478	-0.597821
C	1.529135	10.119494	0.266339
C	0.723482	8.042125	1.230678
C	3.547212	11.635665	-0.939532
H	4.779705	9.884726	-0.785719
C	1.293711	11.473539	-0.097862
C	0.503686	9.347478	0.871084
C	2.281541	12.213380	-0.687744
H	4.326350	12.244248	-1.410444
H	0.308471	11.910516	0.101680
H	-0.474800	9.814556	1.043460
H	2.105006	13.256468	-0.969834
O	2.162487	6.098878	1.275089
O	3.527012	6.540959	-1.915437
C	6.086136	5.375814	-2.499091
H	5.438511	5.670171	-3.345123

H	7.140771	5.456724	-2.828198
C	-0.391723	7.259074	1.865374
H	-0.012070	6.513769	2.591522
H	-1.096978	7.923357	2.401905
O	5.682327	4.023937	-2.313212
C	6.551778	3.115771	-1.778697
O	7.692558	3.446202	-1.514905
C	5.955145	1.764141	-1.597089
C	5.058005	1.238337	-2.528820
C	6.321804	1.016591	-0.476600
C	4.530957	-0.034275	-2.338709
H	4.765099	1.824944	-3.407424
C	5.788574	-0.259987	-0.296476
H	7.024874	1.430780	0.258365
C	4.891648	-0.787990	-1.226925
H	3.826139	-0.446497	-3.068867
H	4.473872	-1.792492	-1.084090
C	6.174674	-1.038696	0.911820
O	6.278148	-0.626532	2.051234
O	6.446537	-2.346205	0.638369
H	10.292686	-6.309559	-0.013898
C	9.401194	-6.929163	-0.164889
C	8.133515	-6.410053	0.215861
C	9.501540	-8.179404	-0.710786
C	6.974912	-7.191492	0.029805
C	8.025656	-5.109854	0.773806
C	8.342500	-8.966635	-0.900317
H	10.475571	-8.583462	-1.005373
C	5.702557	-6.664339	0.415586
C	7.112046	-8.487737	-0.541605
C	6.807750	-4.603939	1.150702
H	8.938354	-4.511884	0.895368
H	8.442822	-9.965957	-1.336765
C	4.489769	-7.480570	0.202796
C	5.632099	-5.398466	0.974334
H	6.211030	-9.098475	-0.681162
C	6.736355	-3.220065	1.733314
C	4.122611	-8.453610	1.184213
C	3.700417	-7.319582	-0.924643
O	4.402448	-4.818349	1.279048
H	5.954936	-3.143996	2.514852
H	7.700142	-2.921723	2.189860
C	4.892272	-8.665264	2.362419
C	2.962924	-9.230331	0.986806
C	2.516796	-8.098621	-1.115170
O	3.983694	-6.320208	-1.854158
C	4.515755	-9.604899	3.282976
H	5.797247	-8.063691	2.514588
C	2.591590	-10.200571	1.957597
C	2.169891	-9.033903	-0.173244
C	1.644094	-7.917541	-2.327147
C	3.352197	-10.382111	3.080014
H	5.112203	-9.765041	4.187312
H	1.685526	-10.794668	1.790207
H	1.261942	-9.640230	-0.301910
H	2.208187	-7.530411	-3.195358
H	1.173009	-8.875650	-2.622598
O	0.688935	-6.878225	-2.145480
H	3.069778	-11.126927	3.831214
C	-0.533289	-7.156636	-1.602241
O	-0.823757	-8.303514	-1.317095

C	-1.399094	-5.956987	-1.438716
C	-1.324613	-4.879575	-2.324215
C	-2.310445	-5.932024	-0.380969
C	-2.160817	-3.782256	-2.150606
H	-0.608973	-4.892120	-3.154780
C	-3.148014	-4.828249	-0.218674
H	-2.368008	-6.776850	0.318637
C	-3.074339	-3.750175	-1.102507
H	-2.100374	-2.936591	-2.844222
C	-4.106877	-4.812843	0.919523
H	-3.734198	-2.883058	-0.973897
O	-3.894197	-5.153744	2.067333
O	-5.347376	-4.373646	0.563692
H	-9.906122	-1.121220	2.467196
C	-9.987000	-0.028552	2.407212
C	-10.587020	0.682874	3.410303
C	-9.460031	0.633397	1.263307
C	-10.692323	2.090373	3.327652
H	-10.992140	0.169273	4.288509
C	-9.568423	2.036657	1.184518
C	-8.827127	-0.079458	0.198374
C	-10.195158	2.754338	2.239777
H	-11.174386	2.638537	4.143677
C	-9.048678	2.723287	0.056694
C	-8.322488	0.619443	-0.886053
C	-8.718903	-1.550245	0.279571
H	-10.268060	3.845672	2.165600
C	-8.434866	2.042590	-0.964336
H	-9.136839	3.818358	0.018189
O	-7.609285	-0.076460	-1.860821
C	-9.765259	-2.357997	-0.264609
C	-7.621836	-2.159281	0.866278
C	-7.908575	2.812305	-2.144969
C	-10.912945	-1.788991	-0.884043
C	-9.664390	-3.762154	-0.189006
C	-7.522785	-3.583639	0.942399
O	-6.556987	-1.367864	1.292596
H	-7.941293	2.206884	-3.074996
H	-8.499248	3.733802	-2.314892
O	-6.515590	3.078287	-2.037532
C	-11.899045	-2.588241	-1.394962
H	-10.993848	-0.695920	-0.938566
C	-10.701556	-4.571797	-0.727570
C	-8.528546	-4.356284	0.419723
C	-6.341661	-4.256088	1.584549
C	-6.082774	4.200329	-1.387846
C	-11.793355	-3.995982	-1.317275
H	-12.781744	-2.145866	-1.868530
H	-10.608784	-5.661990	-0.662238
H	-8.466884	-5.451629	0.461484
H	-5.963109	-3.665290	2.448588
H	-6.600617	-5.266677	1.955234
O	-6.891259	5.002078	-0.958871
C	-4.600538	4.306083	-1.304198
H	-12.594598	-4.615313	-1.733417
C	-3.776889	3.807075	-2.315507
C	-4.039624	4.934881	-0.190665
C	-2.396569	3.939107	-2.211605
H	-4.211692	3.309425	-3.190292
C	-2.653819	5.066165	-0.098585
H	-4.685740	5.323997	0.607844

C	-1.829002	4.567493	-1.108345
H	-1.750885	3.545603	-3.004129
C	-2.071220	5.728944	1.100173
H	-0.739319	4.671692	-1.034318
O	-2.398039	5.570850	2.260666
O	-1.080072	6.612352	0.790654
C	-6.522606	-1.169770	2.690334
H	-7.460322	-0.748760	3.073771
H	-6.290699	-2.108682	3.215849
H	-5.705169	-0.455612	2.813485
C	-8.348615	-0.317230	-3.038788
H	-9.298104	-0.829278	-2.838716
H	-8.536796	0.620554	-3.583340
H	-7.682330	-0.961577	-3.616819
C	2.795463	5.850398	2.512788
H	2.174222	6.172776	3.356754
H	2.898974	4.762644	2.514366
H	3.781241	6.329386	2.578688
C	3.317322	7.556955	-2.873025
H	3.120127	8.532289	-2.408699
H	4.165455	7.645178	-3.562344
H	2.432505	7.204028	-3.408079
C	3.900583	-5.184598	2.547228
H	4.525612	-4.792457	3.358238
H	2.918310	-4.706283	2.563049
H	3.798921	-6.272498	2.655375
C	4.934780	-6.703768	-2.824531
H	5.881545	-7.029178	-2.373431
H	4.550044	-7.495780	-3.477949
H	5.081118	-5.783280	-3.394649

4b, conformation n.2 (E = -0.52240409 Ha)

C	-10.039369	-3.551714	3.273138
C	-9.196534	-3.998154	2.291956
C	-8.898658	-3.181405	1.165943
C	-9.489230	-1.904117	1.081243
C	-10.362409	-1.462497	2.112712
C	-10.629996	-2.270185	3.183909
H	-10.263397	-4.182089	4.140131
H	-8.731683	-4.989526	2.361238
C	-8.025788	-3.618211	0.121491
C	-9.206975	-1.067450	-0.029059
H	-10.811232	-0.465456	2.034089
H	-11.299559	-1.934011	3.982368
C	-8.359071	-1.477677	-1.027169
C	-7.763756	-2.774741	-0.946600
H	-9.676191	-0.074295	-0.074519
C	-7.435120	-4.970115	0.198941
C	-8.118204	-6.053984	-0.437884
C	-6.254255	-5.216005	0.880177
C	-9.346605	-5.868143	-1.132066
C	-7.570941	-7.351396	-0.373417
C	-5.709211	-6.536623	0.954223
C	-9.977220	-6.923637	-1.732628
H	-9.785109	-4.862624	-1.168029
C	-8.241756	-8.431901	-1.008812
C	-6.358752	-7.570911	0.330490
C	-9.417797	-8.220638	-1.674794
H	-10.924097	-6.775220	-2.262335
H	-7.800308	-9.433665	-0.953586

H	-5.950727	-8.589455	0.370227
H	-9.938668	-9.049504	-2.165130
O	-5.636163	-4.220019	1.633065
O	-6.824850	-3.171384	-1.899892
C	-8.090808	-0.552002	-2.182270
H	-7.780003	-1.103182	-3.093925
H	-8.994578	0.037205	-2.434123
C	-4.444058	-6.822003	1.714931
H	-4.377256	-6.222675	2.643283
H	-4.367959	-7.890367	1.995366
O	-6.950916	0.267560	-1.946281
C	-7.102333	1.496210	-1.365934
O	-8.218162	1.911367	-1.114260
C	-5.819794	2.211073	-1.120755
C	-4.676541	1.950201	-1.879164
C	-5.783666	3.177236	-0.111631
C	-3.502027	2.651834	-1.627193
H	-4.696158	1.195038	-2.673951
C	-4.603737	3.880433	0.126532
H	-6.680121	3.383572	0.489351
C	-3.458948	3.617609	-0.628547
H	-2.606076	2.444527	-2.222193
H	-2.529122	4.179807	-0.432762
C	-4.571307	4.907883	1.203709
O	-5.038938	4.826108	2.321854
O	-3.937898	6.050063	0.811481
H	-4.334586	11.508345	-0.435109
C	-3.248637	11.398006	-0.535278
C	-2.630853	10.218441	-0.037027
C	-2.496816	12.376416	-1.125786
C	-1.236879	10.052384	-0.163969
C	-3.405901	9.211855	0.594798
C	-1.096293	12.222275	-1.241646
H	-2.967631	13.287247	-1.509876
C	-0.621890	8.860751	0.335102
C	-0.481353	11.092270	-0.775441
C	-2.816036	8.080693	1.097919
H	-4.490604	9.359314	0.679867
H	-0.509188	13.020957	-1.707125
C	0.838177	8.694722	0.181730
C	-1.402316	7.904725	0.964838
H	0.607033	10.975472	-0.855309
C	-3.672831	7.058041	1.791566
C	1.701365	9.180607	1.212784
C	1.387278	8.086063	-0.935820
O	-0.824662	6.818732	1.618058
H	-3.162916	6.622844	2.672549
H	-4.631048	7.493147	2.135592
C	1.196834	9.809261	2.385075
C	3.096518	9.038538	1.068603
C	2.800601	7.915709	-1.065096
O	0.558071	7.530224	-1.911991
C	2.049595	10.270468	3.350670
H	0.110790	9.911921	2.501930
C	3.962809	9.528310	2.084089
C	3.626415	8.398689	-0.081211
C	3.405758	7.211416	-2.248658
C	3.448435	10.130815	3.199316
H	1.656970	10.751108	4.252928
H	5.045251	9.409888	1.957399
H	4.716485	8.286676	-0.168321

H	2.722330	7.170126	-3.116177
H	4.338556	7.714427	-2.571300
O	3.588700	5.823228	-1.984945
H	4.110899	10.507328	3.985612
C	4.781568	5.367823	-1.497998
O	5.710879	6.140754	-1.356377
C	4.795175	3.908210	-1.204932
C	3.923260	3.022657	-1.842239
C	5.720883	3.428620	-0.274263
C	3.974750	1.664468	-1.545961
H	3.195589	3.389015	-2.576194
C	5.769994	2.064301	0.008260
H	6.407554	4.121865	0.231044
C	4.894345	1.179045	-0.623719
H	3.288180	0.972283	-2.045149
C	6.758607	1.559736	1.000734
H	4.939142	0.100391	-0.392240
O	7.049881	2.049413	2.073645
O	7.377880	0.419850	0.580765
H	8.785169	-4.874024	2.415339
C	8.152548	-5.770397	2.413867
C	8.205878	-6.664897	3.447992
C	7.268323	-5.980333	1.319443
C	7.382983	-7.814671	3.445854
H	8.885434	-6.498007	4.290362
C	6.449308	-7.127795	1.321464
C	7.189956	-5.068084	0.221709
C	6.522998	-8.043229	2.406807
H	7.441856	-8.515035	4.285433
C	5.556380	-7.360523	0.243955
C	6.301947	-5.319132	-0.812454
C	8.072108	-3.883113	0.208333
H	5.877334	-8.929078	2.395512
C	5.468937	-6.480689	-0.805685
H	4.925351	-8.260491	0.266026
O	6.157749	-4.363759	-1.819554
C	9.335713	-3.976579	-0.456090
C	7.715690	-2.697210	0.829230
C	4.506479	-6.773048	-1.924317
C	9.768307	-5.175250	-1.089670
C	10.189984	-2.855624	-0.481168
C	8.589852	-1.564893	0.809602
O	6.566001	-2.609252	1.610993
H	4.808384	-6.281476	-2.872354
H	4.441309	-7.862688	-2.113759
O	3.233293	-6.179557	-1.692959
C	10.982492	-5.235415	-1.717816
H	9.113436	-6.055400	-1.056126
C	11.445018	-2.940402	-1.143661
C	9.794037	-1.653086	0.159358
C	8.224216	-0.279177	1.498184
C	2.254579	-6.890390	-1.055465
C	11.830445	-4.104721	-1.749518
H	11.311681	-6.161649	-2.200435
H	12.095496	-2.058286	-1.158166
H	10.474199	-0.791764	0.127647
H	7.699298	-0.459462	2.456017
H	9.117789	0.338337	1.712675
O	2.461792	-8.048568	-0.743435
C	0.994190	-6.130320	-0.832103
H	12.796268	-4.175364	-2.260353

C	0.706934	-4.952848	-1.526723
C	0.076647	-6.633430	0.095025
C	-0.490573	-4.283829	-1.294852
H	1.417730	-4.547464	-2.256775
C	-1.124680	-5.960541	0.311707
H	0.299234	-7.555825	0.649606
C	-1.411067	-4.782275	-0.380510
H	-0.711587	-3.359756	-1.839814
C	-2.098612	-6.504613	1.297822
H	-2.366211	-4.257462	-0.202717
O	-1.867527	-6.939769	2.408090
O	-3.376354	-6.492047	0.821893
C	5.381320	-2.341377	0.893258
H	5.424779	-1.386981	0.343962
H	5.130101	-3.151997	0.200186
H	4.635515	-2.280200	1.690163
C	6.796988	-4.706163	-3.030399
H	7.859199	-4.942180	-2.890475
H	6.285428	-5.549981	-3.517214
H	6.683288	-3.799755	-3.629481
C	-4.776492	-3.373347	0.901786
H	-5.315973	-2.800078	0.139709
H	-4.393828	-2.704943	1.677596
H	-3.942825	-3.919208	0.430793
C	-7.392311	-3.615815	-3.113324
H	-8.129240	-4.414456	-2.962750
H	-7.851913	-2.778544	-3.659646
H	-6.526535	-3.994061	-3.661747
C	-0.544658	5.707127	0.796012
H	0.223456	5.934969	0.048745
H	-0.166305	4.976302	1.515693
H	-1.441816	5.311050	0.293536
C	0.222362	8.424695	-2.951371
H	-0.306066	9.311070	-2.576838
H	1.103838	8.738812	-3.522829
H	-0.439614	7.823743	-3.579499

4c, conformation n.1 (E = -0.52843019 Ha)

C	-10.311014	0.591573	2.283194
C	-9.367627	-0.338595	1.941066
C	-8.872723	-0.413053	0.609230
C	-9.373650	0.489475	-0.351070
C	-10.351325	1.449087	0.029471
C	-10.808148	1.497448	1.318060
H	-10.691900	0.643911	3.308531
H	-8.981159	-1.045754	2.685907
C	-7.887206	-1.370891	0.219752
C	-8.897101	0.437168	-1.686855
H	-10.727901	2.147715	-0.726705
H	-11.560917	2.234622	1.615857
C	-7.960565	-0.490671	-2.067315
C	-7.452623	-1.407615	-1.095485
H	-9.285842	1.163617	-2.413846
C	-7.321586	-2.291290	1.226538
C	-7.913077	-3.576661	1.424507
C	-6.203051	-1.934985	1.961688
C	-9.077046	-3.988275	0.717689
C	-7.332305	-4.467288	2.350487
C	-5.595227	-2.852375	2.874358
C	-9.624836	-5.223153	0.935664

H	-9.529568	-3.292859	-0.000393
C	-7.918708	-5.745631	2.558076
C	-6.160365	-4.088899	3.056592
C	-9.039911	-6.113136	1.865536
H	-10.522925	-5.535146	0.392335
H	-7.454495	-6.428907	3.278740
H	-5.701954	-4.813135	3.743986
H	-9.494946	-7.096612	2.022054
O	-5.609676	-0.696834	1.717895
O	-6.427747	-2.286710	-1.442263
C	-7.512765	-0.536959	-3.502154
H	-7.450909	-1.586298	-3.861759
H	-8.207459	0.020776	-4.159568
C	-4.341539	-2.494540	3.626110
O	-6.169485	-0.114768	-3.694517
C	-5.873579	1.216340	-3.765944
O	-6.751502	2.050466	-3.677517
C	-4.418352	1.462448	-3.981360
C	-3.830823	1.132949	-5.202813
C	-3.660081	2.045019	-2.967366
C	-2.481859	1.396154	-5.415297
H	-4.428378	0.669412	-5.995670
C	-2.309526	2.303300	-3.177580
H	-4.113828	2.304064	-1.996155
C	-1.723022	1.981257	-4.401988
H	-2.018782	1.149598	-6.377725
H	-1.714778	2.763612	-2.368326
C	-0.288778	2.307577	-4.638698
O	0.169489	2.973320	-5.544496
O	0.554205	1.739273	-3.717353
O	8.172602	-0.730926	4.446093
C	7.009361	-0.996295	4.216199
C	5.825751	-0.128794	4.474114
O	6.671451	-2.210665	3.686433
C	4.963671	0.192714	3.424936
C	5.610611	0.388805	5.751259
C	3.893545	1.051839	3.650251
H	5.126699	-0.227646	2.424032
C	4.533018	1.237973	5.979362
H	6.291898	0.133688	6.571054
C	3.684306	1.574986	4.925876
H	3.222888	1.318767	2.822007
H	4.356201	1.642437	6.982226
C	2.539347	2.500506	5.162276
O	2.753185	3.725362	4.593618
O	1.525657	2.280086	5.791953
C	1.703565	4.681640	4.539949
C	0.781064	4.451673	3.374023
H	2.281857	5.620897	4.414420
H	1.146798	4.738105	5.495325
C	-0.508292	4.048707	3.613843
C	1.215430	4.634714	2.023881
C	-1.403986	3.784811	2.545001
H	-0.859917	3.898522	4.643965
C	0.363073	4.388047	0.959601
O	2.548602	4.940703	1.752748
C	-0.970591	3.937592	1.211987
C	-2.724442	3.328454	2.807657
C	0.810856	4.545070	-0.438387
C	-1.871710	3.609299	0.161557
C	-3.567775	3.018567	1.775737

H	-3.046710	3.214672	3.849135
C	0.818585	5.841790	-1.039123
C	1.201789	3.446464	-1.186187
C	-3.134158	3.159160	0.438512
H	-1.531378	3.684351	-0.885291
H	-4.578877	2.632300	1.973782
C	0.371991	6.999968	-0.343735
C	1.272680	5.984408	-2.366656
C	1.568905	3.583150	-2.560577
O	1.113103	2.160922	-0.655123
H	-3.814000	2.884598	-0.384001
C	0.414887	8.231508	-0.938757
H	-0.018102	6.883950	0.675567
C	1.320182	7.276068	-2.959010
C	1.635251	4.835574	-3.116847
C	1.795411	2.374133	-3.426847
C	0.904016	8.374350	-2.257579
H	0.067436	9.119670	-0.400561
H	1.688396	7.372409	-3.987053
H	1.934354	4.962919	-4.166395
H	0.937198	9.370948	-2.709821
O	-2.739557	-4.546525	2.872470
C	-2.557708	-3.476083	2.327788
C	-1.632489	-3.183582	1.197586
O	-3.221196	-2.361570	2.763044
C	-0.290661	-3.553666	1.286809
C	-2.121609	-2.564910	0.046152
C	0.568019	-3.300241	0.222285
H	0.086713	-4.044400	2.191328
C	-1.265754	-2.322620	-1.022648
H	-3.176032	-2.267036	-0.017392
C	0.076383	-2.689493	-0.930742
H	1.626014	-3.578031	0.292859
H	-1.647520	-1.843268	-1.931438
C	0.979332	-2.439460	-2.090369
O	1.899591	-1.465732	-1.829688
O	0.945708	-2.984686	-3.175650
C	2.839245	-1.086272	-2.827970
C	4.079675	-1.935629	-2.777210
H	3.025173	-0.025587	-2.546211
H	2.394270	-1.089209	-3.842904
C	4.219612	-2.969098	-3.669312
C	5.103285	-1.709874	-1.806411
C	5.354909	-3.819510	-3.629643
H	3.439463	-3.163575	-4.418990
C	6.205990	-2.544892	-1.718769
O	4.911821	-0.693308	-0.871809
C	6.347241	-3.621324	-2.647926
C	5.491301	-4.884352	-4.562019
C	7.219660	-2.352585	-0.662126
C	7.460582	-4.506860	-2.613508
C	6.575326	-5.716963	-4.507268
H	4.711406	-5.025695	-5.319462
C	8.420085	-1.633302	-0.952784
C	7.011852	-2.839566	0.618205
C	7.569933	-5.525279	-3.520636
H	8.232491	-4.350729	-1.849408
H	6.684544	-6.538573	-5.222726
C	8.695324	-1.119228	-2.250717
C	9.363909	-1.421560	0.073190
C	7.947620	-2.582049	1.667553

O	5.826217	-3.496251	0.944412
H	8.429855	-6.202740	-3.492563
C	9.857358	-0.441357	-2.500542
H	7.960288	-1.286047	-3.048324
C	10.564707	-0.715494	-0.211378
C	9.100447	-1.894302	1.385364
C	7.671663	-3.020760	3.080351
C	10.804359	-0.237495	-1.470596
H	10.066938	-0.050649	-3.501881
H	11.289619	-0.559856	0.596150
H	9.830043	-1.683355	2.179531
H	7.190013	-4.014664	3.119310
H	8.599915	-3.059829	3.682998
H	11.727618	0.306901	-1.694422
H	2.333780	1.554135	-2.901253
H	2.359601	2.626337	-4.345345
H	-4.408452	-1.468749	4.046146
H	-4.144658	-3.202325	4.454213
C	2.892010	6.291106	1.973703
H	2.300178	6.973091	1.350609
H	2.787264	6.570253	3.032971
H	3.943564	6.321158	1.678739
C	2.263313	1.757725	0.055847
H	3.145424	1.699779	-0.596267
H	2.477199	2.413674	0.908865
H	1.989968	0.757732	0.404319
C	-5.861511	0.251994	2.732171
H	-6.935077	0.419993	2.882770
H	-5.391749	-0.043932	3.682701
H	-5.383015	1.160339	2.342237
C	-6.878948	-3.436792	-2.125363
H	-7.622240	-3.997166	-1.544441
H	-7.294076	-3.177890	-3.111504
H	-5.964533	-4.022796	-2.242615
C	5.583100	0.505593	-1.198408
H	5.108356	1.006943	-2.051029
H	5.456489	1.105361	-0.292447
H	6.649577	0.349189	-1.407680
C	5.851796	-4.877447	0.651959
H	6.569775	-5.411420	1.285503
H	4.832709	-5.191689	0.889951
H	6.076711	-5.074346	-0.404675

4c, conformation n.2 (E = -0.51285032 Ha)

C	8.845122	-8.169038	-1.906192
C	7.728968	-7.764964	-1.225514
C	7.755940	-6.591575	-0.421684
C	8.954537	-5.853792	-0.340776
C	10.101400	-6.294011	-1.056488
C	10.045556	-7.426825	-1.821376
H	8.819580	-9.071243	-2.526336
H	6.794100	-8.335124	-1.293624
C	6.609390	-6.143496	0.304843
C	9.007933	-4.676856	0.449682
H	11.025263	-5.708304	-0.985640
H	10.925235	-7.769108	-2.376185
C	7.906855	-4.238893	1.141740
C	6.692474	-4.989151	1.066855
H	9.949886	-4.111785	0.492517
C	5.359531	-6.927745	0.232007

C	5.121976	-7.940054	1.213406
C	4.423775	-6.711494	-0.766347
C	6.052742	-8.217859	2.253412
C	3.934551	-8.696716	1.150666
C	3.220471	-7.482901	-0.829819
C	5.796939	-9.193970	3.177530
H	6.985048	-7.640277	2.294444
C	3.689278	-9.703896	2.123864
C	2.997352	-8.454362	0.113701
C	4.600480	-9.944634	3.115277
H	6.517911	-9.406249	3.973936
H	2.759854	-10.281795	2.063283
H	2.084248	-9.062493	0.079315
H	4.416504	-10.719468	3.866628
O	4.703073	-5.830199	-1.808816
O	5.538204	-4.507705	1.685620
C	8.013740	-2.987428	1.969250
H	7.319809	-3.005904	2.835406
H	9.042309	-2.854348	2.358322
C	2.221088	-7.277350	-1.933537
H	2.444936	-6.393192	-2.560676
H	2.194373	-8.164866	-2.595267
O	7.549595	-1.839984	1.266684
C	8.413852	-1.119135	0.491851
O	9.589718	-1.426161	0.443248
C	8.210749	0.347616	-1.500618
C	7.768208	0.021239	-0.217036
C	7.648289	1.424208	-2.176059
C	6.757616	0.771087	0.385882
C	6.646455	2.182936	-1.567291
H	7.989604	1.675598	-3.187972
C	6.197794	1.851169	-0.288160
H	6.400487	0.514507	1.390160
H	5.406752	2.439405	0.192063
C	6.071776	3.336461	-2.314280
O	5.893115	3.416685	-3.514147
O	5.747080	4.391410	-1.513024
H	7.828051	7.769243	1.565717
C	6.845885	8.232190	1.715763
C	5.773633	7.856560	0.860825
C	6.650950	9.156931	2.704663
C	4.501127	8.435079	1.041381
C	5.978332	6.913752	-0.179013
C	5.379632	9.749770	2.881768
H	7.473632	9.450312	3.364902
C	3.427095	8.048577	0.179895
C	4.332018	9.399750	2.074204
C	4.953082	6.547054	-1.014523
H	6.979104	6.481613	-0.307485
H	5.245149	10.495410	3.672429
C	2.096403	8.660227	0.375227
C	3.658876	7.128051	-0.829500
H	3.346758	9.865717	2.203110
C	5.225377	5.575683	-2.128927
C	1.791507	9.881847	-0.302281
C	1.142381	8.079779	1.195531
O	2.666583	6.862110	-1.770248
H	4.321274	5.323306	-2.715479
H	5.975921	5.993679	-2.827617
C	2.726973	10.521494	-1.162454
C	0.527638	10.477608	-0.115350

C	-0.148547	8.670961	1.361023
O	1.388867	6.844962	1.797696
C	2.407356	11.693920	-1.791350
H	3.707507	10.053640	-1.315301
C	0.219619	11.697763	-0.777047
C	-0.431601	9.851687	0.721593
C	-1.206417	8.028618	2.215983
C	1.140706	12.291082	-1.596098
H	3.129356	12.181509	-2.454807
H	-0.767216	12.148754	-0.620849
H	-1.415788	10.325990	0.843181
H	-0.781783	7.346870	2.975289
H	-1.808678	8.795474	2.741699
O	-2.011442	7.123270	1.466470
H	0.907940	13.229600	-2.109718
C	-3.149321	7.563896	0.853458
O	-3.507753	8.718761	0.984407
C	-4.416177	6.843146	-1.156914
C	-3.849474	6.504757	0.073417
C	-5.100704	5.883038	-1.892628
C	-3.964261	5.203592	0.563567
C	-5.228038	4.584489	-1.395476
H	-5.537864	6.144963	-2.864045
C	-4.654664	4.244295	-0.169684
H	-3.512927	4.932091	1.525031
C	-5.976198	3.580735	-2.202634
H	-4.747981	3.224209	0.221434
O	-5.975813	3.465243	-3.412756
O	-6.738370	2.740864	-1.445042
H	-10.656372	-1.829949	-1.478151
C	-10.568934	-2.915288	-1.343689
C	-11.396693	-3.771063	-2.018008
C	-9.573388	-3.416049	-0.459225
C	-11.277429	-5.169424	-1.846287
H	-12.159751	-3.381495	-2.700045
C	-9.454094	-4.811139	-0.295716
C	-8.697075	-2.549058	0.265192
C	-10.327793	-5.680385	-1.004636
H	-11.951358	-5.834350	-2.396277
C	-8.457864	-5.338911	0.565326
C	-7.741588	-3.094992	1.107137
C	-8.836229	-1.088153	0.093794
H	-10.222718	-6.762711	-0.866214
C	-7.604676	-4.510667	1.250275
H	-8.373327	-6.430029	0.668653
O	-6.820930	-2.270589	1.755781
C	-9.742381	-0.373789	0.938560
C	-8.124798	-0.403167	-0.878188
C	-6.545758	-5.115484	2.130878
C	-10.523725	-1.027423	1.932663
C	-9.880673	1.020035	0.780936
C	-8.274099	1.009948	-1.042067
O	-7.358487	-1.108011	-1.803574
H	-6.198436	-4.419079	2.915759
H	-6.921026	-6.032120	2.626991
O	-5.332758	-5.339200	1.418165
C	-11.382314	-0.316269	2.725896
H	-10.431749	-2.115447	2.043208
C	-10.775287	1.738596	1.620628
C	-9.136208	1.693202	-0.221317
C	-7.539435	1.760731	-2.117291

C	-5.115472	-6.533271	0.792286
C	-11.507580	1.083691	2.572406
H	-11.984009	-0.824580	3.486683
H	-10.867226	2.822907	1.489097
H	-9.264448	2.777505	-0.333585
H	-6.891409	1.111500	-2.736504
H	-8.257666	2.264156	-2.793410
O	-5.934471	-7.428270	0.879780
C	-3.778623	-7.244555	-1.175808
H	-12.198560	1.632275	3.220788
C	-3.821047	-6.589086	0.056265
C	-2.578890	-7.337049	-1.871354
C	-2.662404	-6.022369	0.588243
C	-1.416431	-6.781828	-1.332675
H	-2.546340	-7.843404	-2.843994
C	-1.460615	-6.119829	-0.105034
H	-2.693186	-5.499551	1.551363
C	-0.144757	-6.905505	-2.098503
H	-0.551437	-5.677427	0.319202
O	-0.009053	-6.862453	-3.305795
O	0.945768	-7.103241	-1.303603
C	-5.993156	-1.222771	-1.461708
H	-5.517204	-0.247080	-1.310066
H	-5.849096	-1.845115	-0.571806
H	-5.571771	-1.716020	-2.341437
C	-7.255795	-1.816200	3.019729
H	-8.189900	-1.243205	2.952861
H	-7.383617	-2.641851	3.729840
H	-6.434136	-1.169919	3.337598
C	4.272854	-4.504953	-1.578989
H	4.823203	-4.036694	-0.755397
H	4.513572	-4.012421	-2.524584
H	3.195946	-4.445071	-1.384011
C	5.485084	-4.763128	3.072692
H	5.607264	-5.828186	3.305928
H	6.242165	-4.172303	3.609992
H	4.481927	-4.425708	3.343178
C	1.859525	5.743828	-1.466394
H	1.238266	5.921655	-0.581829
H	1.233268	5.657376	-2.358100
H	2.447265	4.829317	-1.326185
C	1.997728	6.942699	3.067672
H	2.964343	7.461303	3.022523
H	1.348271	7.443021	3.795809
H	2.139529	5.895783	3.346436
H	9.006340	-0.241115	-1.973798
H	-4.689636	-7.691528	-1.592267
H	-4.326759	7.866937	-1.540270

C60@**4b** (E = 0.76812553 Ha)

C	-10.166373	-4.443189	1.972135
C	-9.278330	-4.807411	0.996902
C	-9.116702	-4.011285	-0.171201
C	-9.890313	-2.840352	-0.303605
C	-10.805579	-2.481765	0.723597
C	-10.938708	-3.266774	1.836042
H	-10.288348	-5.059434	2.869093
H	-8.679741	-5.721465	1.098269
C	-8.197497	-4.362433	-1.207838
C	-9.748822	-2.026707	-1.457523

H	-11.396855	-1.565889	0.607799
H	-11.640953	-2.994224	2.630617
C	-8.863425	-2.358045	-2.451958
C	-8.074848	-3.543116	-2.318160
H	-10.357232	-1.114718	-1.538637
C	-7.391936	-5.592804	-1.070635
C	-7.904984	-6.823340	-1.586577
C	-6.149662	-5.575054	-0.458196
C	-9.171969	-6.901951	-2.229411
C	-7.138310	-7.999455	-1.458166
C	-5.375401	-6.769981	-0.327337
C	-9.636936	-8.094664	-2.712620
H	-9.771321	-5.987587	-2.324578
C	-7.642246	-9.226857	-1.968870
C	-5.869929	-7.949230	-0.823857
C	-8.864093	-9.271394	-2.582422
H	-10.613781	-8.150855	-3.204303
H	-7.034359	-10.132723	-1.862648
H	-5.286706	-8.875621	-0.740266
H	-9.256410	-10.214236	-2.977250
O	-5.609544	-4.353882	-0.059248
O	-7.094167	-3.836131	-3.264460
C	-8.758318	-1.472360	-3.663472
H	-8.473237	-2.049473	-4.568050
H	-9.721047	-0.964978	-3.870077
C	-4.031581	-6.765957	0.346077
H	-4.006556	-6.039361	1.188907
H	-3.777876	-7.763490	0.753971
O	-7.675768	-0.554849	-3.569016
C	-7.861014	0.661081	-2.972811
O	-8.965842	0.977712	-2.573186
C	-6.624756	1.487178	-2.905298
C	-5.633795	1.397065	-3.885233
C	-6.477014	2.378470	-1.840390
C	-4.500296	2.197848	-3.798771
H	-5.742412	0.697132	-4.722119
C	-5.338262	3.180889	-1.765956
H	-7.253317	2.447833	-1.066310
C	-4.346562	3.091595	-2.744457
H	-3.722550	2.125272	-4.566732
H	-3.451738	3.723794	-2.684840
C	-5.191323	4.118447	-0.619444
O	-5.437124	3.896241	0.550626
O	-4.743895	5.350576	-0.993968
H	-5.790314	10.759201	-1.934030
C	-4.707427	10.777391	-2.102760
C	-3.930424	9.661297	-1.688308
C	-4.109860	11.852793	-2.700959
C	-2.536798	9.663677	-1.900981
C	-4.547032	8.546475	-1.063018
C	-2.711707	11.862807	-2.910441
H	-4.704015	12.714860	-3.021298
C	-1.761200	8.537346	-1.482133
C	-1.944265	10.798239	-2.523031
C	-3.803931	7.471532	-0.646833
H	-5.635207	8.560262	-0.917790
H	-2.250468	12.735017	-3.385545
C	-0.303324	8.535818	-1.720447
C	-2.389631	7.471738	-0.859567
H	-0.857820	10.805336	-2.677802
C	-4.495385	6.319601	0.027471

C	0.559606	9.118703	-0.741147
C	0.242955	7.978759	-2.865602
O	-1.641941	6.344363	-0.522774
H	-3.864555	5.898193	0.842248
H	-5.460981	6.626806	0.473296
C	0.059859	9.682734	0.465885
C	1.950578	9.134612	-0.968922
C	1.654850	7.989969	-3.090929
O	-0.566365	7.300513	-3.775872
C	0.911688	10.233749	1.383965
H	-1.022648	9.669561	0.644764
C	2.815926	9.714452	-0.001072
C	2.478375	8.566447	-2.156929
C	2.259150	7.393347	-4.332857
C	2.305835	10.251388	1.149047
H	0.522456	10.667205	2.311205
H	3.895288	9.718641	-0.193125
H	3.565976	8.588865	-2.315286
H	1.527683	7.300866	-5.156393
H	3.104257	8.012465	-4.693225
O	2.620640	6.029481	-4.143211
H	2.967965	10.697483	1.898295
C	3.885347	5.702176	-3.744227
O	4.712899	6.578024	-3.572048
C	4.100244	4.238491	-3.579911
C	3.375463	3.305737	-4.325324
C	5.063717	3.806180	-2.665970
C	3.615160	1.946790	-4.154440
H	2.616074	3.637001	-5.043631
C	5.299841	2.440393	-2.505015
H	5.633161	4.537728	-2.076192
C	4.574105	1.507368	-3.248229
H	3.044262	1.215929	-4.737446
C	6.319390	1.999927	-1.514713
H	4.757890	0.433051	-3.120479
O	6.542117	2.487962	-0.422856
O	7.063154	0.940889	-1.943532
H	9.166311	-4.174269	0.069698
C	8.589705	-5.101990	0.174366
C	8.803419	-5.940426	1.234417
C	7.619504	-5.418635	-0.817049
C	8.061943	-7.137344	1.363235
H	9.551629	-5.693120	1.994808
C	6.886944	-6.616050	-0.687802
C	7.367666	-4.562601	-1.933478
C	7.124972	-7.470154	0.423665
H	8.247806	-7.790755	2.221895
C	5.920412	-6.962452	-1.667233
C	6.403929	-4.918530	-2.863121
C	8.143389	-3.313661	-2.075569
H	6.542864	-8.394836	0.513085
C	5.675518	-6.142656	-2.739933
H	5.362811	-7.902622	-1.550005
O	6.079591	-4.016381	-3.875104
C	9.360805	-3.333912	-2.825441
C	7.713288	-2.126713	-1.506147
C	4.667223	-6.569501	-3.771587
C	9.856519	-4.524309	-3.427102
C	10.099905	-2.142967	-2.976138
C	8.465764	-0.920238	-1.660519
O	6.477973	-2.091010	-0.861313

H	4.900455	-6.146451	-4.771230
H	4.642226	-7.673028	-3.865896
O	3.378482	-6.017667	-3.532480
C	11.025587	-4.513100	-4.138111
H	9.285894	-5.453567	-3.303526
C	11.310842	-2.155653	-3.720872
C	9.629324	-0.941119	-2.386307
C	8.013485	0.371839	-1.039564
C	2.474081	-6.698681	-2.766738
C	11.761711	-3.315560	-4.288961
H	11.404523	-5.432485	-4.596686
H	11.873350	-1.221370	-3.830924
H	10.215672	-0.023149	-2.523925
H	7.565875	0.193334	-0.035906
H	8.853401	1.081662	-0.913129
O	2.778435	-7.779410	-2.296114
C	1.163744	-6.008447	-2.618820
H	12.693807	-3.330410	-4.863180
C	0.748744	-5.018284	-3.513032
C	0.330586	-6.386855	-1.562763
C	-0.493885	-4.415247	-3.352415
H	1.394999	-4.709316	-4.343358
C	-0.917256	-5.781420	-1.415959
H	0.655863	-7.159146	-0.852080
C	-1.332939	-4.793452	-2.310014
H	-0.815997	-3.637640	-4.053548
C	-1.790915	-6.193831	-0.283611
H	-2.315953	-4.320216	-2.194000
O	-1.467506	-6.351163	0.877987
O	-3.080521	-6.418502	-0.663675
C	6.577484	-2.109341	0.547284
H	7.092966	-3.006519	0.911617
H	7.083938	-1.207197	0.923667
H	5.530293	-2.110578	0.868104
C	6.657036	-4.331623	-5.123866
H	7.746727	-4.445298	-5.063814
H	6.208327	-5.244070	-5.544987
H	6.397197	-3.466087	-5.737533
C	-5.706626	-4.118741	1.329770
H	-5.063680	-4.812290	1.892956
H	-5.336497	-3.095640	1.428545
H	-6.739756	-4.189179	1.692163
C	-7.598994	-4.447838	-4.432005
H	-8.182105	-5.350772	-4.211832
H	-8.209738	-3.740678	-5.013633
H	-6.691884	-4.704831	-4.983683
C	-1.321529	6.278161	0.851302
H	-2.227818	6.153810	1.464005
H	-0.699609	5.379402	0.918650
H	-0.761266	7.159470	1.186967
C	-1.139590	8.135042	-4.759601
H	-1.745772	8.938177	-4.320158
H	-0.379256	8.570964	-5.418658
H	-1.772900	7.444095	-5.321133
C	-0.694995	-2.067199	6.175698
C	-1.807473	-1.744375	5.291076
C	-0.211560	-1.114628	7.055588
C	0.232397	-2.918277	5.440919
C	-2.380259	-0.485181	5.330813
C	-1.567497	-2.395947	4.009559
C	-0.814746	0.211530	7.097386

C	1.225115	-0.962196	7.247181
C	1.596677	-2.773645	5.622996
C	-0.306904	-3.121635	4.102147
C	-1.870969	0.518061	6.257348
C	-2.743683	0.189756	4.091165
C	-1.912480	-1.755034	2.832447
C	0.249183	1.183585	7.314886
C	1.509885	0.458194	7.407349
C	2.105745	-1.770085	6.549187
C	2.494326	-2.824243	4.475771
C	0.545492	-3.169092	3.013066
C	-1.919429	1.812954	5.590103
C	-2.458806	1.610072	4.251412
C	-2.515589	-0.428707	2.874297
C	-1.014819	-1.805577	1.685274
C	0.203233	2.413152	6.681276
C	2.661051	0.999062	6.861816
C	3.317995	-1.200452	5.974565
C	1.982371	-3.016730	3.204593
C	3.557916	-1.851739	4.693035
C	0.182404	-2.494012	1.773500
C	-0.909176	2.735997	5.796701
C	-1.960026	2.340093	3.186738
C	-1.990779	0.340403	1.753010
C	-1.063141	-0.510422	1.018381
C	1.415530	2.982755	6.106858
C	2.612672	2.293923	6.194644
C	3.588478	0.148245	6.126820
C	2.507235	-2.247457	2.083263
C	4.056561	-1.121669	3.628327
C	1.394761	-1.924518	1.198682
C	-0.384276	3.504810	4.675334
C	-0.896314	3.312328	3.404117
C	-1.720089	1.689060	1.905209
C	0.087878	0.030409	0.472557
C	1.052401	3.657494	4.867076
C	3.510416	2.243544	5.047534
C	4.113380	0.917285	5.005674
C	3.519524	-1.325811	2.288231
C	4.340861	0.298748	3.788681
C	1.348680	-0.695021	0.565265
C	0.000670	3.264185	2.255467
C	-0.508139	2.258839	1.330233
C	0.372733	1.450749	0.632912
C	1.904530	3.609417	3.777760
C	3.165460	2.884166	3.870312
C	3.468903	-0.029574	1.622561
C	3.977823	0.973650	2.549101
C	2.412623	0.277020	0.782698
C	1.365361	3.406608	2.438840
C	1.809511	1.603258	0.824402
C	3.405343	2.232897	2.588717
C	2.293071	2.555876	1.704047

C60@2x**4b** (E = 0.2426138 Ha)

C	2.583297	9.916293	0.271771
C	3.871542	9.483596	0.110910
C	4.595442	8.934778	1.206240
C	3.963691	8.861457	2.463909
C	2.619954	9.303618	2.602837

C	1.945741	9.818616	1.530103
H	2.030191	10.338526	-0.573892
H	4.368013	9.556058	-0.865011
C	5.933938	8.452750	1.068861
C	4.670288	8.347110	3.581457
H	2.129161	9.203534	3.584695
H	0.908146	10.153926	1.632990
C	5.959309	7.893652	3.456028
C	6.588510	7.929380	2.172360
H	4.161659	8.315785	4.556201
C	6.589618	8.518139	-0.253075
C	7.371775	9.668298	-0.584342
C	6.463866	7.490359	-1.173185
C	7.529555	10.758583	0.316370
C	8.007573	9.733272	-1.840845
C	7.099931	7.565351	-2.452006
C	8.286387	11.845279	-0.028046
H	7.025932	10.713894	1.290418
C	8.791122	10.871488	-2.175119
C	7.859193	8.664620	-2.762551
C	8.927199	11.902971	-1.286941
H	8.402382	12.683129	0.667426
H	9.282147	10.905864	-3.154466
H	8.364925	8.734879	-3.734538
H	9.529375	12.781689	-1.539845
O	5.792552	6.325771	-0.805018
O	7.838047	7.338203	1.993738
C	6.680985	7.394145	4.678185
H	7.783258	7.446880	4.559438
H	6.406497	7.995110	5.567533
C	6.940594	6.475084	-3.474145
H	5.902410	6.073125	-3.464242
H	7.150791	6.841868	-4.497454
O	6.488918	5.999079	4.882300
C	5.455318	5.559426	5.659086
O	4.732729	6.363420	6.219740
C	5.345492	4.077406	5.733803
C	6.463264	3.248821	5.613697
C	4.081909	3.520893	5.939837
C	6.312067	1.869062	5.698030
H	7.458622	3.678592	5.449984
C	3.939529	2.134275	6.023040
H	3.200747	4.173940	6.032953
C	5.056495	1.305495	5.900195
H	7.188789	1.219303	5.601281
H	4.948858	0.215069	5.959620
C	2.573636	1.579534	6.215422
O	1.528808	2.095798	5.859538
O	2.534005	0.388214	6.874907
H	1.380164	-1.967069	11.759439
C	1.495313	-2.901452	11.198372
C	1.546799	-2.846507	9.778610
C	1.587792	-4.101480	11.848217
C	1.703413	-4.036124	9.038742
C	1.426538	-1.606648	9.100144
C	1.731724	-5.298960	11.110426
H	1.548591	-4.149182	12.941259
C	1.772287	-3.971084	7.612043
C	1.788571	-5.269590	9.743706
C	1.475757	-1.543345	7.730562
H	1.283698	-0.694565	9.694013

H	1.794885	-6.250992	11.647714
C	1.931610	-5.225016	6.848029
C	1.683125	-2.742066	6.978418
H	1.892835	-6.198474	9.168486
C	1.251147	-0.219931	7.057281
C	0.763168	-5.913216	6.393911
C	3.184085	-5.746853	6.569383
O	1.899765	-2.662839	5.605291
H	0.728805	-0.347808	6.081035
H	0.617193	0.440971	7.683912
C	-0.548829	-5.416202	6.632773
C	0.909632	-7.121195	5.682093
C	3.328619	-6.980560	5.861093
O	4.313507	-5.000041	6.901408
C	-1.647412	-6.092522	6.175133
H	-0.664943	-4.476194	7.187692
C	-0.245592	-7.806611	5.217308
C	2.205709	-7.641768	5.431690
C	4.679954	-7.584930	5.594253
C	-1.493727	-7.301102	5.458396
H	-2.657639	-5.703346	6.355494
H	-0.118665	-8.740542	4.656932
H	2.297499	-8.586364	4.877204
H	5.417144	-7.299969	6.373870
H	4.621709	-8.690817	5.567398
O	5.290965	-7.046566	4.428333
H	-2.387923	-7.825931	5.087006
C	5.074047	-7.628353	3.211048
O	4.399216	-8.639251	3.139877
C	5.742204	-6.930015	2.079029
C	6.793920	-6.033216	2.284243
C	5.298126	-7.196910	0.781459
C	7.395461	-5.409775	1.196645
H	7.150065	-5.811558	3.297510
C	5.912545	-6.571257	-0.303881
H	4.466452	-7.896016	0.615256
C	6.962097	-5.673703	-0.097932
H	8.216977	-4.703812	1.360365
C	5.414454	-6.861935	-1.675286
H	7.443912	-5.178161	-0.950242
O	4.260679	-7.042076	-2.016400
O	6.409183	-6.938765	-2.604770
H	7.695477	-5.446053	-8.138270
C	8.093115	-4.485122	-8.488331
C	7.698238	-3.962826	-9.689822
C	9.030400	-3.794952	-7.670038
C	8.215589	-2.726156	-10.139295
H	6.976559	-4.497384	-10.316386
C	9.545488	-2.563703	-8.123419
C	9.462583	-4.311035	-6.409190
C	9.119843	-2.040701	-9.375160
H	7.882824	-2.326744	-11.102886
C	10.484464	-1.855631	-7.329690
C	10.359525	-3.583064	-5.644148
C	8.949590	-5.619138	-5.953614
H	9.526664	-1.079953	-9.711811
C	10.890463	-2.340552	-6.111866
H	10.881006	-0.902071	-7.706545
O	10.666377	-4.034006	-4.361522
C	9.673818	-6.802756	-6.299848
C	7.791762	-5.723379	-5.200696

C	11.901494	-1.560891	-5.315534
C	10.871465	-6.757458	-7.066992
C	9.193376	-8.057203	-5.872610
C	7.304414	-6.998424	-4.773332
O	7.156358	-4.560834	-4.768548
H	12.456688	-2.207512	-4.604540
H	12.641394	-1.079545	-5.985086
O	11.285208	-0.634223	-4.429136
C	11.542677	-7.907199	-7.383039
H	11.243242	-5.782012	-7.405663
C	9.908461	-9.238053	-6.212312
C	8.001871	-8.131740	-5.105770
C	6.039252	-7.130435	-3.972443
C	11.037783	0.644665	-4.842638
C	11.057595	-9.162767	-6.950649
H	12.462462	-7.867123	-7.975928
H	9.522833	-10.205797	-5.871514
H	7.647876	-9.118359	-4.779144
H	5.282409	-6.379578	-4.292095
H	5.587192	-8.134501	-4.088796
O	11.391359	1.004368	-5.950078
C	10.345590	1.478649	-3.822793
H	11.611821	-10.069245	-7.214914
C	10.592824	1.316387	-2.458178
C	9.445075	2.451474	-4.260894
C	9.940936	2.128486	-1.536633
H	11.295909	0.550964	-2.109265
C	8.797260	3.262294	-3.328191
H	9.246685	2.577533	-5.334021
C	9.044026	3.102099	-1.963402
H	10.133921	2.000378	-0.465979
C	7.824821	4.277094	-3.816351
H	8.534722	3.739772	-1.229838
O	7.030394	4.151109	-4.729077
O	7.890030	5.459423	-3.140148
C	6.000234	-4.236053	-5.511246
H	6.223812	-4.084638	-6.574371
H	5.222318	-5.006720	-5.397979
H	5.667928	-3.300339	-5.049973
C	11.922552	-4.670577	-4.267474
H	12.034796	-5.485410	-4.993567
H	12.739413	-3.943512	-4.390904
H	11.920025	-5.065162	-3.248859
C	4.481190	6.240701	-1.322193
H	4.486603	6.192969	-2.422084
H	4.114661	5.294885	-0.909595
H	3.852768	7.075699	-0.988311
C	8.917893	8.151837	2.398347
H	8.899528	9.140074	1.921991
H	8.935135	8.263927	3.492978
H	9.789003	7.583699	2.064091
C	0.714041	-2.582778	4.840442
H	0.158968	-1.656876	5.056937
H	1.089085	-2.563352	3.811883
H	0.063428	-3.451860	4.998133
C	4.968309	-5.445975	8.069223
H	4.294975	-5.492358	8.934374
H	5.437132	-6.428573	7.907985
H	5.735447	-4.683847	8.223947
C	0.347739	2.777560	-3.580054
C	0.824027	3.324539	-2.315828

C	-0.815273	2.028296	-3.615287
C	1.508584	2.358110	-4.355103
C	0.113364	3.094734	-1.150812
C	2.279175	3.243048	-2.309652
C	-1.563872	1.786364	-2.388307
C	-0.878911	0.819825	-4.427604
C	1.448101	1.210863	-5.126825
C	2.702331	2.645980	-3.570071
C	-1.111654	2.305845	-1.188031
C	0.820348	2.771555	0.082101
C	2.951632	2.938967	-1.138238
C	-2.090205	0.428213	-2.442356
C	-1.666909	-0.169114	-3.702645
C	0.223398	0.421711	-5.163694
C	2.577985	0.290527	-5.154214
C	3.774683	1.771736	-3.595871
C	-1.161611	1.494766	0.021984
C	0.032279	1.782642	0.806996
C	2.202182	2.695119	0.088239
C	4.080230	2.016466	-1.166262
C	-2.137822	-0.341825	-1.293414
C	-1.312967	-1.506133	-3.750499
C	0.596282	-0.986381	-5.213886
C	3.711389	0.563670	-4.408677
C	2.051418	-1.067450	-5.207755
C	4.481481	1.448907	-2.362970
C	-1.661474	0.205307	-0.029231
C	0.665831	0.766462	1.500692
C	2.869058	1.624732	0.818763
C	4.029676	1.205462	0.043589
C	-1.764891	-1.749864	-1.343766
C	-1.363195	-2.317036	-2.540559
C	-0.152003	-1.925305	-4.525572
C	4.378801	-0.506396	-3.677862
C	2.685301	-2.083652	-4.514267
C	4.854595	0.040825	-2.413492
C	-0.994031	-0.864603	0.701541
C	0.139217	-0.591437	1.447368
C	2.120897	0.685402	1.506808
C	4.383734	-0.131620	-0.004087
C	-1.058117	-2.073038	-0.110716
C	-0.233406	-3.237486	-2.567885
C	0.515169	-2.995197	-3.794771
C	3.881054	-1.797005	-3.730662
C	1.897032	-3.071917	-3.788934
C	4.806911	-0.728904	-1.264472
C	1.268995	-1.512879	1.422664
C	2.493748	-0.722633	1.457163
C	3.595907	-1.120523	0.720821
C	0.014651	-2.946846	-0.136534
C	0.437746	-3.544007	-1.397066
C	3.828553	-2.606261	-2.519070
C	2.603521	-3.394873	-2.555978
C	4.280552	-2.086815	-1.318595
C	1.208363	-2.659116	0.648873
C	3.532134	-2.328898	-0.091490
C	1.892880	-3.624766	-1.391016
C	2.369120	-3.078065	-0.126697
H	-9.018238	-12.400263	0.690674
C	-8.875430	-11.569182	-0.007923
C	-8.137780	-10.476079	0.357111

C	-9.461622	-11.642319	-1.292428
C	-7.945665	-9.394673	-0.547556
H	-7.676634	-10.418794	1.351309
C	-9.292234	-10.619151	-2.184478
H	-10.048892	-12.526232	-1.561766
C	-7.182064	-8.238563	-0.195733
C	-8.528339	-9.474033	-1.828842
H	-9.741329	-10.665419	-3.183267
C	-6.575052	-8.157367	1.148388
C	-7.026713	-7.216680	-1.118047
C	-8.347675	-8.412601	-2.753154
C	-5.243887	-8.641100	1.340626
C	-7.265706	-7.613442	2.219251
C	-7.609837	-7.305009	-2.420661
O	-6.378906	-6.045802	-0.729155
H	-8.812025	-8.494187	-3.744673
C	-4.484752	-9.210867	0.280482
C	-4.655865	-8.548414	2.618107
C	-6.678146	-7.549609	3.521361
O	-8.510122	-7.029239	1.988732
C	-7.421631	-6.218100	-3.441608
C	-5.047239	-5.953819	-1.190518
H	-4.946340	-9.295634	-0.711433
C	-3.206047	-9.648809	0.494352
C	-3.321205	-8.997341	2.812470
C	-5.396527	-8.006119	3.699900
C	-7.435066	-7.012310	4.705435
C	-9.599370	-7.837833	2.378161
O	-8.432576	-5.240264	-3.183234
H	-6.404576	-5.771770	-3.367013
H	-7.545944	-6.603006	-4.472310
H	-4.439960	-6.813445	-0.880471
H	-5.014471	-5.847426	-2.285545
H	-4.688089	-5.040273	-0.711114
C	-2.613417	-9.535474	1.773185
H	-2.625753	-10.087782	-0.324173
H	-2.865544	-8.884543	3.809822
H	-4.919859	-7.953291	4.689854
H	-8.533296	-7.088729	4.563542
H	-7.171689	-7.569181	5.626213
O	-7.271324	-5.606609	4.854220
H	-9.564044	-8.835632	1.923251
H	-9.648636	-7.927262	3.473944
H	-10.461792	-7.279796	2.006497
C	-8.384745	-4.070077	-3.881338
H	-1.583308	-9.877995	1.918095
C	-6.251199	-5.115918	5.618247
C	-9.440139	-3.101367	-3.478720
O	-7.540318	-3.918685	-4.743743
O	-5.521187	-5.885334	6.217110
C	-6.164482	-3.630543	5.634493
C	-10.091716	-2.366920	-4.470378
C	-9.761266	-2.909804	-2.133649
C	-7.272443	-2.822243	5.369272
C	-4.931601	-3.047262	5.934223
C	-11.068310	-1.437997	-4.108874
H	-9.836235	-2.517741	-5.527679
C	-10.735528	-1.980604	-1.784367
H	-9.249481	-3.488729	-1.354676
C	-7.142006	-1.438212	5.402562
H	-8.244659	-3.270146	5.131312

C	-4.810750	-1.656662	5.969086
H	-4.056716	-3.683166	6.139220
C	-11.762683	-0.677695	-5.184201
C	-11.390169	-1.243016	-2.764709
H	-10.987277	-1.828300	-0.729265
C	-5.917501	-0.849111	5.699631
H	-8.010726	-0.805344	5.190393
C	-3.477043	-1.074226	6.273680
O	-11.939052	0.642682	-4.881617
O	-12.170231	-1.123216	-6.240072
H	-12.153353	-0.509433	-2.480119
H	-5.825809	0.244245	5.718544
O	-2.395202	-1.584036	6.040190
O	-3.520535	0.138547	6.893470
C	-12.522386	1.522138	-5.836590
C	-2.272280	0.770762	7.192021
C	-11.494974	2.106339	-6.767547
H	-12.966166	2.284726	-5.170824
H	-13.342923	1.040122	-6.403557
C	-2.573398	2.152708	7.696589
H	-1.614610	0.813204	6.292032
H	-1.743696	0.171223	7.960614
C	-10.755005	3.279654	-6.421098
C	-11.263545	1.499320	-7.975995
C	-2.709307	3.261706	6.803794
C	-2.659966	2.362435	9.049580
C	-9.794227	3.798132	-7.274458
O	-10.953563	3.828929	-5.155541
C	-10.294487	2.011983	-8.876672
H	-11.822138	0.595755	-8.258953
C	-2.851296	4.551558	7.289822
O	-2.802943	3.033426	5.433907
C	-2.846163	3.666722	9.575587
H	-2.576215	1.520864	9.749428
C	-9.010909	4.997652	-6.913972
C	-9.550926	3.158269	-8.529955
C	-11.833725	4.932762	-5.150285
C	-10.060200	1.371386	-10.124241
C	-2.919697	5.713093	6.380106
C	-2.923941	4.769511	8.700801
C	-1.555186	2.893822	4.785160
C	-2.937910	3.873611	10.979207
C	-9.436632	6.277493	-7.389684
C	-7.877582	4.908945	-6.121830
C	-8.575992	3.641387	-9.447260
H	-11.500952	5.733811	-5.823588
H	-12.856329	4.636317	-5.412311
H	-11.793320	5.267437	-4.111001
C	-9.117162	1.860122	-10.986271
H	-10.645544	0.479785	-10.377827
C	-1.703207	6.347877	5.976540
C	-4.130462	6.195016	5.911184
C	-3.075488	6.070619	9.257152
H	-1.045795	1.969866	5.100177
H	-1.838150	2.830559	3.731878
H	-0.898589	3.756398	4.955068
C	-3.091786	5.135537	11.484053
H	-2.882808	3.005525	11.645957
C	-8.699706	7.426941	-7.038550
C	-10.588981	6.431629	-8.210623
C	-7.140018	6.078252	-5.756869

O	-7.486350	3.692169	-5.567235
C	-8.367364	3.008402	-10.642208
H	-7.998980	4.535376	-9.179146
H	-8.931768	1.369536	-11.947392
C	-0.428722	5.886349	6.410215
C	-1.761650	7.463052	5.116124
C	-4.186647	7.331136	5.044654
O	-5.296593	5.493071	6.212860
C	-3.156747	6.246256	10.611622
H	-3.118549	6.931573	8.577852
H	-3.163024	5.300051	12.564075
C	-9.117054	8.701754	-7.509868
C	-7.553182	7.304623	-6.211600
C	-10.971822	7.668659	-8.652420
H	-11.159707	5.536461	-8.488536
C	-5.926187	5.994748	-4.873890
C	-6.696190	2.902477	-6.431213
H	-7.616776	3.384778	-11.345189
C	0.718663	6.508389	5.997525
H	-0.381242	5.017363	7.078998
C	-0.557305	8.095481	4.704003
C	-3.018555	7.941410	4.663277
C	-5.495834	7.886791	4.555320
C	-6.065483	6.082615	7.238851
H	-3.270971	7.249688	11.034845
H	-8.533428	9.585886	-7.228550
C	-10.228476	8.818176	-8.298748
H	-7.002818	8.213990	-5.936900
H	-11.857611	7.781340	-9.286335
O	-6.414567	6.059076	-3.530872
H	-5.358751	5.057917	-5.038670
H	-5.236492	6.842517	-5.053128
H	-5.722744	3.367475	-6.626940
H	-6.565729	1.980191	-5.859972
H	-7.202146	2.695308	-7.383387
C	0.653263	7.627031	5.136160
H	1.700225	6.143258	6.324663
H	-0.613745	8.957549	4.028252
H	-3.041578	8.808730	3.988550
H	-6.306864	7.731537	5.297515
H	-5.417758	8.973378	4.354978
O	-6.006449	7.169328	3.438839
H	-5.487819	6.233711	8.159412
H	-6.498317	7.039233	6.908793
H	-6.857064	5.347769	7.402166
H	-10.553638	9.797696	-8.664209
C	-5.525722	5.886946	-2.511604
H	1.585975	8.112401	4.808237
C	-5.647212	7.529774	2.170590
C	-6.178831	5.886101	-1.173912
O	-4.340474	5.771291	-2.755829
O	-4.924073	8.494448	2.001569
C	-6.236265	6.668644	1.108900
C	-5.633539	6.662435	-0.151720
C	-7.313959	5.107743	-0.941837
C	-7.372244	5.889188	1.341919
H	-4.735091	7.266890	-0.337191
C	-7.902419	5.112074	0.317970
H	-7.741328	4.498709	-1.748103
H	-7.851499	5.881520	2.328203
H	-8.791088	4.499292	0.504214

C60@**4c** (E = 0.76332958 Ha)

C	10.471103	3.826462	-1.980098
C	9.219015	4.371491	-1.895059
C	8.216705	4.038950	-2.848698
C	8.536671	3.129193	-3.876547
C	9.845989	2.579051	-3.946863
C	10.790545	2.921537	-3.018561
H	11.240012	4.086103	-1.244894
H	8.968376	5.075844	-1.091911
C	6.901487	4.595369	-2.792713
C	7.550310	2.763179	-4.828165
H	10.080868	1.876756	-4.755227
H	11.800000	2.500368	-3.067868
C	6.277287	3.271256	-4.760158
C	5.956050	4.208238	-3.728866
H	7.824834	2.058637	-5.625647
C	6.579057	5.567986	-1.728827
C	6.849834	6.955950	-1.940928
C	6.018164	5.159106	-0.530641
C	7.440335	7.434439	-3.143852
C	6.530223	7.884134	-0.929080
C	5.681975	6.104304	0.488479
C	7.691720	8.768607	-3.315255
H	7.697735	6.710588	-3.927454
C	6.798183	9.265585	-1.131385
C	5.938367	7.435547	0.280504
C	7.365931	9.696201	-2.299260
H	8.149453	9.131879	-4.241442
H	6.540034	9.975480	-0.336888
H	5.677068	8.177888	1.047532
H	7.574244	10.759088	-2.459795
O	5.687878	3.815221	-0.364619
O	4.639023	4.653900	-3.621404
C	5.257802	2.845362	-5.781319
H	4.342987	3.465068	-5.755572
H	5.685624	2.907336	-6.801392
C	5.051005	5.669046	1.782990
O	4.714576	1.561132	-5.486340
C	5.226876	0.445536	-6.082908
O	6.172486	0.539493	-6.843319
C	4.515205	-0.812560	-5.721182
C	3.132419	-0.837644	-5.532889
C	5.258065	-1.990341	-5.613578
C	2.490783	-2.041814	-5.263797
H	2.546411	0.086412	-5.601839
C	4.618020	-3.193005	-5.338787
H	6.345200	-1.969207	-5.758420
C	3.231946	-3.221397	-5.179328
H	1.395537	-2.067602	-5.128937
H	5.200587	-4.118189	-5.251350
C	2.560555	-4.528265	-4.928405
O	2.964303	-5.441227	-4.235499
O	1.385967	-4.648166	-5.614817
O	-13.029594	0.811382	-0.648736
C	-12.091988	0.202318	-0.176256
C	-11.292641	-0.876948	-0.821834
O	-11.671629	0.458628	1.101050
C	-9.919597	-0.690730	-0.991411
C	-11.910223	-2.045745	-1.263430

C	-9.164049	-1.680929	-1.605488
H	-9.436386	0.227971	-0.634873
C	-11.148888	-3.044227	-1.864242
H	-12.990549	-2.180396	-1.137116
C	-9.777708	-2.859521	-2.033227
H	-8.080844	-1.538294	-1.752622
H	-11.625507	-3.973058	-2.198032
C	-8.938820	-3.933971	-2.634031
O	-8.226310	-3.497388	-3.723511
O	-8.854849	-5.089367	-2.274221
C	-7.075495	-4.213675	-4.142566
C	-5.821563	-3.801504	-3.418221
H	-7.016559	-3.923937	-5.207426
H	-7.222675	-5.315711	-4.081393
C	-5.759488	-2.649909	-2.677066
C	-4.648116	-4.615050	-3.529855
C	-4.566654	-2.266737	-2.010812
H	-6.639736	-1.993379	-2.572478
C	-3.462391	-4.257779	-2.910595
O	-4.669200	-5.736256	-4.358441
C	-3.410567	-3.064137	-2.124425
C	-4.531885	-1.084532	-1.222467
C	-2.255493	-5.099829	-3.038604
C	-2.232489	-2.657875	-1.438573
C	-3.385017	-0.721092	-0.570881
H	-5.439374	-0.473197	-1.142065
C	-1.984208	-6.074449	-2.028038
C	-1.400758	-4.985237	-4.122998
C	-2.223386	-1.518830	-0.679240
H	-1.334179	-3.283560	-1.519053
H	-3.362626	0.194122	0.041216
C	-2.837686	-6.253250	-0.903587
C	-0.843027	-6.893147	-2.146614
C	-0.266507	-5.845427	-4.260738
O	-1.692586	-4.121001	-5.176667
H	-1.313181	-1.221895	-0.141300
C	-2.547904	-7.190117	0.050674
H	-3.731982	-5.623278	-0.815259
C	-0.559267	-7.855573	-1.139419
C	0.002535	-6.764951	-3.278823
C	0.595364	-5.822075	-5.492722
C	-1.393842	-7.998633	-0.064969
H	-3.207420	-7.323317	0.914757
H	0.337197	-8.478127	-1.241541
H	0.879529	-7.422157	-3.358467
H	-1.180006	-8.738480	0.713283
O	2.986461	7.413324	1.948264
C	2.723843	6.280140	1.598148
C	1.398628	5.764157	1.152524
O	3.685955	5.309565	1.613795
C	0.288822	5.906622	1.985574
C	1.271243	5.171200	-0.103840
C	-0.954129	5.451324	1.560796
H	0.394474	6.379825	2.968578
C	0.024419	4.729304	-0.534552
H	2.149514	5.050682	-0.750547
C	-1.083255	4.870744	0.299210
H	-1.829824	5.550014	2.213958
H	-0.082725	4.273792	-1.525547
C	-2.425583	4.422683	-0.168334
O	-2.837303	3.279608	0.463981

O	-3.122231	4.943190	-1.013951
C	-4.157898	2.798205	0.260435
C	-5.179820	3.439769	1.158259
H	-4.027644	1.720989	0.504161
H	-4.457946	2.879390	-0.808534
C	-4.814315	4.057089	2.327260
C	-6.567147	3.388578	0.806545
C	-5.780945	4.661316	3.172601
H	-3.760370	4.099377	2.635012
C	-7.533796	3.971112	1.608914
O	-6.966580	2.645951	-0.304153
C	-7.144308	4.626341	2.818188
C	-5.384363	5.304892	4.376687
C	-8.964822	3.920286	1.245875
C	-8.090996	5.244309	3.681711
C	-6.317338	5.889981	5.188405
H	-4.320834	5.322659	4.641186
C	-9.519403	4.956724	0.432664
C	-9.775227	2.882064	1.674354
C	-7.685803	5.859806	4.834814
H	-9.151902	5.222114	3.401937
H	-6.016540	6.387171	6.116400
C	-8.738181	6.051561	-0.031287
C	-10.882896	4.899900	0.078584
C	-11.153619	2.817198	1.298816
O	-9.198937	1.837149	2.394699
H	-8.417321	6.336688	5.495596
C	-9.300030	7.030832	-0.804636
H	-7.677471	6.098004	0.246995
C	-11.443626	5.928731	-0.726540
C	-11.683222	3.813434	0.518716
C	-12.034216	1.677043	1.734623
C	-10.667759	6.969886	-1.157503
H	-8.695256	7.872531	-1.158564
H	-12.504545	5.869563	-0.996115
H	-12.737573	3.777312	0.211523
H	-11.860775	1.422468	2.801378
H	-13.107219	1.913240	1.599035
H	-11.094835	7.764257	-1.778386
H	-0.017658	-5.747203	-6.409564
H	1.220826	-6.733400	-5.562378
H	5.483621	4.710621	2.139644
H	5.185401	6.429097	2.576899
C	3.490963	-0.171175	5.701602
C	2.694054	-1.149122	6.270721
C	4.924286	-0.392260	5.556969
C	3.026301	0.554789	4.526368
C	3.288175	-2.399967	6.725428
C	1.390145	-1.452895	5.694828
C	5.488433	-1.580006	5.988646
C	5.345338	0.196961	4.292260
C	4.172423	0.782390	3.655316
C	1.788166	0.266346	3.979421
C	4.649201	-2.609848	6.588114
C	2.351372	-3.476852	6.430611
C	1.178359	-2.891546	5.793665
C	0.948971	-0.763518	4.578805
C	6.503694	-2.241369	5.178714
C	6.309270	-0.431141	3.523074
C	4.022584	0.709778	2.281534
C	1.630308	0.190406	2.532485

C	5.145830	-3.907687	6.148561
C	2.822932	-4.709186	6.013103
C	0.536111	-3.568150	4.771458
C	0.272505	-1.476039	3.502253
C	6.291977	-3.679958	5.277502
C	6.903552	-1.681746	3.977743
C	6.151719	-0.507114	2.076155
C	2.718786	0.406176	1.705525
C	5.038895	0.050525	1.470121
C	0.693630	-0.886490	2.237600
C	4.256299	-4.930193	5.868422
C	2.146455	-5.421833	4.936654
C	1.032679	-4.866021	4.331859
C	0.071630	-2.842049	3.596090
C	6.490696	-4.486164	4.170303
C	7.113139	-2.530749	2.811850
C	6.648424	-1.804796	1.636651
C	2.928153	-0.442676	0.539543
C	4.361541	-0.663466	0.394554
C	0.890518	-1.692009	1.128971
C	4.465694	-5.779377	4.702526
C	3.161765	-6.083202	4.126630
C	0.874978	-4.942046	2.884868
C	0.281202	-3.691120	2.430258
C	5.553961	-5.563118	3.875356
C	6.911909	-3.896779	2.905598
C	6.005990	-2.481317	0.614500
C	2.038380	-1.464925	0.259183
C	4.833010	-1.895839	-0.022549
C	0.681005	-3.131468	1.229372
C	3.012063	-6.155313	2.752743
C	1.839006	-5.569872	2.115758
C	5.396335	-5.639362	2.428419
C	6.235610	-4.609405	1.829006
C	5.794284	-3.920022	0.713107
C	2.535132	-2.762871	-0.180125
C	3.896159	-2.972845	-0.317286
C	1.696115	-3.792738	0.419313
C	4.158213	-5.927679	1.881543
C	2.260254	-4.980433	0.851063
C	4.490252	-4.223783	0.137065
C	3.693471	-5.201732	0.706063
C	6.600427	3.111532	0.450581
H	7.619422	3.138133	0.045931
H	6.596302	3.499708	1.480876
H	6.204746	2.090449	0.435159
C	4.402797	5.883615	-4.274233
H	5.055845	6.683187	-3.900160
H	4.517898	5.796160	-5.361071
H	3.360697	6.093497	-4.021465
C	-6.847889	3.345473	-1.526807
H	-7.382267	4.303461	-1.511451
H	-5.790387	3.508947	-1.783645
H	-7.311193	2.661711	-2.241850
C	-9.490381	1.875060	3.775340
H	-9.175561	2.818887	4.237734
H	-10.562075	1.707157	3.962508
H	-8.903445	1.042103	4.168972
C	-1.308626	-2.782711	-4.946258
H	-1.724032	-2.383072	-4.011687
H	-0.213125	-2.662294	-4.940482

H	-1.734992	-2.261356	-5.806779
C	-5.227272	-6.878137	-3.740060
H	-4.732576	-7.121024	-2.791787
H	-6.307795	-6.745811	-3.577247
H	-5.047836	-7.664528	-4.476633

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