

16

1 scf done: -496.127554
C -0.788441 0.032829 -2.454144
C -1.955393 -0.207950 -1.717690
C 0.415677 0.295440 -1.804240
H -2.892743 -0.412242 -2.219190
H 1.309698 0.479822 -2.385661
C -1.903255 -0.183286 -0.342970
C 0.465777 0.319800 -0.417777
O -2.978567 -0.403854 0.473984
H 1.385512 0.520699 0.113090
C -0.688857 0.081485 0.311372
O -0.639338 0.105493 1.668292
C -0.808872 0.014522 -3.915863
H 0.156360 0.215250 -4.401265
O -1.801827 -0.203089 -4.591272
H -3.768436 -0.577061 -0.051993
H -1.518360 -0.077859 2.025191

3

H00. scf done: -150.913426
O -0.767852 0.000000 -2.406362
O -0.322127 0.000000 -1.144366
H -0.823390 0.000000 -0.234266

19

Complejo 1(H) scf done: -647.076417
C 0.292315 -0.309688 -0.118789
C -0.479377 0.853385 0.019546
C -1.848901 0.748908 0.069043
C -2.462874 -0.513607 -0.015354
C -1.698902 -1.662938 -0.153339
C -0.317817 -1.561039 -0.204984
O -3.812701 -0.614302 0.035981
H -2.200572 -2.617924 -0.217237
C 1.739878 -0.241697 -0.169825
O 2.381984 0.804341 -0.090424
O 5.112924 -0.514857 0.668500
O 4.958903 0.555499 -0.058961
O -2.703289 1.808560 0.198051
H -0.006910 1.824813 0.086038
H 0.291802 -2.448708 -0.310191
H -4.199889 0.267293 0.121039
H 2.265354 -1.196208 -0.287616
H 3.960905 0.709041 -0.117061
H -2.211118 2.637768 0.224184

19

TS1-H scf done: -647.041895
C 0.069058 -3.968754 1.860024
C 0.810792 -3.371994 2.890000
C 1.906832 -4.033056 3.392686
C 2.268697 -5.289407 2.872922
C 1.530814 -5.874106 1.853809
C 0.425391 -5.212522 1.343517
O 3.348085 -5.940082 3.368882
H 1.835216 -6.840187 1.476716
C -1.094398 -3.287869 1.315020
O -1.560180 -2.227681 1.614846
O -2.505727 -4.234548 -0.557539
O -3.426908 -3.213895 -0.527333
O 2.709332 -3.560723 4.392618

H	0.528487	-2.405187	3.287147
H	-0.161035	-5.654566	0.549420
H	3.754007	-5.410024	4.068795
H	-1.686754	-3.910370	0.394590
H	-3.078752	-2.548208	-1.138245
H	2.403263	-2.699544	4.701913

15

1R(H)	scf done:	-495.468925	
C	-0.794527	0.031853	-2.447061
C	-1.964590	-0.209717	-1.710620
C	0.413398	0.295034	-1.805621
H	-2.901976	-0.413993	-2.211851
H	1.302056	0.478222	-2.393373
C	-1.907534	-0.184056	-0.336128
C	0.463702	0.319371	-0.420212
O	-2.978706	-0.403760	0.484855
H	1.384288	0.520346	0.108935
C	-0.689876	0.081273	0.312368
O	-0.634628	0.106350	1.666761
C	-0.834177	0.009094	-3.904846
O	-1.741778	-0.191185	-4.644877
H	-3.771508	-0.577515	-0.036618
H	-1.511569	-0.076569	2.029416

19

Complejo 1(H2)	scf done:	-647.071798	
C	-1.839507	0.210489	0.002970
C	-1.988380	-1.158796	0.156009
C	-0.566877	0.776353	-0.192762
H	2.101491	2.116341	1.155195
O	-0.542966	2.135257	-0.324134
C	-0.867822	-1.976408	0.108726
C	0.544822	-0.035201	-0.244319
C	0.392912	-1.419705	-0.092260
C	1.549816	-2.310659	-0.143497
O	-2.936261	1.011310	0.046765
O	2.700023	-1.942660	-0.320493
H	-2.667647	1.930323	-0.087778
H	0.366542	2.454865	-0.457681
H	1.325115	-3.378017	-0.009842
O	2.722047	2.701762	0.678313
O	2.129789	3.098929	-0.406685
H	-2.979230	-1.563329	0.308662
H	1.525037	0.396514	-0.402393
H	-0.968903	-3.047370	0.225206

19

TS1-H2	scf done:	-647.014660	
C	-2.095186	-0.032384	-0.048460
C	-2.011508	-1.399533	0.174831
C	-0.927354	0.736061	-0.233086
H	2.004484	2.727716	1.014726
O	-1.099445	2.072568	-0.430258
C	-0.774421	-2.026095	0.214445
C	0.265221	0.069886	-0.202935
C	0.400035	-1.292340	0.025042
C	1.696706	-1.966735	0.081253
O	-3.309302	0.566401	-0.084249
O	2.766788	-1.401108	-0.055181
H	-3.204893	1.512994	-0.250221
H	-0.245123	2.521463	-0.481397

H	1.650347	-3.048643	0.264473
O	2.575336	2.010010	0.706298
O	2.101816	1.734238	-0.572925
H	-2.926379	-1.956422	0.319215
H	1.397887	0.893902	-0.441523
H	-0.705294	-3.091093	0.396076

15

1R(H2) scf done: -495.432017

C	1.299110	1.414911	0.612484
C	1.151593	2.800691	0.400422
C	0.327769	0.521865	0.174621
O	2.153202	3.604184	0.862553
C	0.020002	3.191098	-0.246515
C	-0.803658	0.984974	-0.479116
H	-1.561996	0.291927	-0.821400
C	-0.981726	2.356606	-0.706185
C	-2.175040	2.841351	-1.395371
O	2.398521	0.946201	1.249773
O	-2.401461	4.016195	-1.629304
H	-2.885080	2.062466	-1.703759
H	2.975364	1.683902	1.489978
H	1.955132	4.529264	0.671475
H	0.478205	-0.532456	0.356468

19

Complejo 1(H3) scf done: -647.075710

C	-0.981659	-0.589913	0.089736
C	-0.062350	0.175291	-0.642693
C	1.242950	-0.246345	-0.734965
C	1.649312	-1.429353	-0.092126
C	0.739606	-2.187592	0.629343
C	-0.579088	-1.769478	0.716335
O	2.937813	-1.840466	-0.180520
O	2.223485	0.410176	-1.425905
C	-2.371360	-0.187821	0.225281
O	-2.854859	0.859133	-0.194471
O	-1.058986	3.406503	0.334698
O	-1.865758	3.259321	-0.677327
H	1.079543	-3.095189	1.108014
H	-0.367596	1.083447	-1.144995
H	-1.300318	-2.352751	1.273378
H	-3.017822	-0.898328	0.753609
H	1.863532	1.183719	-1.875692
H	-2.224044	2.329620	-0.607786
H	3.441514	-1.211446	-0.714673

19

TS1-H3 scf done: -647.047751

C	-1.112877	-0.193713	-0.346540
C	-0.787112	1.152065	-0.346251
C	0.547313	1.538540	-0.180662
C	1.547000	0.538530	0.002521
C	1.209310	-0.810375	0.005741
C	-0.112939	-1.167161	-0.170208
O	2.819184	0.910254	0.178198
O	0.929315	2.809638	-0.210318
C	-2.501499	-0.633952	-0.529707
O	-3.441375	0.123027	-0.689979
O	0.975202	3.212904	2.120634
O	0.671757	1.927824	2.425361
H	1.984112	-1.550083	0.145701

H	-1.541838	1.915167	-0.480449
H	-0.393563	-2.212648	-0.172613
H	-2.656330	-1.721402	-0.515066
H	0.997035	3.174648	0.841898
H	-0.296070	1.897485	2.512004
H	2.881618	1.876331	0.118925

15

1R(H3)	scf done:	-495.481514	
C	-0.813853	-0.000743	-2.470001
C	-1.961827	-0.314222	-1.788577
C	0.376507	0.334180	-1.777310
H	-2.876755	-0.571566	-2.304042
H	1.260533	0.575233	-2.353074
C	-1.964918	-0.304759	-0.355464
C	0.430014	0.358701	-0.395628
O	-2.965059	-0.576269	0.347155
H	1.337145	0.613861	0.132252
C	-0.715043	0.045904	0.316647
O	-0.724766	0.051778	1.643288
C	-0.788054	-0.004039	-3.945977
H	0.175399	0.259263	-4.402437
O	-1.749826	-0.274887	-4.636819
H	-1.619709	-0.192435	1.938276

19

Complejo 1(H4)	scf done:	-647.071101	
C	1.137187	-0.394398	-0.961239
C	0.568412	0.884464	-0.834156
C	0.437947	-1.518697	-0.544027
O	1.352615	1.920028	-1.260300
H	0.899579	-2.490126	-0.652254
C	-0.692797	1.029678	-0.302557
C	-0.837535	-1.373905	-0.010322
H	-1.126771	2.016390	-0.201793
H	-1.394527	-2.243122	0.313860
C	-1.401743	-0.105383	0.110087
C	-2.742860	0.016194	0.682078
O	2.379423	-0.540261	-1.484590
O	-3.335950	1.071778	0.829840
H	-3.211777	-0.930472	0.983907
H	2.733069	0.325570	-1.728560
O	2.261978	0.452718	1.985124
O	1.186313	-0.116678	2.445028
H	0.891986	-0.765242	1.773684
H	0.895451	2.761460	-1.143812

19

TS1-H4	scf done:	-647.043891	
C	1.505850	0.395729	0.021867
C	0.516486	1.422479	0.084820
C	1.103298	-0.953298	-0.004683
O	0.975396	2.685499	0.126059
H	1.872855	-1.711252	-0.045646
C	-0.828232	1.090234	0.104318
C	-0.233319	-1.272538	0.006313
H	-1.578018	1.869493	0.151577
H	-0.556120	-2.304674	-0.021737
C	-1.195106	-0.249475	0.062338
C	-2.618983	-0.631582	0.076105
O	2.782004	0.726358	-0.031603
O	-3.532990	0.168027	0.118741

H	-2.816938	-1.711022	0.044488
H	3.076741	1.120626	0.967118
O	3.088084	1.335813	2.234021
O	1.815468	1.009992	2.573866
H	1.848881	0.080144	2.855609
H	0.241861	3.311365	0.187656

15

1R(H4) scf done: -495.478078

C	-0.759075	0.008547	-2.476609
C	-1.916520	-0.355487	-1.800549
C	0.432139	0.365490	-1.783679
H	-2.812927	-0.623741	-2.344320
H	1.305837	0.641176	-2.359921
C	-1.911659	-0.371658	-0.418970
C	0.465208	0.358232	-0.426900
O	-2.966669	-0.704935	0.322784
H	1.352326	0.623468	0.130525
C	-0.705181	-0.011006	0.338112
O	-0.715695	-0.030246	1.580215
C	-0.743721	0.032366	-3.950239
H	0.206579	0.330513	-4.411218
O	-1.706459	-0.254558	-4.634944
H	-3.722960	-0.930347	-0.236936

19

Complejo 1(H5) scf done: -647.073387

C	0.708777	-0.347741	0.442959
C	0.762198	1.051301	0.349345
C	-0.269051	-1.069346	-0.220706
O	1.772361	1.651259	1.048488
C	-0.169123	1.721880	-0.412231
C	-1.208013	-0.393755	-0.988029
H	-0.131289	2.801122	-0.487969
H	-1.980247	-0.940844	-1.512430
C	-1.159564	0.994687	-1.082861
C	-2.166711	1.675270	-1.897834
O	1.633071	-1.010348	1.194931
O	-2.228122	2.883227	-2.053503
H	-2.897640	1.014933	-2.384735
O	1.447348	-4.177612	1.279342
O	1.018851	-3.434681	2.259508
H	1.202841	-2.500453	1.993768
H	2.221120	-0.382798	1.638523
H	1.724127	2.610339	0.959438
H	-0.280936	-2.146444	-0.126005

19

TS1-H5 scf done: -647.015209

C	1.248194	1.409921	0.709851
C	1.132158	2.778195	0.394558
C	0.223923	0.582354	0.305877
O	2.168156	3.561004	0.813703
C	0.028008	3.241930	-0.288327
C	-0.893765	0.993634	-0.374750
H	-0.049507	4.295748	-0.523752
H	-1.675728	0.306761	-0.672559
C	-0.983995	2.356176	-0.674331
C	-2.164891	2.827922	-1.403419
O	2.317674	0.929864	1.380651
O	-2.355279	3.987618	-1.722908
H	-2.897850	2.050522	-1.658955

O	0.490509	-1.844138	0.917236
O	0.463876	-1.857110	2.309541
H	-0.472051	-1.974642	2.524196
H	2.924933	1.655557	1.580454
H	2.010177	4.484876	0.583854
H	0.378841	-0.780359	0.630948

15

1R(H5) scf done: -495.432715

C	1.248920	1.406162	0.713766
C	1.130418	2.774404	0.399589
C	0.223243	0.592017	0.304135
O	2.164343	3.561247	0.818677
C	0.026671	3.239439	-0.285979
C	-0.893982	0.987205	-0.376015
H	-0.051082	4.293010	-0.520569
H	-1.676478	0.301549	-0.676747
C	-0.984226	2.353806	-0.674527
C	-2.163642	2.830182	-1.403337
O	2.324967	0.931599	1.386028
O	-2.352719	3.991729	-1.718204
H	-2.899181	2.056530	-1.662462
H	2.925445	1.664448	1.579057
H	2.011631	4.480611	0.567743

19

Complejo 1(H6) scf done: -647.071195

C	1.575685	-0.087165	-0.566315
C	0.733589	-0.619020	-1.531351
C	1.064135	0.738559	0.450466
H	-1.292922	-0.751424	-2.229665
O	1.983434	1.211641	1.342888
C	-0.623747	-0.335732	-1.487797
C	-0.284359	1.016557	0.499970
C	-1.134613	0.478707	-0.478186
C	-2.577182	0.727857	-0.440189
O	2.901097	-0.370482	-0.610198
H	-3.153277	0.254978	-1.247183
H	3.349916	0.058449	0.130841
H	1.561270	1.789082	1.989842
O	-3.138270	1.401841	0.406817
O	-2.362906	-2.385574	0.696167
O	-1.267754	-2.133074	1.351395
H	-0.940789	-1.265004	1.035024
H	1.155098	-1.250507	-2.300618
H	-0.678640	1.647374	1.286623

19

TS1-H6 scf done: -647.016184

C	2.296795	-6.505269	2.842420
C	1.593358	-5.565952	3.589959
C	2.021763	-6.676022	1.472612
H	-0.066243	-3.890602	3.681741
O	2.777232	-7.628141	0.847225
C	0.640721	-4.836370	2.922670
C	1.055544	-5.918538	0.848632
C	0.329700	-4.966157	1.584137
C	-0.714854	-4.148280	0.961864
O	3.248954	-7.254148	3.444633
O	-1.020993	-4.224506	-0.214469
H	3.642622	-7.859465	2.801255
H	2.533609	-7.701827	-0.083039

H	-1.224742	-3.443241	1.629947
O	-0.585120	-3.128394	4.307467
O	-0.224544	-1.897621	3.765333
H	0.570690	-1.649184	4.257119
H	1.808927	-5.438078	4.641782
H	0.851525	-6.060216	-0.205688

15

1R(H6)	scf done:	-495.432715	
C	1.248920	1.406162	0.713766
C	1.130418	2.774404	0.399589
C	0.223243	0.592017	0.304135
O	2.164343	3.561247	0.818677
C	0.026671	3.239439	-0.285979
C	-0.893982	0.987205	-0.376015
H	-0.051082	4.293010	-0.520569
H	-1.676478	0.301549	-0.676747
C	-0.984226	2.353806	-0.674527
C	-2.163642	2.830182	-1.403337
O	2.324967	0.931599	1.386028
O	-2.352719	3.991729	-1.718204
H	-2.899181	2.056530	-1.662462
H	2.925445	1.664448	1.579057
H	2.011631	4.480611	0.567743

4

H202	scf done:	-151.586197	
O	-1.333796	0.068206	-4.054637
O	-1.240556	0.519720	-2.711006
H	-0.519268	-0.014440	-2.353441
H	-2.055084	-0.573486	-4.017069

19

Complejo 1(C)	scf done:	-647.076463	
C	2.303277	-0.836364	0.214608
C	1.819224	0.413705	0.640726
C	1.449843	-1.765158	-0.362212
O	2.751927	1.242978	1.198570
H	1.851438	-2.717707	-0.677295
C	0.490511	0.728216	0.484162
C	0.108681	-1.452666	-0.518678
H	0.119158	1.690732	0.811502
H	-0.570337	-2.166424	-0.965998
C	-0.371609	-0.212183	-0.098969
C	-1.779821	0.078986	-0.278183
O	3.613685	-1.142353	0.369002
O	-2.309205	1.140388	0.048502
H	-2.385095	-0.713904	-0.732591
O	-4.828013	1.453052	-1.765003
O	-4.823825	1.344612	-0.466612
H	-3.849268	1.258889	-0.198585
H	4.070581	-0.404924	0.795489
H	2.338850	2.060126	1.501567

19

TS1-C	scf done:	-647.030753	
C	-1.997134	0.623127	-0.085369
C	-1.059763	1.562705	-0.544730
C	-1.603870	-0.731467	0.182991
H	-1.392421	2.571672	-0.739910
O	-2.604117	-1.524240	0.592897
C	0.235922	1.170611	-0.720958
C	-0.303499	-1.116861	-0.004346

H	0.982358	1.874686	-1.061284
H	-0.003391	-2.139581	0.178300
C	0.625516	-0.176274	-0.466942
C	2.038793	-0.576517	-0.689858
O	-3.249615	0.996132	0.095077
H	2.632987	0.181030	-1.212349
O	2.373152	-1.786549	-0.723744
O	2.338867	0.081305	0.966310
O	2.892973	1.363844	0.893262
H	2.258820	1.917721	1.367590
H	-3.791818	0.259282	0.419850
H	-2.298676	-2.428004	0.749627

19

1A(C) scf done: -647.041327

C	0.849726	0.738754	-0.103532
C	0.217997	2.029492	-0.269248
C	0.072462	-0.430267	-0.104866
O	1.054829	3.046565	-0.245291
H	0.564083	-1.384075	0.016151
C	-1.161096	2.122254	-0.436725
C	-1.275096	-0.311132	-0.272260
H	-1.627430	3.089180	-0.564459
H	-1.901302	-1.192699	-0.287919
C	-1.904213	0.969827	-0.429208
C	-3.420126	1.012151	-0.598410
O	2.149459	0.664637	0.046538
O	-3.939768	2.194722	-0.843224
H	-3.685623	0.210111	-1.311763
O	-3.952999	0.354956	0.636883
O	-3.633235	1.169153	1.761805
H	-2.865073	0.721871	2.141353
H	2.563262	1.544249	0.019398
H	0.607365	3.897122	-0.371543

19

Complejo 1(C1) scf done: -647.071208

C	1.744804	-0.141334	-0.403156
C	1.170616	1.011675	0.160647
C	0.947952	-1.093003	-1.021853
O	2.049741	1.881573	0.741586
C	-0.192159	1.201670	0.109100
C	-0.427181	-0.902487	-1.077638
H	-0.632332	2.086175	0.551688
H	-1.061705	-1.639685	-1.552188
C	-0.996989	0.240089	-0.515760
C	-2.452547	0.393540	-0.566554
O	3.086803	-0.332000	-0.345120
O	-3.062332	1.343591	-0.106208
H	-2.990797	-0.425219	-1.063295
O	-2.225001	-1.609061	1.940337
O	-0.938985	-1.719374	2.102456
H	-0.518695	-1.385020	1.283798
H	3.498681	0.403310	0.128332
H	1.585025	2.655326	1.081352
H	1.415098	-1.969767	-1.447524

19

TS1-C1 scf done: -647.038468

C	1.040483	0.851444	0.284674
C	0.883981	2.263344	0.372416
C	0.103852	0.077035	-0.409776

O	1.901662	2.903448	1.014989
C	-0.192644	2.875221	-0.187776
C	-0.991611	0.677377	-0.967805
H	-0.297740	3.950997	-0.146702
H	-1.721387	0.100406	-1.519401
C	-1.241235	2.079930	-0.761048
C	-2.132860	2.722775	-1.779098
O	2.110955	0.256337	0.836828
O	-2.076444	3.894958	-2.068900
H	-2.866344	2.050734	-2.243896
O	-2.559700	2.082959	0.463616
O	-2.062487	1.496236	1.626965
H	-2.202367	0.547551	1.497220
H	2.669182	0.919832	1.267527
H	1.733328	3.852981	1.056983
H	0.280843	-0.984982	-0.507663

19

1A(C1) scf done: -647.043899

C	0.865131	0.730542	-0.283048
C	0.290302	2.037779	-0.217887
C	0.039974	-0.401392	-0.215918
O	1.196413	3.050457	-0.345047
H	0.499677	-1.376441	-0.306910
C	-1.039930	2.214207	-0.074199
C	-1.304792	-0.276288	-0.046225
H	-1.465527	3.208721	-0.066242
H	-1.940389	-1.148992	-0.009233
C	-1.953869	1.058460	0.101636
C	-3.149907	1.119952	-0.841825
O	2.197761	0.574778	-0.438774
O	-3.170776	1.808900	-1.834025
H	-3.994428	0.471399	-0.578306
O	-2.503162	1.239774	1.469129
O	-3.375817	0.163356	1.795435
H	-2.798412	-0.440587	2.283383
H	2.626888	1.440751	-0.479588
H	0.758072	3.905650	-0.260174

19

Complejo 1(C2) scf done: -647.070714

C	1.620358	-1.289441	0.637730
C	1.827073	0.058360	0.293761
C	0.463485	-1.944953	0.245969
O	3.006785	0.601179	0.723190
C	0.873262	0.741294	-0.427633
C	-0.496127	-1.260428	-0.486676
H	1.032187	1.779954	-0.687711
H	-1.406713	-1.759498	-0.791662
C	-0.295091	0.075806	-0.823430
C	-1.345238	0.780854	-1.556159
O	2.557728	-1.961001	1.353540
O	-1.294283	1.957274	-1.875920
H	-2.224941	0.174437	-1.813089
H	3.304575	-1.376877	1.540118
H	3.092739	1.509322	0.409991
H	0.332620	-2.981643	0.522183
O	-1.763922	1.643329	1.639159
O	-1.285539	0.641642	2.318898
H	-0.363477	0.508657	2.024297

19

TS1-C2 scf done: -647.042305
C 0.714679 0.869581 0.487175
C 0.710942 2.265913 0.410648
C -0.257324 0.133277 -0.170206
O 1.678529 2.913923 1.088118
C -0.348367 2.949060 -0.238836
C -1.229484 0.786982 -0.935633
H -0.192533 3.986007 -0.508046
H -1.954236 0.204935 -1.490076
C -1.252075 2.163905 -1.023191
C -2.214692 2.807017 -1.901966
O 1.684553 0.222489 1.184739
O -2.279709 4.012770 -2.093676
H -2.900902 2.125264 -2.422073
O -1.301164 3.367385 1.332654
O -2.535010 3.890966 0.998919
H -2.360051 4.818589 0.784673
H 2.275175 0.864690 1.599500
H 1.609141 3.869986 0.967422
H -0.233408 -0.944641 -0.098789

19

1A(C2) scf done: -647.058016
C -1.887201 0.448687 0.112135
C -1.090229 -0.572905 -0.362015
C -1.317229 1.638729 0.562442
O -1.693269 -1.689871 -0.809699
C 0.394361 -0.520889 -0.265147
C 0.069749 1.839144 0.445273
H 0.857984 -0.992049 -1.134608
H 0.478093 2.814215 0.681315
C 0.908851 0.862064 -0.027072
C 2.269969 1.217064 -0.339892
O -3.246967 0.330507 0.116173
O 3.077341 0.494328 -0.918992
H 2.558345 2.236345 -0.047918
O 0.654998 -1.395546 0.883899
O 2.046683 -1.653005 0.965902
H 2.157674 -2.431978 0.401633
H -3.498573 -0.546707 -0.199264
H -1.046580 -2.353932 -1.082690
H -1.962690 2.420027 0.935170

19

Complejo 1(C3) scf done: -647.073616
C 0.769714 -0.925771 0.504067
C 0.659503 0.446099 0.228777
C 0.065052 -1.846699 -0.257709
O 1.385076 1.282377 1.046015
C -0.138245 0.890568 -0.798682
C -0.740017 -1.403475 -1.296221
H -0.215845 1.950951 -1.003093
H -1.290613 -2.113289 -1.899692
C -0.840683 -0.041340 -1.571442
C -1.690850 0.393415 -2.678700
O 1.561206 -1.368866 1.513324
O -1.850769 1.556444 -3.010690
H -2.199976 -0.413490 -3.223274
O -0.531151 0.451325 3.447714
O 0.538037 1.167201 3.651694
H 0.935337 1.320162 2.759924

H	2.023258	-0.627689	1.926097
H	1.396195	2.180238	0.689490
H	0.164772	-2.898159	-0.027600

19

TS1-C3 scf done: -647.042720

C	0.476929	0.974199	0.566473
C	0.329428	2.410363	0.539950
C	-0.409279	0.170078	-0.114023
O	1.419785	3.085625	0.981416
C	-0.562637	2.973039	-0.415386
C	-1.374537	0.752864	-0.931208
H	-0.582038	4.047484	-0.541712
H	-2.071819	0.126495	-1.471505
C	-1.438692	2.146746	-1.091679
C	-2.431801	2.704832	-2.017992
O	1.441348	0.440878	1.331025
O	-2.555168	3.893243	-2.252264
H	-3.081125	1.968195	-2.510325
O	-0.774490	2.491873	2.073484
O	-0.703021	3.802564	2.531127
H	0.106635	3.828518	3.059796
H	1.973455	1.143510	1.731752
H	1.289266	4.039934	0.906080
H	-0.323364	-0.903022	-0.022310

19

1A(C3) scf done: -647.057122

C	-1.141735	1.156003	0.049913
C	-0.847340	-0.292338	-0.214478
C	-0.177026	2.046087	0.414503
O	-1.552221	-0.672677	-1.367840
C	0.608443	-0.592650	-0.283397
C	1.168127	1.647650	0.466349
H	0.896076	-1.585492	-0.599878
H	1.932487	2.353189	0.759078
C	1.539243	0.339564	0.089277
C	2.973976	0.003452	0.076437
O	-2.431945	1.534637	-0.055226
O	3.418404	-1.079803	-0.251767
H	3.648832	0.811581	0.389603
O	-1.442259	-0.954734	0.938005
O	-1.298591	-2.357394	0.773566
H	-2.144991	-2.614311	0.380892
H	-2.967420	0.806553	-0.399448
H	-1.274950	-1.557715	-1.638083
H	-0.463268	3.064993	0.634210

19

Complejo 1(C4) scf done: -647.071122

C	1.256091	-0.834544	0.296233
C	1.226599	0.566368	0.188649
C	0.254965	-1.604008	-0.279629
O	2.254319	1.223421	0.805143
C	0.203801	1.186507	-0.492880
C	-0.775446	-0.979861	-0.972590
H	0.182342	2.266243	-0.568437
H	-1.558774	-1.569825	-1.430163
C	-0.803517	0.409682	-1.078672
C	-1.905547	1.033959	-1.810421
O	2.259423	-1.445701	0.972420
O	-2.035382	2.235971	-1.971521

H	-2.644875	0.336147	-2.227335
O	-0.384991	-0.464300	2.976725
O	-1.484686	-0.311629	2.298248
H	-1.360494	-0.765596	1.440059
H	2.856793	-0.780097	1.339258
H	2.159473	2.176725	0.695287
H	0.299906	-2.679461	-0.180374

19

TS1-C4 scf done: -647.047508

C	0.476004	0.802508	0.638098
C	0.480788	2.238023	0.495198
C	-0.357719	0.032685	-0.224363
O	1.430600	2.865929	1.216770
C	-0.474443	2.856940	-0.265611
C	-1.316677	0.663090	-0.964561
H	-0.508675	3.937135	-0.321285
H	-2.011285	0.092260	-1.566850
C	-1.392166	2.073985	-0.979436
C	-2.433594	2.706936	-1.786896
O	1.559853	0.192753	1.164449
O	-2.587606	3.914293	-1.877793
H	-3.095567	2.018258	-2.328158
O	-0.562971	0.751596	2.233022
O	-1.837948	1.246322	2.089500
H	-2.364245	0.492829	1.784922
H	2.073318	0.828745	1.682321
H	1.333493	3.825352	1.157178
H	-0.254456	-1.042655	-0.200358

19

1A(C4) scf done: -647.065967

C	0.741137	0.671498	0.308652
C	0.049206	1.994541	0.108478
C	-0.135796	-0.504242	0.041245
O	0.890285	3.024602	0.283448
H	0.340674	-1.471312	0.129414
C	-1.266994	2.100323	-0.209223
C	-1.438975	-0.364515	-0.260719
H	-1.717454	3.076670	-0.332924
H	-2.059597	-1.235362	-0.428165
C	-2.036749	0.931711	-0.383366
C	-3.446004	1.017910	-0.708094
O	1.900547	0.568030	-0.465666
O	-4.058651	2.075020	-0.826380
H	-3.961968	0.059544	-0.847816
O	1.252283	0.611224	1.672178
O	0.176589	0.812981	2.570544
H	-0.139762	-0.085419	2.747037
H	2.414061	1.381941	-0.367084
H	0.449930	3.868029	0.112299

19

Complejo 1(C5) scf done: -647.070344

C	1.369063	-0.596668	0.168980
C	1.106314	0.760925	0.423345
C	0.528368	-1.334399	-0.652368
O	2.000342	1.383425	1.250242
C	0.012652	1.370341	-0.147642
C	-0.581881	-0.722060	-1.220514
H	-0.188377	2.415996	0.048664
H	-1.247562	-1.287560	-1.859259

C	-0.837580	0.624238	-0.973966
C	-2.013523	1.238024	-1.588973
O	2.448587	-1.196293	0.730832
O	-2.339529	2.404920	-1.444679
H	-2.618247	0.568289	-2.215748
O	-1.489101	-0.800684	2.108448
O	-1.032745	-2.017890	2.173558
H	-0.534919	-2.176312	1.346763
H	2.924236	-0.555442	1.276379
H	1.735697	2.296258	1.413247
H	0.758203	-2.375109	-0.837309

19

TS1-C5 scf done: -647.039413

C	0.825551	0.877895	0.469178
C	0.757855	2.277327	0.439627
C	-0.207058	0.085684	-0.107590
O	1.750125	2.928730	1.118597
C	-0.239641	2.903603	-0.267810
C	-1.143042	0.754773	-0.956540
H	-0.287226	3.984152	-0.299403
H	-1.857707	0.172050	-1.521335
C	-1.181267	2.126380	-0.984538
C	-2.209171	2.777724	-1.805775
O	1.821770	0.241339	1.103218
O	-2.346510	3.983672	-1.897121
H	-2.873350	2.095314	-2.352971
O	-1.283051	-0.268228	1.350267
O	-0.604379	-1.133561	2.201868
H	-0.769171	-2.012057	1.831680
H	2.426980	0.882143	1.504029
H	1.653082	3.883202	1.018731
H	0.024827	-0.954410	-0.292817

19

1A(C5) scf done: -647.054316

C	0.761255	0.716027	-0.143729
C	0.187514	1.968022	-0.151078
C	-0.032033	-0.535460	-0.240434
O	1.053772	3.023696	0.015359
H	0.421931	-1.215167	-0.967494
C	-1.181761	2.125309	-0.329002
C	-1.467747	-0.286475	-0.541157
H	-1.624759	3.110980	-0.325027
H	-2.099407	-1.146860	-0.719992
C	-1.986350	0.972273	-0.543564
C	-3.428526	1.114992	-0.796843
O	2.091680	0.534571	0.002435
O	-4.014178	2.181079	-0.809001
H	-3.968475	0.176164	-0.978755
O	0.110609	-1.325412	0.980849
O	-0.403937	-0.577467	2.072462
H	-1.331542	-0.851761	2.110458
H	2.529117	1.393226	0.090479
H	0.588990	3.860138	-0.102248

19

Complejo 1(C6) scf done: -647.071154

C	1.581181	-0.693028	0.371300
C	1.259844	0.652331	0.618270
C	0.812761	-1.449626	-0.501315
O	2.082915	1.302314	1.494968

C	0.174063	1.229557	-0.002279
C	-0.280712	-0.868087	-1.130889
H	-0.075380	2.263897	0.197398
H	-0.892041	-1.448914	-1.809563
C	-0.598860	0.466799	-0.884891
C	-1.786468	1.032485	-1.526955
O	2.647683	-1.264233	0.986497
O	-2.177034	2.176705	-1.368814
H	-2.333608	0.344964	-2.186435
O	-3.087016	-0.626169	0.822311
O	-2.148189	-1.120394	1.575169
H	-1.364602	-1.261542	1.004851
H	3.069351	-0.618306	1.568995
H	1.802903	2.218528	1.605618
H	1.080700	-2.482499	-0.673355

19

TS1-C6 scf done: -647.045366

C	0.984698	0.823377	0.298524
C	0.728316	2.211347	0.491742
C	0.190733	0.084389	-0.530571
O	1.568077	2.838802	1.339816
C	-0.301451	2.841152	-0.191873
C	-0.963817	0.680004	-1.111458
H	-0.453634	3.905956	-0.068306
H	-1.451530	0.165693	-1.928954
C	-1.108936	2.099486	-1.035607
C	-2.201232	2.720438	-1.778876
O	2.044254	0.251984	0.927502
O	-2.456109	3.913952	-1.753208
H	-2.805227	2.034803	-2.388284
O	-2.353946	0.153333	0.061555
O	-2.083334	0.635813	1.323375
H	-1.478435	-0.012190	1.713409
H	2.520329	0.922037	1.435561
H	1.359154	3.779905	1.407334
H	0.399307	-0.965588	-0.676738

19

1A(C6) scf done: -647.059198

C	0.981923	0.750501	-0.299441
C	0.372115	2.060935	-0.358947
C	0.227936	-0.349186	-0.138343
O	1.236057	3.077702	-0.493031
H	0.689995	-1.325254	-0.100645
C	-1.006484	2.204800	-0.351639
C	-1.236534	-0.243191	0.109875
H	-1.434781	3.187103	-0.508027
H	-1.787615	-1.043759	-0.384757
C	-1.818992	1.095889	-0.221204
C	-3.251314	1.212927	-0.387127
O	2.333733	0.663693	-0.442175
O	-3.847192	2.281666	-0.517887
H	-3.809334	0.269163	-0.410478
O	-1.345260	-0.505100	1.551809
O	-2.714748	-0.717666	1.871444
H	-2.972866	0.112466	2.296140
H	2.704659	1.542693	-0.593563
H	0.777331	3.925195	-0.572104

15

2 scf done: -495.669693

C	-2.373833	-0.392264	0.123044
C	-1.560885	0.793079	0.048497
C	-1.724861	-1.622583	-0.138381
O	-2.208996	1.979131	0.305940
H	-2.313175	-2.529468	-0.089010
C	-0.232120	0.755601	-0.256647
C	-0.378456	-1.664027	-0.447826
H	0.342238	1.671857	-0.301964
H	0.102998	-2.614847	-0.645315
C	0.385387	-0.491612	-0.512482
C	1.782157	-0.590503	-0.838828
O	-3.617826	-0.262124	0.417423
O	2.567009	0.356622	-0.929221
H	2.149152	-1.611995	-1.016858
H	-3.127994	1.722403	0.490889

18

Complejo 2(H) scf done: -646.621795

C	-0.134900	-0.423535	0.036152
C	0.505950	0.782926	-0.351250
C	1.859712	0.873574	-0.263449
C	2.681655	-0.213715	0.216622
C	2.009535	-1.407519	0.589575
C	0.639772	-1.502559	0.500226
O	3.944225	-0.038600	0.275826
H	2.605889	-2.235004	0.949905
C	-1.542175	-0.573248	-0.014167
O	-2.344408	0.313331	-0.386735
O	-4.797431	-0.606733	1.172922
O	-4.721943	-0.343978	-0.101752
O	2.533969	2.014355	-0.624375
H	-0.075956	1.620815	-0.711875
H	0.138063	-2.416958	0.793592
H	-1.943645	-1.542420	0.301482
H	-3.725264	-0.061078	-0.276678
H	3.471708	1.813206	-0.468157

18

TS2-H scf done: -646.587088

C	-0.245109	-0.169663	-0.034977
C	0.809861	-1.118328	-0.024545
C	2.095861	-0.673297	0.002450
C	2.431921	0.730169	0.020775
C	1.350011	1.647181	0.008921
C	0.045678	1.203110	-0.018234
O	3.667644	1.056123	0.046443
H	1.577653	2.704851	0.021767
C	-1.607453	-0.592230	-0.062665
O	-2.087540	-1.701704	-0.080639
O	-3.562801	1.038628	-0.025190
O	-4.519258	0.056632	-0.140734
O	3.161540	-1.539740	0.014166
H	0.593409	-2.178722	-0.037547
H	-0.771720	1.913767	-0.027174
H	-2.428876	0.338722	-0.061162
H	-4.712805	-0.209563	0.769633
H	3.947304	-0.967570	0.033516

14

2R(H) scf done: -495.012401

C	-0.780932	0.034523	-2.470903
C	-1.941885	-0.204696	-1.690379

C	0.439945	0.300374	-1.837315
H	-2.890204	-0.411070	-2.169488
H	1.316217	0.480728	-2.447157
C	-1.846542	-0.171065	-0.330869
C	0.528728	0.332786	-0.459878
O	-2.938519	-0.395375	0.474020
H	1.470749	0.537935	0.031236
C	-0.608227	0.098988	0.352358
O	-0.609977	0.111203	1.634850
C	-0.842197	0.007442	-3.901529
O	-1.750535	-0.193154	-4.658187
H	-2.598542	-0.314162	1.380977

18

Complejo 2(H2) scf done: -646.620195

C	2.347611	0.178577	0.017911
C	2.084855	-1.215017	0.056221
C	1.200087	1.052156	-0.039330
H	-3.066824	0.658986	0.325308
O	1.474916	2.397650	-0.083347
C	0.792385	-1.690543	0.039273
C	-0.078396	0.585237	-0.053060
C	-0.307383	-0.814806	-0.010493
C	-1.609199	-1.386394	-0.013197
O	3.513117	0.702831	0.026938
H	-1.643058	-2.481617	-0.018661
O	-2.696282	-0.774934	-0.012452
O	-3.450097	1.595331	0.478167
O	-3.638970	2.099564	-0.707872
H	2.928245	-1.891676	0.097374
H	0.607757	-2.757809	0.068708
H	-0.902990	1.282974	-0.106156
H	2.444225	2.459491	-0.065332

18

TS2-H2 scf done: -646.565351

C	-2.571169	-0.253816	-0.075324
C	-2.450100	1.141475	0.149316
C	-1.331968	-1.004712	-0.196694
H	2.803214	-0.445653	0.747684
O	-1.451488	-2.344651	-0.435606
C	-1.217049	1.748421	0.253607
C	-0.151116	-0.360818	-0.081085
C	-0.015178	1.020518	0.146923
C	1.227007	1.719113	0.284244
O	-3.664226	-0.895812	-0.189093
H	1.127672	2.802899	0.426341
O	2.359688	1.221755	0.255693
O	2.637677	-1.406480	0.850152
O	1.953104	-1.707641	-0.329498
H	-3.360004	1.719833	0.235812
H	-1.150870	2.816274	0.428234
H	0.980930	-1.142598	-0.247175
H	-2.409243	-2.509464	-0.470694

14

2R(H2) scf done: -494.977996

C	1.371991	1.360603	0.608403
C	1.173892	2.781868	0.387480
C	0.352115	0.490484	0.139644
O	2.163553	3.616377	0.843274
C	0.052449	3.184127	-0.239177

C	-0.773560	0.972267	-0.495782
H	-1.537584	0.286114	-0.844200
C	-0.966968	2.351815	-0.710840
C	-2.149402	2.822055	-1.375306
O	2.440386	0.994460	1.203937
O	-2.413373	4.002522	-1.611436
H	-2.853044	2.035851	-1.683543
H	2.821998	3.021356	1.240170
H	0.485374	-0.571267	0.296955

18

Complejo 2(H3) scf done: -646.614855

C	-1.008538	-0.683604	-0.468756
C	-0.735666	0.694851	-0.655056
C	0.558137	1.133896	-0.602989
C	1.671072	0.246604	-0.361258
C	1.358490	-1.120354	-0.171424
C	0.051097	-1.566554	-0.225913
O	2.849885	0.747780	-0.329744
O	0.876983	2.455478	-0.781447
C	-2.350265	-1.201800	-0.516714
O	-3.367155	-0.538115	-0.726294
O	0.922155	1.208783	2.707794
O	-0.265518	0.711367	2.517775
H	2.172663	-1.807244	0.018431
H	-1.540528	1.393431	-0.845069
H	-0.168266	-2.617356	-0.076866
H	-2.436795	-2.285429	-0.351382
H	1.843339	2.493597	-0.680313
H	-0.431089	0.734669	1.549225

18

TS2-H3 scf done: -646.595498

C	-1.159213	-0.219816	-0.380554
C	-0.866385	1.144361	-0.364422
C	0.430876	1.570949	-0.150621
C	1.517156	0.628557	0.067009
C	1.159969	-0.758390	0.083967
C	-0.128114	-1.159929	-0.145554
O	2.697143	1.047131	0.237932
O	0.734661	2.888397	-0.173558
C	-2.503142	-0.700115	-0.624752
O	-3.478711	0.012759	-0.843402
O	1.362640	3.034500	2.237869
O	0.710843	1.879558	2.493621
H	1.949808	-1.477318	0.256807
H	-1.644826	1.878713	-0.526952
H	-0.376260	-2.214831	-0.151896
H	-2.621368	-1.792877	-0.605686
H	1.182084	3.112673	0.713650
H	-0.233319	2.105570	2.538107

14

2R(H3) scf done: -495.033472

C	-0.815287	-0.001566	-2.461456
C	-1.959453	-0.331164	-1.769715
C	0.385127	0.334746	-1.766215
H	-2.869885	-0.586096	-2.296957
H	1.263998	0.588440	-2.346796
C	-1.983070	-0.347419	-0.345221
C	0.432692	0.338867	-0.405671
O	-3.017654	-0.645154	0.312026

H	1.339655	0.592888	0.126858
C	-0.723235	0.004318	0.379518
O	-0.708517	-0.001014	1.631856
C	-0.793725	0.014544	-3.921245
H	0.168403	0.290835	-4.375084
O	-1.751306	-0.252225	-4.633919

18

Complejo 2(H5) scf done: -646.620195

C	2.347611	0.178577	0.017911
C	2.084855	-1.215017	0.056221
C	1.200087	1.052156	-0.039330
H	-3.066824	0.658986	0.325308
O	1.474916	2.397650	-0.083347
C	0.792385	-1.690543	0.039273
C	-0.078396	0.585237	-0.053060
C	-0.307383	-0.814806	-0.010493
C	-1.609199	-1.386394	-0.013197
O	3.513117	0.702831	0.026938
H	-1.643058	-2.481617	-0.018661
O	-2.696282	-0.774934	-0.012452
O	-3.450097	1.595331	0.478167
O	-3.638970	2.099564	-0.707872
H	2.928245	-1.891676	0.097374
H	0.607757	-2.757809	0.068708
H	-0.902990	1.282974	-0.106156
H	2.444225	2.459491	-0.065332

18

TS2-H5 scf done: -646.563340

C	1.482949	1.505300	0.841048
C	1.286670	2.793386	0.213748
C	0.351365	0.674833	0.744160
O	2.357821	3.649899	0.280089
C	0.124880	3.151027	-0.410000
C	-0.830895	0.979988	0.131245
H	0.038414	4.129977	-0.863060
H	-1.655957	0.277206	0.097729
C	-0.958976	2.246505	-0.462144
C	-2.204344	2.578205	-1.108851
O	2.598354	1.241078	1.400771
O	-2.451398	3.644313	-1.670078
H	-2.969485	1.789331	-1.077202
O	0.459296	-1.627869	1.733881
O	-0.812389	-2.110967	1.417465
H	-0.696001	-2.522672	0.549980
H	3.045052	3.166744	0.767724
H	0.468154	-0.570609	1.329560

14

2R(H5) scf done: -494.978122

C	1.293718	1.333182	0.698888
C	1.145713	2.727646	0.348920
C	0.199888	0.560755	0.286154
O	2.184920	3.544130	0.726042
C	0.055178	3.222085	-0.312913
C	-0.912047	0.987759	-0.374233
H	0.003276	4.277137	-0.547293
H	-1.715009	0.316311	-0.658208
C	-0.997432	2.358790	-0.687892
C	-2.164801	2.834616	-1.386282
O	2.347158	0.949623	1.317853

O	-2.369030	4.001344	-1.721374
H	-2.913160	2.064523	-1.622913
H	2.820298	2.957502	1.168864

18

Complejo 2(H6) scf done: -646.620195

C	2.347611	0.178577	0.017911
C	2.084855	-1.215017	0.056221
C	1.200087	1.052156	-0.039330
H	-3.066824	0.658986	0.325308
O	1.474916	2.397650	-0.083347
C	0.792385	-1.690543	0.039273
C	-0.078396	0.585237	-0.053060
C	-0.307383	-0.814806	-0.010493
C	-1.609199	-1.386394	-0.013197
O	3.513117	0.702831	0.026938
H	-1.643058	-2.481617	-0.018661
O	-2.696282	-0.774934	-0.012452
O	-3.450097	1.595331	0.478167
O	-3.638970	2.099564	-0.707872
H	2.928245	-1.891676	0.097374
H	0.607757	-2.757809	0.068708
H	-0.902990	1.282974	-0.106156
H	2.444225	2.459491	-0.065332

18

TS2-H6 scf done: -646.563357

C	1.791085	-1.026130	-0.057635
C	0.450112	-1.479329	-0.229355
C	1.974355	0.397700	0.090195
H	-1.817316	-1.029259	-0.402508
O	3.274204	0.811621	0.257245
C	-0.545104	-0.544624	-0.244480
C	0.942437	1.288565	0.067706
C	-0.389706	0.828651	-0.112372
C	-1.516363	1.723844	-0.165316
O	2.815222	-1.785591	-0.024076
H	-2.492521	1.245695	-0.318909
H	3.802667	-0.003457	0.234278
O	-1.446336	2.947739	-0.054095
O	-2.865197	-1.474883	-0.496983
O	-3.506751	-1.165665	0.700210
H	-3.308368	-1.918371	1.274413
H	0.261962	-2.539357	-0.335489
H	1.132198	2.348772	0.179716

14

2R(H6) scf done: -494.980384

C	1.246324	1.334336	0.693763
C	1.110626	2.733675	0.357046
C	0.177485	0.475443	0.292495
O	2.152321	3.541230	0.754115
C	0.034873	3.241097	-0.307375
C	-0.866161	1.045688	-0.366850
H	-0.017245	4.298454	-0.535440
C	-1.027336	2.378734	-0.704810
C	-2.189002	2.848051	-1.407597
O	2.291015	0.952069	1.317600
O	-2.391716	4.018533	-1.736742
H	-2.931657	2.077343	-1.653890
H	2.778694	2.945740	1.196998
H	0.238635	-0.579850	0.525128

18

Complejo 2(C) scf done: -646.614967

C	1.839486	-0.564260	-0.008741
C	0.965990	-1.300832	-0.845932
C	1.361503	0.712452	0.459732
H	1.299878	-2.262635	-1.212041
O	2.223797	1.410800	1.268623
C	-0.279283	-0.804503	-1.185097
C	0.131243	1.202124	0.134262
H	-0.936932	-1.378758	-1.827174
H	-0.194967	2.160441	0.516768
C	-0.720135	0.437207	-0.700774
C	-2.039102	0.894956	-1.059473
O	3.006873	-0.947581	0.355372
H	-2.608318	0.212763	-1.707360
O	-2.547805	1.956093	-0.698219
O	-2.007749	-0.276192	2.379752
O	-1.390666	-1.288415	1.843451
H	-1.113713	-1.007606	0.943483
H	3.009904	0.843945	1.343369

18

TS2-C scf done: -646.596533

C	2.017797	-0.622645	-0.132195
C	1.033068	-1.488892	-0.713418
C	1.590781	0.725829	0.221942
H	1.342672	-2.487272	-0.990696
O	2.537561	1.531140	0.757659
C	-0.243178	-1.051422	-0.907478
C	0.313181	1.155367	0.016780
H	-0.987459	-1.704860	-1.343875
H	0.022088	2.162075	0.283167
C	-0.628118	0.264383	-0.537391
C	-1.998532	0.700111	-0.799795
O	3.212228	-0.951493	0.085656
H	-2.651845	-0.064067	-1.235725
O	-2.381253	1.868332	-0.690990
O	-2.213320	-0.265201	1.157221
O	-2.608931	-1.605936	1.027608
H	-1.842771	-2.110186	1.329578
H	3.356264	1.009425	0.798797

18

2A(C) scf done: -646.614700

C	2.207664	-0.422700	0.141372
C	1.448527	-1.628051	0.324341
C	1.467431	0.785812	-0.205647
H	1.988901	-2.528098	0.583717
O	2.180503	1.906396	-0.373266
C	0.093350	-1.612502	0.178073
C	0.097861	0.775614	-0.352414
H	-0.483409	-2.517500	0.319585
H	-0.425723	1.685825	-0.613073
C	-0.594516	-0.416493	-0.157153
C	-2.091903	-0.471931	-0.407985
O	3.454620	-0.347645	0.262347
H	-2.512400	-1.343117	0.117028
O	-2.388382	-0.379017	-1.703768
O	-2.714997	0.702875	0.259916
O	-2.501307	0.598038	1.665315
H	-1.694546	1.112815	1.806587

H	3.114843	1.683324	-0.222094
18			
Complejo 2(C1)	scf done:	-646.615200	
C	1.747173	-0.196902	-0.181589
C	1.218279	1.034720	0.349116
C	0.829727	-1.034564	-0.867199
O	2.114479	1.825479	1.025145
C	-0.084879	1.404321	0.188666
C	-0.491322	-0.649856	-1.046179
H	-0.440685	2.339023	0.603045
H	-1.173881	-1.295101	-1.586291
C	-0.966372	0.556855	-0.523149
C	-2.351804	0.897779	-0.720828
O	2.986492	-0.461254	0.006492
O	-2.900257	1.922460	-0.314137
H	-2.937651	0.158262	-1.285875
O	-1.473118	-2.400692	1.631767
O	-0.319791	-1.877059	1.929977
H	0.091613	-1.594817	1.079742
H	2.954044	1.337259	0.989175
H	1.197953	-1.965911	-1.277882
18			
TS2-C1	scf done:	-646.588918	
C	1.094456	0.813002	0.300772
C	0.888301	2.248425	0.395071
C	0.105313	0.074320	-0.408561
O	1.892836	2.946183	1.004664
C	-0.198692	2.872011	-0.116181
C	-1.006177	0.683226	-0.921104
H	-0.300639	3.946916	-0.054420
H	-1.742840	0.117255	-1.477933
C	-1.275649	2.086334	-0.677227
C	-2.094188	2.718319	-1.759267
O	2.154003	0.311663	0.811979
O	-1.977257	3.872066	-2.115104
H	-2.831110	2.053531	-2.230769
O	-2.579053	2.116532	0.469883
O	-2.150262	1.429719	1.627291
H	-2.185401	0.497277	1.371173
H	2.554491	2.280088	1.254928
H	0.276135	-0.984479	-0.556905
18			
2A(C1)	scf done:	-646.591168	
C	-1.784628	-0.231854	0.546068
C	-1.234560	0.606834	-0.510386
C	-0.847091	-0.879170	1.389786
O	-2.168052	1.270863	-1.260038
C	0.086100	0.761397	-0.728888
C	0.502559	-0.771931	1.194015
H	0.447515	1.424766	-1.503464
H	1.204789	-1.272372	1.848915
C	1.071821	-0.014404	0.050792
C	2.209094	0.817345	0.617418
O	-3.066324	-0.303331	0.665357
O	2.235038	2.028056	0.595898
H	3.000748	0.238570	1.113443
O	1.854196	-0.945231	-0.838469
O	0.984397	-1.939254	-1.354337
H	0.870692	-2.548466	-0.609813

H	-3.025054	1.003913	-0.885149
H	-1.232491	-1.464516	2.215952

18

Complejo 2(C2) scf done: -646.614788

C	-1.856281	0.373921	-0.074927
C	-1.143161	-0.658226	-0.784185
C	-1.081710	1.442513	0.440413
O	-1.910729	-1.688731	-1.268846
C	0.208419	-0.628380	-0.962633
C	0.287729	1.475893	0.265345
H	0.708036	-1.426463	-1.496141
H	0.867783	2.297471	0.668935
C	0.954826	0.450225	-0.424213
C	2.385842	0.528948	-0.574753
O	-3.127060	0.262647	0.047371
O	3.087781	-0.294086	-1.162837
H	2.855368	1.409619	-0.113348
O	0.785243	-2.443126	1.760098
O	0.640092	-1.238227	2.229322
H	0.749797	-0.622296	1.471416
H	-2.818731	-1.472260	-0.998039
H	-1.593244	2.230559	0.977022

18

TS2-C2 scf done: -646.592801

C	0.532024	0.902981	0.653799
C	0.736850	2.300663	0.324587
C	-0.557538	0.260932	0.023157
O	1.799579	2.898019	0.878885
C	-0.169280	3.046687	-0.452625
C	-1.366998	0.958267	-0.857917
H	0.149527	4.010521	-0.824809
H	-2.177528	0.437029	-1.355455
C	-1.180386	2.315202	-1.149998
C	-2.073210	2.970461	-2.049086
O	1.360166	0.364172	1.455677
O	-2.058718	4.177556	-2.324565
H	-2.827503	2.320874	-2.516771
O	-1.086262	3.922478	1.013809
O	-2.095680	3.087557	1.480007
H	-2.791581	3.148589	0.810603
H	2.230083	2.217348	1.429901
H	-0.732424	-0.785458	0.231566

18

2A(C2) scf done: -646.608276

C	-1.811166	0.649363	-0.035764
C	-1.069277	-0.483779	-0.510125
C	-1.059428	1.781500	0.379925
O	-1.763268	-1.553763	-0.916582
C	0.406479	-0.615101	-0.486940
C	0.318800	1.773835	0.272222
H	0.769998	-1.065198	-1.414543
H	0.863627	2.675862	0.531964
C	1.071705	0.684184	-0.181297
C	2.464683	0.813748	-0.333109
O	-3.082053	0.564768	-0.036204
O	3.243775	-0.071403	-0.751864
H	2.877579	1.795325	-0.056481
O	0.788558	-1.661607	0.473428
O	0.407456	-1.246778	1.776696

H	1.096018	-0.607087	2.014234
H	-2.704828	-1.324162	-0.805760
H	-1.588926	2.653035	0.737330

18

Complejo 2(C3) scf done: -646.614814

C	-1.561162	0.694026	-0.414813
C	-0.920913	-0.473715	-0.970603
C	-0.721095	1.625543	0.239035
O	-1.751956	-1.362242	-1.602309
C	0.423627	-0.694028	-0.869479
C	0.641028	1.408385	0.337570
H	0.863993	-1.585473	-1.297766
H	1.269061	2.130922	0.845309
C	1.234341	0.261657	-0.205333
C	2.654973	0.078362	-0.062846
O	-2.831684	0.805486	-0.544212
O	3.298097	-0.882744	-0.487614
H	3.177001	0.883971	0.473546
O	-1.606002	-1.769486	1.971911
H	0.005030	-1.204945	1.274980
O	-0.358435	-1.447097	2.154567
H	-2.640885	-0.979009	-1.507474
H	-1.175020	2.510385	0.665532

18

TS2-C3 scf done: -646.598699

C	0.575774	0.693553	0.441978
C	0.253081	2.129365	0.552117
C	-0.190867	-0.068553	-0.479092
O	1.161017	2.875378	1.233834
C	-0.548733	2.750791	-0.424514
C	-1.091113	0.548315	-1.311184
H	-0.640159	3.828449	-0.429824
H	-1.665198	-0.037883	-2.018826
C	-1.275005	1.956016	-1.298957
C	-2.196064	2.535617	-2.259347
O	1.488677	0.240503	1.185235
O	-2.431641	3.734207	-2.373329
H	-2.701055	1.815418	-2.918295
O	-0.956836	1.968096	2.040822
H	-2.702759	2.122420	1.342782
O	-2.190534	1.391111	1.711087
H	1.728827	2.241360	1.703750
H	-0.016435	-1.134775	-0.529530

18

2A(C3) scf done: -646.608705

C	-1.347594	0.880384	-0.199350
C	-0.835127	-0.544134	-0.398977
C	-0.440106	1.886172	0.178249
O	-1.467568	-1.139229	-1.498339
C	0.629962	-0.682936	-0.465905
C	0.917664	1.629261	0.253563
H	1.029767	-1.644611	-0.757795
H	1.601604	2.416584	0.544926
C	1.451171	0.361396	-0.079955
C	2.895543	0.218717	-0.046704
O	-2.586244	1.040670	-0.383490
O	3.511139	-0.805384	-0.329776
H	3.447790	1.118416	0.259690
O	-1.378903	-1.371683	0.715413

H	-0.034095	-1.316799	2.044680
O	-0.888175	-0.871211	1.946805
H	-2.362947	-0.766363	-1.519678
H	-0.833186	2.874318	0.377749

18

Complejo 2(C4) scf done: -646.615274

C	1.476518	0.236738	-0.719420
C	0.757989	1.285866	-0.040549
C	0.718542	-0.896638	-1.110796
O	1.511496	2.363344	0.354887
C	-0.583560	1.223605	0.196840
C	-0.649204	-0.952833	-0.884425
H	-1.083118	2.034850	0.710448
H	-1.214808	-1.819525	-1.205485
C	-1.313958	0.089084	-0.230308
C	-2.732426	-0.028574	-0.009458
O	2.734874	0.381370	-0.911197
O	-3.441923	0.810152	0.546590
H	-3.185939	-0.958647	-0.381971
O	1.830658	-0.970025	2.320285
O	0.837060	-1.718407	1.936741
H	0.690956	-1.532425	0.980732
H	2.416392	2.153713	0.068753
H	1.230454	-1.701647	-1.621667

18

TS2-C4 scf done: -646.595788

C	0.501244	0.743029	0.654606
C	0.457285	2.216437	0.514079
C	-0.409432	0.000300	-0.213588
O	1.396758	2.876649	1.209544
C	-0.479877	2.854860	-0.245659
C	-1.341173	0.651038	-0.954240
H	-0.500627	3.934406	-0.305057
H	-2.045236	0.099674	-1.565209
C	-1.400104	2.077455	-0.973551
C	-2.417947	2.706771	-1.790137
O	1.560928	0.240025	1.146448
O	-2.573633	3.921041	-1.894348
H	-3.076551	2.020523	-2.338791
O	-0.603883	0.741990	2.224401
O	-1.932076	1.198174	2.103997
H	-2.394805	0.462475	1.682488
H	1.968411	2.187467	1.597120
H	-0.337542	-1.078926	-0.196627

18

2A(C4) scf done: -646.600739

C	1.353778	-0.173478	-0.461021
C	0.504683	1.027606	-0.094068
C	0.520528	-1.360577	-0.838035
O	1.211778	2.155775	0.069566
C	-0.846748	0.992050	0.051300
C	-0.818573	-1.374282	-0.688456
H	-1.397001	1.881738	0.326175
H	-1.396831	-2.253114	-0.947739
C	-1.526185	-0.217474	-0.212831
C	-2.958831	-0.304575	-0.069753
O	2.342081	0.151569	-1.282414
O	-3.678504	0.620656	0.311327
H	-3.404596	-1.274689	-0.326048

O	2.070577	-0.558426	0.840212
O	1.149453	-0.851741	1.884805
H	0.894961	-1.768939	1.711690
H	2.104355	1.955733	-0.270687
H	1.064781	-2.217730	-1.213919

18

Complejo 2(C5) scf done: -646.615200

C	1.688984	-0.018958	0.541003
C	1.152365	-0.987364	-0.382297
C	0.753725	0.636107	1.383403
O	2.067780	-1.599134	-1.202810
C	-0.176377	-1.290203	-0.439680
C	-0.595277	0.314670	1.337562
H	-0.537156	-2.025101	-1.148011
H	-1.292747	0.814020	1.999449
C	-1.077825	-0.636550	0.433284
C	-2.490333	-0.917573	0.414256
O	2.951703	0.197044	0.535106
O	-3.047795	-1.726182	-0.328446
H	-3.089387	-0.343766	1.136197
O	-1.240092	2.866136	-0.730011
O	-0.091004	2.373656	-1.090972
H	0.226232	1.816390	-0.342183
H	2.923125	-1.209260	-0.956096
H	1.127042	1.367972	2.088146

18

TS2-C5 scf done: -646.592553

C	0.788194	0.854713	0.455222
C	0.724744	2.294900	0.408932
C	-0.312088	0.120947	-0.143270
O	1.710803	2.963045	1.087234
C	-0.224364	2.955699	-0.306667
C	-1.183588	0.823450	-1.022601
H	-0.235657	4.036608	-0.340978
H	-1.899850	0.272571	-1.618406
C	-1.178596	2.202683	-1.051542
C	-2.153593	2.872061	-1.896651
O	1.746017	0.291942	1.060216
O	-2.272772	4.087010	-2.002668
H	-2.817008	2.204315	-2.464060
O	-1.408182	-0.135014	1.332850
O	-0.762386	-0.990916	2.250024
H	-0.927145	-1.875297	1.898401
H	2.265446	2.278072	1.493054
H	-0.138506	-0.934887	-0.306090

18

2A(C5) scf done: -646.599126

C	-1.117212	0.637723	0.410190
C	-0.055650	1.428795	-0.103039
C	-0.899933	-0.839970	0.553220
O	-0.350366	2.751121	-0.370043
C	1.219702	0.951234	-0.269966
C	0.525686	-1.228424	0.605434
H	2.006937	1.590927	-0.642724
H	0.779154	-2.221293	0.952516
C	1.502446	-0.382953	0.135767
C	2.871719	-0.883058	0.116981
O	-2.247568	1.163365	0.674710
O	3.841139	-0.254600	-0.288029

H	3.002749	-1.904558	0.501137
O	-1.420858	-1.539096	-0.664564
O	-2.846605	-1.486520	-0.674786
H	-3.094748	-2.259500	-0.148542
H	-1.287907	2.859727	-0.149586
H	-1.492661	-1.239549	1.377374

18

Complejo 2(C6) scf done: -646.615191

C	-1.741202	0.022766	-0.361649
C	-1.162162	-1.134404	0.273524
C	-0.836338	0.917420	-0.989678
O	-2.049850	-1.980197	0.891525
C	0.178198	-1.386963	0.259794
C	0.525115	0.651715	-1.018017
H	0.571286	-2.269090	0.748889
H	1.199725	1.338345	-1.515471
C	1.049693	-0.486470	-0.397092
C	2.473349	-0.701678	-0.437440
O	-3.011808	0.176291	-0.309979
O	3.065935	-1.654886	0.069054
H	3.046417	0.069417	-0.972623
O	1.119947	2.620269	1.655830
O	0.006366	1.976716	1.853086
H	-0.272296	1.618899	0.978222
H	-2.920898	-1.573628	0.747855
H	-1.241479	1.795479	-1.475828

18

TS2-C6 scf done: -646.590405

C	0.991409	0.721566	0.293771
C	0.738230	2.158252	0.448872
C	0.134237	0.023276	-0.549516
O	1.587845	2.801379	1.266109
C	-0.273134	2.822322	-0.211523
C	-0.992957	0.659156	-1.116479
H	-0.397062	3.889843	-0.088399
H	-1.514444	0.164662	-1.926138
C	-1.116146	2.090851	-1.041065
C	-2.204760	2.719185	-1.761272
O	2.000621	0.254500	0.934842
O	-2.445333	3.922697	-1.750359
H	-2.835579	2.038058	-2.348642
O	-2.479214	0.259348	0.051240
O	-2.082188	0.578149	1.345216
H	-1.406893	-0.082654	1.558571
H	2.206613	2.109237	1.573727
H	0.292459	-1.035623	-0.702642

18

2A(C6) scf done: -646.603528

C	-1.754366	0.268953	-0.374779
C	-1.205725	-0.998364	0.154191
C	-0.857769	1.183575	-0.845998
O	-2.126528	-1.853357	0.608072
C	0.137672	-1.312428	0.149788
C	0.610860	0.991111	-0.734849
H	0.465740	-2.283719	0.496508
H	1.130634	1.301165	-1.644824
C	1.049496	-0.384296	-0.328921
C	2.450869	-0.679134	-0.397237
O	-3.050232	0.346660	-0.349356

O	2.971151	-1.738039	-0.021779
H	3.083100	0.109955	-0.826229
O	1.188259	1.974789	0.209348
O	0.665871	1.736304	1.507010
H	-0.266474	1.991725	1.421743
H	-2.976364	-1.383402	0.456508
H	-1.211906	2.117824	-1.263299

14

3	scf done:	-495.186450	
C	-0.792329	0.032275	-2.465916
C	-1.957709	-0.208005	-1.691905
C	0.420062	0.296428	-1.818721
H	-2.894034	-0.412081	-2.199174
H	1.311825	0.480329	-2.407182
C	-1.953800	-0.193616	-0.303283
C	0.470874	0.320733	-0.436284
O	-3.026459	-0.414632	0.424040
H	1.402764	0.523937	0.078197
C	-0.673585	0.085196	0.367556
O	-0.613006	0.110644	1.654481
C	-0.801995	0.016271	-3.895933
H	0.170082	0.218032	-4.370900
O	-1.786957	-0.200593	-4.618309

17

Complejo 3(H)	scf done:	-646.135471	
C	-0.437081	-0.536769	-0.710886
C	0.481475	-1.057676	0.245768
C	1.599096	-0.345648	0.678872
C	1.782882	1.021740	0.142868
C	0.831926	1.511601	-0.785215
C	-0.249731	0.755348	-1.207270
O	2.788869	1.722075	0.522377
H	0.980549	2.516182	-1.163005
C	-1.588585	-1.267168	-1.145163
O	-1.911279	-2.405343	-0.776438
O	-2.269984	-0.097751	2.018160
O	-1.147875	0.535198	2.203035
O	2.466137	-0.810981	1.534577
H	0.333871	-2.062113	0.626744
H	-0.958443	1.160878	-1.920098
H	-2.224539	-0.741974	-1.873604
H	-0.477283	0.102401	1.609278

17

TS3-H	scf done:	-646.103826	
C	-0.188413	-3.844639	2.127849
C	0.730300	-3.421316	3.130866
C	1.946508	-4.053147	3.337562
C	2.278819	-5.190632	2.458140
C	1.334807	-5.584089	1.470984
C	0.130446	-4.932738	1.302625
O	3.397675	-5.798120	2.601414
H	1.596516	-6.427373	0.843173
C	-1.429536	-3.176462	1.944264
O	-1.913817	-2.233420	2.540975
O	-2.791501	-4.017366	-0.096234
O	-2.070937	-3.543658	-1.167724
O	2.803055	-3.694938	4.262171
H	0.468328	-2.579153	3.761184
H	-0.572104	-5.257222	0.545561

H -2.088969 -3.635409 1.018510
H -1.474453 -4.267903 -1.405068
13

3R(H) scf done: -494.529912
C -0.795281 0.031628 -2.454811
C -1.963788 -0.209220 -1.677140
C 0.420660 0.296492 -1.814970
H -2.899826 -0.413262 -2.184940
H 1.306795 0.479088 -2.410056
C -1.953501 -0.193396 -0.289186
C 0.472218 0.321024 -0.433777
O -3.023199 -0.413695 0.441405
H 1.405505 0.524519 0.077787
C -0.670601 0.085945 0.375434
O -0.605968 0.112313 1.659955
C -0.837991 0.008554 -3.879048
O -1.734051 -0.189668 -4.659897

17
Complejo 3(H2) scf done: -646.145774
C 1.804702 -0.997790 -0.082997
C 2.295136 0.352955 -0.072367
C 0.326268 -1.203358 -0.035222
H -1.927679 -2.514128 0.377427
O -0.134026 -2.381391 -0.039270
C 1.440443 1.410116 -0.019989
C -0.510556 -0.052844 0.015811
C 0.026459 1.214513 0.023949
C -0.828419 2.397837 0.076773
O 2.566168 -1.990631 -0.129567
O -2.049743 2.373101 0.118500
H -0.298840 3.360779 0.076759
O -2.887160 -2.558175 0.528121
O -3.429708 -2.127751 -0.761968
H 3.367072 0.495117 -0.107870
H -1.582506 -0.202135 0.043623
H 1.822389 2.423785 -0.011716

17
TS3-H2 scf done: -646.099075
C 1.949149 -0.715431 0.069363
C 2.424930 0.625784 0.021806
C 0.477917 -0.910402 -0.098263
H -1.408695 -2.229132 0.070032
O 0.052206 -2.111542 -0.365157
C 1.562102 1.696066 -0.062948
C -0.338991 0.203404 0.019036
C 0.158925 1.510993 -0.082873
C -0.678101 2.673991 -0.001388
O 2.711265 -1.724798 0.123349
O -1.912403 2.673635 0.081958
H -0.147507 3.637181 -0.034217
O -2.362876 -2.184691 0.431302
O -2.885929 -1.021656 -0.223505
H 3.495312 0.779822 0.073203
H -2.169068 -0.354449 -0.045889
H 1.951854 2.708420 -0.033953

13
3R(H2) scf done: -494.498293
C 1.369224 1.394883 0.624488
C 1.208989 2.858600 0.429005

C	0.353957	0.520059	0.142109
O	2.132789	3.681522	0.865901
C	0.049158	3.188729	-0.221086
C	-0.778812	0.973702	-0.502608
H	-1.532483	0.279248	-0.857339
C	-0.969101	2.353911	-0.708049
C	-2.145338	2.808572	-1.376268
O	2.413775	0.954794	1.220622
O	-2.433736	3.989722	-1.619782
H	-2.837154	2.013244	-1.690143
H	0.506742	-0.539897	0.303479

17

Complejo 3(H5) scf done: -646.143508

C	2.097829	-0.849012	-0.118008
C	0.940600	-1.457239	-0.712991
C	1.991475	0.574992	0.323551
H	-1.085545	-1.229059	-1.320088
O	2.991910	1.140195	0.844924
C	-0.218521	-0.759921	-0.870162
C	0.745921	1.241249	0.133721
C	-0.324502	0.599372	-0.445766
C	-1.603023	1.281200	-0.641430
O	3.177840	-1.465362	0.039394
O	-1.828380	2.438153	-0.315181
H	-2.387706	0.682043	-1.122279
O	-3.664610	-1.470869	0.153503
O	-2.924495	-0.877741	1.266246
H	-2.013356	-1.135555	1.092932
H	1.026110	-2.487687	-1.031660
H	0.663705	2.271420	0.456507

17

TS3-H5 scf done: -646.084710

C	1.329124	1.365406	0.748673
C	1.189972	2.807438	0.411740
C	0.255241	0.563524	0.321234
O	2.145410	3.614887	0.777722
C	0.050900	3.212458	-0.275308
C	-0.870436	0.957740	-0.357401
H	-0.043798	4.263901	-0.519754
H	-1.647479	0.259675	-0.645605
C	-0.978497	2.320912	-0.666123
C	-2.150341	2.750576	-1.374052
O	2.360066	0.942445	1.373934
O	-2.402918	3.911040	-1.718772
H	-2.866844	1.952045	-1.617170
O	0.456811	-1.865583	0.907927
O	0.370080	-1.899837	2.302445
H	-0.576811	-1.989822	2.475145
H	0.387251	-0.736464	0.626705

13

3R(H5) scf done: -494.498180

C	1.284407	1.365144	0.738846
C	1.176564	2.808328	0.414230
C	0.204873	0.593740	0.294917
O	2.142200	3.605524	0.791032
C	0.045598	3.236586	-0.278898
C	-0.909961	0.992845	-0.383851
H	-0.032261	4.291171	-0.515791
H	-1.697798	0.311998	-0.686118

C	-0.995573	2.366010	-0.683661
C	-2.153833	2.819590	-1.396191
O	2.304360	0.909876	1.376375
O	-2.385984	3.986687	-1.737404
H	-2.883163	2.034908	-1.647289

17

Complejo 3(H6) scf done: -646.143508

C	1.692946	-1.571002	0.511461
C	0.752000	-0.936959	1.392218
C	1.446953	-1.478407	-0.959929
H	-1.034130	0.203786	1.577523
O	2.251866	-2.029439	-1.760325
C	-0.330845	-0.271160	0.903675
C	0.297105	-0.760642	-1.400386
C	-0.566483	-0.177566	-0.501578
C	-1.746623	0.559076	-0.951486
O	2.698127	-2.190730	0.931740
O	-2.057320	0.721005	-2.123241
H	-2.374775	0.975584	-0.152813
O	-1.569758	3.132958	1.456790
O	-0.529943	3.139908	0.428927
H	0.016735	2.381138	0.657161
H	0.936033	-1.010001	2.455929
H	0.118113	-0.687550	-2.465667

17

TS3-H6 scf done: -646.082608

C	2.337008	-6.561164	2.977548
C	1.578027	-5.564845	3.666111
C	2.049269	-6.797322	1.547493
H	-0.045806	-3.922469	3.692244
O	2.751155	-7.703327	0.911903
C	0.621930	-4.866287	2.983993
C	1.052199	-6.038171	0.950785
C	0.281801	-5.064658	1.653313
C	-0.780813	-4.316981	1.052508
O	3.253445	-7.223989	3.569568
O	-1.155397	-4.422808	-0.122787
H	-1.284572	-3.599222	1.714021
O	-0.577449	-3.117763	4.332219
O	-0.234767	-1.902868	3.738207
H	0.584919	-1.646908	4.183059
H	1.810621	-5.371033	4.705572
H	0.839470	-6.198735	-0.100440

13

3R(H6) scf done: -494.498103

C	1.250383	1.349310	0.718882
C	1.158587	2.792495	0.406956
C	0.181986	0.493871	0.293459
O	2.136769	3.580964	0.794871
C	0.043204	3.243042	-0.280382
C	-0.865703	1.047016	-0.375837
H	-0.027851	4.300474	-0.510748
C	-1.020821	2.383297	-0.702359
C	-2.172746	2.839247	-1.410334
O	2.260694	0.891839	1.351137
O	-2.397408	4.012537	-1.745315
H	-2.903593	2.059373	-1.666236
H	0.253281	-0.562198	0.523697

17

Complejo 3(C) scf done: -646.145184

C	2.524956	-0.255450	0.302308
C	1.896361	1.097622	0.289710
C	1.720318	-1.374878	-0.098315
O	2.579356	2.105760	0.626691
H	2.184295	-2.352356	-0.085326
C	0.531197	1.194463	-0.111922
C	0.422983	-1.210159	-0.479320
H	0.071138	2.174416	-0.120996
H	-0.174757	-2.062657	-0.778998
C	-0.181785	0.081148	-0.484951
C	-1.584963	0.179133	-0.901639
O	3.724701	-0.381134	0.654245
O	-2.230601	1.224134	-0.903048
H	-2.020393	-0.739616	-1.306603
O	-2.601163	-0.822123	1.253006
O	-3.523366	0.286058	1.452940
H	-3.338278	0.855639	0.692216

17

TS3-C scf done: -646.145066

C	1.216781	0.748742	-0.621924
C	0.527542	2.067311	-0.531164
C	0.412315	-0.437497	-0.541179
O	1.205291	3.132165	-0.599893
H	0.922224	-1.389906	-0.604996
C	-0.890265	2.068486	-0.371621
C	-0.939893	-0.364505	-0.391729
H	-1.394387	3.024482	-0.308643
H	-1.536695	-1.266893	-0.332373
C	-1.600559	0.895763	-0.303535
C	-3.061903	0.897761	-0.147088
O	2.465253	0.706396	-0.768942
O	-3.737184	1.921208	-0.041925
H	-3.547504	-0.076205	-0.254336
O	-3.031507	0.233288	2.218256
O	-3.869045	1.321006	2.692489
H	-4.064987	1.806043	1.876281

17

3A(C) scf done: -646.161099

C	-2.393746	-0.503405	-0.051197
C	-1.819959	0.861601	-0.117903
C	-1.499504	-1.588922	0.219820
O	-2.576239	1.851405	-0.353376
H	-1.924364	-2.583377	0.275408
C	-0.410857	1.007575	0.087261
C	-0.163301	-1.379496	0.407820
H	0.005843	2.005647	0.042278
H	0.495909	-2.212933	0.618711
C	0.393873	-0.068126	0.335271
C	1.889393	0.092864	0.534370
O	-3.636342	-0.676920	-0.227766
O	2.373719	1.327024	0.648601
H	2.220981	-0.592087	1.332852
O	2.418352	-0.553224	-0.719263
O	3.836833	-0.406317	-0.652988
H	3.895737	0.513544	-0.325945

17

Complejo 3(C1) scf done: -646.145072

C	2.082726	-0.086791	-0.290082
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C	1.538207	1.201703	0.236358
C	1.159484	-1.012140	-0.888724
O	2.322612	2.040412	0.758150
C	0.135169	1.428858	0.125173
C	-0.170240	-0.726585	-0.971716
H	-0.263514	2.354946	0.519690
H	-0.856702	-1.433582	-1.421614
C	-0.693580	0.500250	-0.461719
C	-2.136172	0.718980	-0.550877
O	3.308979	-0.326139	-0.197687
O	-2.713092	1.721310	-0.155076
H	-2.706902	-0.097129	-1.015155
O	-1.935668	-1.625028	1.827913
O	-0.552543	-1.480482	2.279449
H	-0.080053	-1.236760	1.475379
H	1.561290	-1.941818	-1.269460

17

TS3-C1 scf done: -646.110632

C	1.794638	-0.238025	-0.524544
C	1.197752	0.927766	0.186741
C	0.911649	-1.194631	-1.097160
O	2.001401	1.847215	0.636870
C	-0.177691	0.990217	0.293637
C	-0.450016	-1.125956	-0.955461
H	-0.623256	1.850278	0.780221
H	-1.100935	-1.869056	-1.400352
C	-1.060479	-0.084819	-0.124870
C	-2.374999	0.322995	-0.737784
O	3.070093	-0.338660	-0.642253
O	-2.718986	1.472340	-0.929498
H	-3.018844	-0.512177	-1.049491
O	-1.707330	-0.841332	1.171362
O	-0.668290	-1.512967	1.868317
H	-0.377698	-2.190912	1.239322
H	1.358426	-1.994614	-1.677261

17

3A(C1) scf done: -646.110773

C	-1.845216	0.162016	-0.497727
C	-1.285759	-0.754242	0.538357
C	-0.932463	0.865969	-1.326880
O	-2.122864	-1.454005	1.251584
C	0.084177	-0.841812	0.660678
C	0.428782	0.793861	-1.171592
H	0.498766	-1.533807	1.385311
H	1.100756	1.349554	-1.814366
C	1.020556	0.009896	-0.071160
C	2.240723	-0.683378	-0.635133
O	-3.119128	0.270944	-0.645005
O	2.412385	-1.886007	-0.629528
H	2.968129	-0.016032	-1.119890
O	1.761994	1.007650	0.884015
O	0.820279	1.938423	1.399288
H	0.500737	2.393764	0.604439
H	-1.354521	1.476631	-2.117597

17

Complejo 3(C2) scf done: -646.143891

C	1.355687	-1.194030	0.912539
C	1.647075	0.222024	0.528572
C	0.245113	-1.849248	0.277538

O	2.617292	0.823210	1.062843
C	0.798233	0.839962	-0.435949
C	-0.523095	-1.201333	-0.640707
H	0.999031	1.868310	-0.707656
H	-1.360112	-1.704663	-1.109304
C	-0.254505	0.154591	-1.003037
C	-1.131161	0.793352	-1.981168
O	2.075209	-1.762365	1.764981
O	-1.005339	1.941217	-2.382442
H	-1.949722	0.165949	-2.360731
O	-0.828916	2.193505	2.282357
O	-1.526257	0.928158	2.048762
H	-1.201373	0.655500	1.184177
H	0.042839	-2.874141	0.559221

17

TS3-C2 scf done: -646.131992

C	0.577332	0.917189	0.643654
C	0.807696	2.351034	0.367926
C	-0.524366	0.278889	-0.003747
O	1.822220	2.940305	0.857315
C	-0.167411	3.066159	-0.414929
C	-1.349341	0.969667	-0.854033
H	0.121999	4.047071	-0.765920
H	-2.158501	0.453272	-1.358962
C	-1.174582	2.351414	-1.111285
C	-2.060043	3.006864	-2.014939
O	1.371962	0.294548	1.412837
O	-2.053876	4.217124	-2.291927
H	-2.807518	2.356243	-2.492821
O	-1.158521	4.007911	1.094172
O	-2.229676	3.147178	1.476732
H	-2.629591	2.895927	0.630029
H	-0.677162	-0.775602	0.186771

17

3A(C2) scf done: -646.146517

C	-1.860089	0.545587	-0.079375
C	-1.120308	-0.599639	-0.547056
C	-1.127177	1.711978	0.352026
O	-1.706825	-1.648820	-0.976823
C	0.388468	-0.623469	-0.473951
C	0.234842	1.771936	0.272144
H	0.786115	-1.092476	-1.377506
H	0.746324	2.689205	0.546606
C	1.031806	0.688985	-0.185505
C	2.406662	0.851216	-0.342640
O	-3.144891	0.526379	-0.069172
O	3.228584	-0.018434	-0.756161
H	2.795463	1.847540	-0.081544
O	0.797166	-1.637273	0.523814
O	0.411248	-1.182692	1.815275
H	0.967143	-0.395799	1.939327
H	-1.702522	2.558694	0.703805

17

Complejo 3(C3) scf done: -646.143576

C	1.648682	-0.877566	0.654322
C	1.503641	0.610999	0.608775
C	0.761392	-1.665966	-0.156334
O	2.278982	1.331092	1.292151
C	0.478664	1.155411	-0.219262

C	-0.188888	-1.079954	-0.935031
H	0.361197	2.231351	-0.244355
H	-0.852153	-1.684885	-1.541543
C	-0.341329	0.340188	-0.970288
C	-1.389600	0.898632	-1.819981
O	2.529003	-1.389599	1.382023
O	-1.615408	2.093122	-1.952444
H	-1.995995	0.161809	-2.365041
O	-0.867644	0.563707	3.042305
H	-1.385522	0.103949	1.246290
O	-1.802876	-0.051195	2.100331
H	0.877857	-2.741095	-0.121917

17

TS3-C3 scf done: -646.126435

C	0.559091	0.706175	0.514783
C	0.279260	2.198141	0.667134
C	-0.184052	-0.036927	-0.442531
O	1.222684	2.931186	1.167779
C	-0.591321	2.772827	-0.361869
C	-1.079158	0.574112	-1.291839
H	-0.700939	3.849673	-0.366832
H	-1.629020	-0.014901	-2.016581
C	-1.286800	1.977123	-1.266095
C	-2.188662	2.534337	-2.244803
O	1.436632	0.184206	1.251299
O	-2.456572	3.732099	-2.372685
H	-2.660278	1.803423	-2.917688
O	-0.820567	2.111514	2.063120
H	-2.453788	1.959822	1.102063
O	-2.053454	1.433527	1.808191
H	-0.002205	-1.102716	-0.500560

17

3A(C3) scf done: -646.127693

C	-1.371331	0.869394	-0.188173
C	-0.861629	-0.541930	-0.541108
C	-0.451936	1.880564	0.179604
O	-1.380705	-1.031012	-1.670117
C	0.617968	-0.686621	-0.425462
C	0.905959	1.633806	0.260892
H	1.028195	-1.650460	-0.699751
H	1.583380	2.428508	0.550372
C	1.447751	0.362063	-0.041551
C	2.880942	0.225243	0.029112
O	-2.614840	1.067985	-0.266156
O	3.518604	-0.800613	-0.229490
H	3.423047	1.129384	0.342504
O	-1.476372	-1.451807	0.552796
H	-0.121854	-1.285109	1.874849
O	-1.055234	-1.027351	1.849574
H	-0.849616	2.864169	0.397350

17

Complejo 3(C4) scf done: -646.143607

C	1.564813	-0.743607	0.454055
C	1.605274	0.746480	0.324460
C	0.482093	-1.443141	-0.181416
O	2.549920	1.389945	0.856169
C	0.558870	1.381948	-0.404810
C	-0.492764	-0.769401	-0.855363
H	0.584419	2.460438	-0.495654

H	-1.309743	-1.308309	-1.319865
C	-0.461382	0.651785	-0.973363
C	-1.535584	1.303063	-1.715999
O	2.459701	-1.332791	1.101596
O	-1.616170	2.507899	-1.911524
H	-2.307835	0.629406	-2.113265
O	-0.857751	0.058686	2.771690
O	-0.967180	-1.399712	2.734600
H	-0.723718	-1.610155	1.826212
H	0.467036	-2.522535	-0.097525

17

TS3-C4 scf done: -646.131235

C	0.324662	0.827413	0.709326
C	0.489141	2.318001	0.474307
C	-0.652506	0.129940	-0.146256
O	1.420177	2.924430	1.078249
C	-0.426024	2.956016	-0.387917
C	-1.466646	0.806236	-0.981772
H	-0.339700	4.027437	-0.520946
H	-2.186460	0.280980	-1.599108
C	-1.390408	2.239485	-1.097637
C	-2.308241	2.889884	-1.987277
O	1.273060	0.173396	1.229489
O	-2.363097	4.111509	-2.198180
H	-3.009019	2.225237	-2.511684
O	-0.902752	1.269852	2.202653
O	-1.257410	0.002494	2.770658
H	-1.949548	-0.322221	2.182552
H	-0.685320	-0.949178	-0.065210

17

3A(C4) scf done: -646.136028

C	-1.219452	0.047836	0.393527
C	-0.247547	1.201418	0.047918
C	-0.539540	-1.288959	0.541101
O	-0.748112	2.357520	-0.068836
C	1.123868	0.936630	-0.102171
C	0.781888	-1.456551	0.389777
H	1.779849	1.769767	-0.323495
H	1.236282	-2.429652	0.540890
C	1.654001	-0.349444	0.049748
C	3.045434	-0.613400	-0.093384
O	-2.046789	0.328062	1.395284
O	3.922936	0.234744	-0.369062
H	3.347567	-1.659004	0.057340
O	-1.958900	0.007214	-0.949520
O	-2.954832	-1.009138	-0.908978
H	-2.490999	-1.784767	-1.250337
H	-1.179940	-2.113761	0.830126

17

Complejo 3(C5) scf done: -646.145066

C	1.922320	0.239808	0.412688
C	1.440288	-0.812088	-0.532969
C	0.987308	0.758606	1.374298
O	2.236504	-1.294596	-1.383845
C	0.080379	-1.227886	-0.431679
C	-0.296784	0.305150	1.425211
H	-0.275726	-1.977675	-1.126843
H	-0.991845	0.704629	2.153769
C	-0.761189	-0.692942	0.516039

C	-2.164351	-1.093091	0.597145
O	3.108194	0.638075	0.346081
O	-2.690923	-1.930608	-0.120803
H	-2.753920	-0.584687	1.372571
O	-2.266681	2.051959	-0.667216
O	-0.913803	2.240386	-1.188779
H	-0.356680	1.841681	-0.509869
H	1.343773	1.518960	2.056672

17

TS3-C5 scf done: -646.115488

C	0.860912	0.840096	0.470323
C	0.792492	2.315401	0.479250
C	-0.258396	0.071545	-0.081546
O	1.717236	2.978228	1.108538
C	-0.243557	2.908290	-0.236927
C	-1.155307	0.745413	-0.962663
H	-0.306407	3.988590	-0.271104
H	-1.862271	0.182216	-1.557835
C	-1.174106	2.130710	-0.973754
C	-2.180079	2.767736	-1.805914
O	1.846754	0.235970	0.986267
O	-2.355757	3.980044	-1.907595
H	-2.822555	2.079394	-2.373711
O	-1.275937	-0.251371	1.351442
O	-0.617114	-1.149021	2.242707
H	-0.764014	-2.014058	1.840417
H	-0.022439	-0.968571	-0.280260

17

3A(C5) scf done: -646.117604

C	-1.133840	0.660577	0.461068
C	-0.108258	1.507840	-0.141827
C	-0.896747	-0.813446	0.589895
O	-0.404150	2.747520	-0.440373
C	1.165733	0.960268	-0.310160
C	0.516892	-1.190985	0.686914
H	1.951710	1.576756	-0.727234
H	0.788848	-2.160997	1.081564
C	1.473059	-0.342934	0.161741
C	2.841442	-0.831348	0.146408
O	-2.258924	1.135286	0.825107
O	3.806545	-0.236203	-0.329607
H	2.989890	-1.822355	0.599637
O	-1.375281	-1.511949	-0.687417
O	-2.794645	-1.379304	-0.819461
H	-3.131986	-2.098747	-0.269065
H	-1.536511	-1.237293	1.364859

17

Complejo 3(C6) scf done: -646.145066

C	1.891092	-0.558253	0.651095
C	1.523918	0.874351	0.865663
C	1.102391	-1.322518	-0.277267
O	2.199477	1.575370	1.667556
C	0.407453	1.391887	0.145987
C	0.055045	-0.759781	-0.943343
H	0.129065	2.424829	0.312641
H	-0.532138	-1.346530	-1.639375
C	-0.302202	0.606333	-0.732559
C	-1.468287	1.126319	-1.443608
O	2.859558	-1.051059	1.274448

O	-1.884475	2.271958	-1.351911
H	-1.978584	0.406726	-2.098762
O	-2.774270	-0.992914	0.859521
O	-1.698204	-1.115021	1.841722
H	-0.904878	-1.172987	1.296300
H	1.375038	-2.358712	-0.428110

17

TS3-C6 scf done: -646.128203

C	1.009627	0.775355	0.366198
C	0.788101	2.256279	0.528497
C	0.124826	0.065997	-0.462024
O	1.566180	2.919614	1.279007
C	-0.274643	2.853874	-0.190515
C	-0.986659	0.676017	-1.067537
H	-0.405745	3.925614	-0.103872
H	-1.480574	0.170112	-1.886478
C	-1.110598	2.114219	-1.009561
C	-2.171799	2.723880	-1.766407
O	2.000793	0.246934	0.960984
O	-2.433746	3.931071	-1.789013
H	-2.779482	2.030157	-2.364512
O	-2.557324	0.156518	0.045776
O	-2.132003	0.403724	1.383000
H	-1.203050	0.113597	1.367015
H	0.299177	-0.993945	-0.599423

17

3A(C6) scf done: -646.140022

C	-1.795756	0.114750	-0.406102
C	-1.195465	-1.128218	0.223265
C	-0.935722	1.078203	-0.867668
O	-1.968901	-1.998274	0.721020
C	0.207391	-1.293857	0.190631
C	0.536013	1.017910	-0.707924
H	0.606978	-2.233239	0.554832
H	1.062039	1.406917	-1.582123
C	1.066713	-0.326290	-0.316309
C	2.462654	-0.531030	-0.426498
O	-3.085445	0.166450	-0.491788
O	3.088186	-1.566759	-0.084620
H	3.029594	0.305126	-0.860000
O	0.981584	2.042011	0.285627
O	0.377597	1.762517	1.541640
H	-0.569157	1.721756	1.315171
H	-1.351186	1.963635	-1.335617

16

1 scf done: -496.123145

C	-0.740004	0.018909	-2.515600
C	-1.913583	-0.307052	-1.825798
C	0.417817	0.348678	-1.818167
H	-2.808046	-0.561945	-2.380757
H	1.319453	0.598977	-2.362777
C	-1.910616	-0.297937	-0.450087
C	0.418416	0.357263	-0.429431
O	-2.985429	-0.595415	0.336538
H	1.304652	0.609932	0.135271
C	-0.742137	0.034955	0.255854
O	-0.750916	0.040455	1.605155
C	-0.720592	0.015243	-3.985166
H	0.248443	0.285036	-4.436369

O	-1.671810	-0.256727	-4.683678
H	-1.631447	-0.204039	1.915016
H	-3.754622	-0.815233	-0.199065

3

H00.	scf done:	-150.907446	
O	-0.763134	0.000000	-2.418707
O	-0.329821	0.000000	-1.143248
H	-0.820415	0.000000	-0.223038

19

Complejo 1(H)	scf done:	-647.073964	
C	0.080376	-0.352776	-0.123665
C	-0.653060	0.839303	-0.043959
C	-2.022972	0.778189	0.035638
C	-2.680784	-0.465879	0.033035
C	-1.952554	-1.643372	-0.047733
C	-0.569192	-1.585633	-0.126266
O	-4.023238	-0.511508	0.110388
H	-2.481644	-2.585698	-0.047370
C	1.531910	-0.320581	-0.205149
O	2.191944	0.709429	-0.204143
O	5.044303	-0.457695	0.509820
O	4.826408	0.638389	-0.167466
O	-2.851548	1.857064	0.121326
H	-0.137000	1.791064	-0.043954
H	0.010621	-2.497490	-0.187574
H	-4.368302	0.388882	0.162601
H	2.028653	-1.297430	-0.272039
H	3.833321	0.718105	-0.224475
H	-2.351277	2.679963	0.118561

19

TS1-H	scf done:	-647.034904	
C	0.118406	-3.930986	1.794867
C	0.842120	-3.344438	2.843520
C	1.897163	-4.034479	3.390690
C	2.242121	-5.309006	2.904748
C	1.521776	-5.882422	1.868092
C	0.456628	-5.191306	1.310643
O	3.276860	-5.973379	3.450699
H	1.805256	-6.863691	1.514602
C	-1.009340	-3.216230	1.201894
O	-1.454671	-2.150690	1.494419
O	-2.369796	-4.144433	-0.715237
O	-3.526155	-3.468284	-0.399485
O	2.683282	-3.584486	4.408894
H	0.570360	-2.363273	3.212467
H	-0.113232	-5.632251	0.503811
H	3.658159	-5.439355	4.159414
H	-1.584127	-3.823766	0.239471
H	-3.428920	-2.612239	-0.838175
H	2.388401	-2.722700	4.721693

15

1R(H)	scf done:	-495.467676	
C	-0.793762	0.031987	-2.448979
C	-1.963817	-0.209588	-1.712985
C	0.410746	0.294475	-1.803981
H	-2.896891	-0.413048	-2.223516
H	1.299508	0.477677	-2.392055
C	-1.905817	-0.183722	-0.338530
C	0.462230	0.319074	-0.417965

O	-2.964368	-0.400620	0.493985
H	1.383607	0.520208	0.109729
C	-0.690391	0.081196	0.315224
O	-0.644355	0.104242	1.661481
C	-0.830802	0.009754	-3.913777
O	-1.739730	-0.190715	-4.643896
H	-3.768713	-0.576619	-0.005038
H	-1.524870	-0.079552	2.011432

19

Complejo 1(H2) scf done: -647.065303

C	1.664672	-0.482852	0.069910
C	1.763133	0.783236	0.625728
C	0.497472	-0.864876	-0.616859
H	-1.428441	-0.957761	1.107106
O	0.517109	-2.127405	-1.131818
C	0.701853	1.670725	0.500909
C	-0.551627	0.020600	-0.753796
C	-0.451611	1.296345	-0.180563
C	-1.556399	2.259872	-0.313678
O	2.683466	-1.354435	0.188328
O	-2.600788	2.027201	-0.878539
H	2.427365	-2.189368	-0.225071
H	-0.380988	-2.476336	-1.175714
H	-1.369704	3.243394	0.146967
O	-1.944658	-1.728148	1.425007
O	-1.970621	-2.581708	0.441201
H	2.667711	1.053094	1.152527
H	-1.436991	-0.251809	-1.316294
H	0.769049	2.660228	0.934649

19

TS1-H2 scf done: -647.005543

C	-2.100564	0.077922	0.056429
C	-2.122768	-1.300475	0.213548
C	-0.877367	0.746803	-0.146790
H	2.236501	2.430823	1.285991
O	-0.943339	2.096257	-0.285146
C	-0.939880	-2.027015	0.168103
C	0.259723	-0.010521	-0.186581
C	0.285265	-1.388749	-0.036035
C	1.530074	-2.169561	-0.091517
O	-3.246151	0.784739	0.100688
O	2.622125	-1.690888	-0.287436
H	-3.049201	1.720342	-0.034004
H	-0.059285	2.448649	-0.455111
H	1.398812	-3.252626	0.060413
O	2.733426	1.825189	0.719112
O	1.965314	1.756818	-0.438774
H	-3.073942	-1.789766	0.368958
H	1.437470	0.783016	-0.385926
H	-0.957287	-3.103046	0.290193

15

1R(H2) scf done: -495.428089

C	1.335600	1.424606	0.604109
C	1.160854	2.808799	0.406748
C	0.376857	0.524924	0.154074
O	2.153089	3.610884	0.881936
C	0.024635	3.194568	-0.234695
C	-0.761274	0.983334	-0.493863
H	-1.508063	0.281210	-0.844388

C	-0.963760	2.352835	-0.705042
C	-2.172478	2.829389	-1.392429
O	2.439116	0.975170	1.232853
O	-2.423008	3.991298	-1.613905
H	-2.863568	2.030144	-1.705870
H	2.996117	1.724971	1.476780
H	1.953021	4.536769	0.704886
H	0.540011	-0.530074	0.320800

19

Complejo 1(H3) scf done: -647.065302

C	-1.063210	-0.777365	-0.423317
C	-0.607773	0.548486	-0.454760
C	0.749134	0.796482	-0.429559
C	1.666009	-0.270462	-0.396625
C	1.211092	-1.579659	-0.376446
C	-0.155116	-1.830507	-0.387483
O	2.987106	-0.013367	-0.380724
O	1.310304	2.038741	-0.459105
C	-2.505805	-1.068720	-0.450522
O	-3.372346	-0.224612	-0.473493
O	-0.306314	2.580423	1.993564
O	-0.536888	1.420018	2.539263
H	1.934009	-2.382877	-0.347030
H	-1.319305	1.363293	-0.520828
H	-0.519089	-2.849793	-0.368723
H	-2.760765	-2.140777	-0.450223
H	0.711228	2.678679	-0.056958
H	-0.539327	0.768117	1.807142
H	3.117055	0.943902	-0.364173

19

TS1-H3 scf done: -647.042458

C	-1.068536	-0.183519	-0.315458
C	-0.710187	1.154493	-0.302805
C	0.637367	1.507692	-0.163346
C	1.620272	0.481134	-0.041581
C	1.252092	-0.858506	-0.062382
C	-0.085788	-1.180312	-0.199098
O	2.899045	0.830457	0.085316
O	1.063013	2.758129	-0.163879
C	-2.482075	-0.582905	-0.450849
O	-3.403892	0.195088	-0.526101
O	0.651582	3.316516	2.089394
O	0.462988	2.030167	2.472358
H	2.012572	-1.620453	0.030711
H	-1.456483	1.932130	-0.404536
H	-0.388688	-2.219999	-0.216529
H	-2.656608	-1.670744	-0.476468
H	0.886231	3.195117	0.853442
H	-0.499065	1.895405	2.453376
H	2.951638	1.797736	0.043420

15

1R(H3) scf done: -495.480934

C	-0.813025	-0.000670	-2.466469
C	-1.961276	-0.313724	-1.784330
C	0.377190	0.333600	-1.776032
H	-2.872797	-0.569647	-2.306801
H	1.261317	0.574332	-2.352872
C	-1.962953	-0.303919	-0.350574
C	0.435132	0.359299	-0.392590

O	-2.949961	-0.571410	0.362471
H	1.344619	0.614739	0.131482
C	-0.709633	0.047175	0.319601
O	-0.733645	0.049446	1.642411
C	-0.795696	-0.005603	-3.947753
H	0.171596	0.259508	-4.403122
O	-1.752208	-0.274980	-4.632488
H	-1.638870	-0.198146	1.905357

19

Complejo 1(H4) scf done: -647.068314

C	0.778844	-0.102530	-0.088446
C	0.082934	1.035850	-0.516895
C	0.104175	-1.252985	0.274910
O	0.873760	2.095885	-0.845098
H	0.666947	-2.117999	0.597940
C	-1.292068	1.019232	-0.580830
C	-1.283953	-1.269987	0.213619
H	-1.845164	1.890094	-0.910505
H	-1.827748	-2.162324	0.494328
C	-1.978190	-0.142178	-0.210685
C	-3.449423	-0.183717	-0.268545
O	2.139317	-0.061705	-0.035280
O	-4.145257	0.739776	-0.624328
H	-3.898944	-1.140681	0.042494
H	2.450100	0.810358	-0.317106
O	4.886929	-0.057459	1.247565
O	4.112735	-1.062655	1.559150
H	3.280084	-0.897161	1.065510
H	0.344925	2.860189	-1.097796

19

TS1-H4 scf done: -647.035725

C	1.504071	0.367412	0.016687
C	0.512756	1.394012	0.097767
C	1.091450	-0.980283	-0.037969
O	0.970649	2.651822	0.139925
H	1.860182	-1.737818	-0.100868
C	-0.831243	1.060488	0.119889
C	-0.246485	-1.298634	-0.030110
H	-1.591933	1.828923	0.182572
H	-0.568901	-2.330478	-0.084053
C	-1.205277	-0.277128	0.053148
C	-2.637979	-0.642769	0.061318
O	2.770934	0.684634	-0.031842
O	-3.538115	0.160710	0.120268
H	-2.844835	-1.723244	0.006583
H	3.057846	1.173346	0.940405
O	3.134057	1.395361	2.179463
O	1.865317	1.127251	2.592011
H	1.923721	0.258729	3.020573
H	0.241002	3.269584	0.265457

15

1R(H4) scf done: -495.472391

C	-0.766121	0.010549	-2.470817
C	-1.932675	-0.330795	-1.788674
C	0.426095	0.349065	-1.780563
H	-2.822259	-0.582981	-2.352280
H	1.307579	0.607495	-2.353849
C	-1.936606	-0.342192	-0.410261
C	0.453269	0.346791	-0.421404

O	-3.001217	-0.654504	0.326337
H	1.343261	0.599235	0.137696
C	-0.724534	0.001355	0.352578
O	-0.727882	-0.009058	1.585507
C	-0.762370	0.022676	-3.946475
H	0.194876	0.301991	-4.412280
O	-1.728926	-0.250420	-4.620505
H	-3.752095	-0.866373	-0.242536

19

Complejo 1(H5) scf done: -647.064855

C	0.733442	1.203701	-0.756869
C	-0.312322	1.429238	0.156409
C	0.894386	-0.047116	-1.336259
O	-0.360352	2.691783	0.662393
C	-1.186505	0.415040	0.479171
C	0.009882	-1.072037	-1.014528
H	-1.993641	0.577475	1.182788
H	0.126893	-2.049428	-1.465296
C	-1.026898	-0.844254	-0.111055
C	-1.957376	-1.939374	0.214665
O	1.582980	2.200758	-1.064202
O	-2.891888	-1.833872	0.974564
H	-1.747311	-2.893356	-0.294532
O	3.045944	-1.305797	1.100551
O	1.879697	-1.125037	1.658368
H	1.246546	-0.987644	0.926618
H	1.336585	2.991253	-0.567580
H	-1.089393	2.789765	1.284172
H	1.709331	-0.201096	-2.029380

19

TS1-H5 scf done: -647.005831

C	1.326402	1.458623	0.711001
C	1.158169	2.820206	0.388828
C	0.317470	0.598985	0.337770
O	2.186943	3.619356	0.784834
C	0.029164	3.252016	-0.273233
C	-0.823431	0.979667	-0.326205
H	-0.097397	4.298481	-0.521981
H	-1.589977	0.267796	-0.605859
C	-0.963353	2.334606	-0.632667
C	-2.174295	2.781357	-1.343403
O	2.427212	1.033801	1.351871
O	-2.395064	3.928368	-1.655130
H	-2.892412	1.980459	-1.583188
O	0.451625	-1.860289	0.897966
O	0.189777	-1.929401	2.265863
H	-0.761580	-2.094079	2.301524
H	3.000187	1.791578	1.526122
H	2.028360	4.537077	0.538633
H	0.475581	-0.792774	0.669121

15

1R(H5) scf done: -495.428501

C	1.251981	1.404201	0.714457
C	1.128158	2.771250	0.395654
C	0.226468	0.589270	0.306836
O	2.168549	3.542774	0.817752
C	0.024979	3.238132	-0.289393
C	-0.890895	0.987239	-0.373266
H	-0.068131	4.289208	-0.533487

H	-1.671939	0.298327	-0.671240
C	-0.985144	2.351203	-0.674661
C	-2.167127	2.838226	-1.406478
O	2.326500	0.944508	1.383395
O	-2.347840	3.993145	-1.716721
H	-2.904956	2.061375	-1.664764
H	2.915071	1.686403	1.571005
H	2.028654	4.468674	0.592067

19

Complejo 1(H6) scf done: -647.065026

C	1.253844	-1.048803	-0.137585
C	0.124716	-1.328316	-0.896974
C	1.448405	0.241711	0.387191
H	-1.682632	-0.528905	-1.740348
O	2.587680	0.390220	1.116845
C	-0.802970	-0.320146	-1.145333
C	0.525614	1.236245	0.150586
C	-0.606172	0.954895	-0.622606
C	-1.606038	2.003608	-0.887875
O	2.160019	-2.015178	0.099893
H	-2.470280	1.677089	-1.488336
H	2.868682	-1.657138	0.649476
H	2.670077	1.288960	1.453664
O	-1.517608	3.143399	-0.493952
O	-2.858155	-1.520308	1.381988
O	-1.659028	-1.292683	1.844785
H	-1.095016	-1.128912	1.063089
H	-0.005994	-2.326613	-1.290962
H	0.664854	2.230879	0.556456

19

TS1-H6 scf done: -647.007678

C	2.236145	-6.529111	2.935785
C	1.524605	-5.595170	3.681462
C	1.977076	-6.680004	1.560898
H	-0.101494	-3.852946	3.755645
O	2.744630	-7.625195	0.947669
C	0.584098	-4.853469	3.006536
C	1.021134	-5.915791	0.931319
C	0.289651	-4.967371	1.664792
C	-0.741474	-4.139204	1.012642
O	3.174631	-7.287872	3.529365
H	-1.266632	-3.432953	1.670936
H	3.564805	-7.878014	2.871928
H	2.530202	-7.693256	0.011244
O	-1.011156	-4.215484	-0.163590
O	-0.549182	-3.020678	4.321548
O	-0.094505	-1.871805	3.673232
H	0.676413	-1.611242	4.194648
H	1.725981	-5.478308	4.737642
H	0.818342	-6.036059	-0.126421

15

1R(H6) scf done: -495.430218

C	1.217646	1.385448	0.695125
C	1.107738	2.755931	0.386739
C	0.215656	0.497618	0.311237
O	2.159532	3.511865	0.819807
C	0.017285	3.244962	-0.294437
C	-0.843474	1.044552	-0.363431
H	-0.067764	4.298708	-0.532154

C	-1.009516	2.368161	-0.693124
C	-2.188447	2.859252	-1.422943
O	2.294740	0.933667	1.362958
O	-2.357288	4.019085	-1.724805
H	-2.928919	2.089616	-1.686219
H	2.882233	1.676781	1.551436
H	2.030627	4.441105	0.603598
H	0.301631	-0.553955	0.548965

4

HOOH	scf done:	-151.579881	
O	-1.305503	0.026692	-4.043248
O	-1.268849	0.479752	-2.695015
H	-0.485208	0.030058	-2.355949
H	-2.089144	-0.536503	-4.041942

19

Complejo 1(C)	scf done:	-647.073973	
C	2.318860	-0.850716	0.259554
C	1.816140	0.395318	0.678152
C	1.490491	-1.762844	-0.377069
O	2.731330	1.199009	1.290126
H	1.901291	-2.712642	-0.688501
C	0.499460	0.720642	0.460157
C	0.160470	-1.437697	-0.598728
H	0.100956	1.675926	0.777305
H	-0.496155	-2.140945	-1.094450
C	-0.335470	-0.203462	-0.183594
C	-1.733540	0.114301	-0.427361
O	3.610384	-1.157315	0.478946
O	-2.257850	1.169998	-0.099931
H	-2.320223	-0.661380	-0.936258
O	-5.242115	0.695473	-1.137074
O	-4.790872	1.763222	-0.534411
H	-3.828396	1.575845	-0.351961
H	4.039705	-0.418157	0.928115
H	2.335536	2.035425	1.556985

19

TS1-C	scf done:	-647.021041	
C	1.136261	0.204538	-0.040253
C	0.657297	1.315133	0.665220
C	0.244695	-0.693270	-0.605007
O	1.625699	2.127944	1.183418
H	0.633666	-1.547415	-1.141406
C	-0.699596	1.527237	0.800770
C	-1.122243	-0.483404	-0.469632
H	-1.072612	2.382692	1.350284
H	-1.823032	-1.182364	-0.908184
C	-1.593008	0.622537	0.226981
C	-3.057989	0.851134	0.346936
O	2.469427	0.005713	-0.165017
O	-3.507538	1.665109	1.239245
H	-3.671619	-0.016312	0.090336
O	-3.400689	1.844613	-0.955972
O	-4.711604	1.706765	-1.308524
H	-5.092373	2.578771	-1.125686
H	2.933288	0.725092	0.279935
H	1.233953	2.872852	1.650185

19

1A(C)	scf done:	-647.042823	
C	2.294057	-0.391053	-0.097762

C	1.573062	0.801039	0.034224
C	1.623368	-1.603280	-0.137462
O	2.332774	1.934623	0.062722
H	2.196145	-2.513578	-0.246710
C	0.195333	0.779817	0.127816
C	0.237841	-1.633212	-0.043068
H	-0.356563	1.706351	0.224109
H	-0.286518	-2.578087	-0.075475
C	-0.471434	-0.446444	0.079808
C	-1.976261	-0.463954	0.214791
O	3.643310	-0.361208	-0.191396
O	-2.268289	-0.037871	1.465908
H	-2.375892	-1.475034	0.074554
O	-2.500113	0.394155	-0.791715
O	-3.915245	0.351976	-0.671618
H	-4.092409	1.076773	-0.056715
H	3.939127	0.555643	-0.141476
H	1.780820	2.717059	0.160419

19

Complejo 1(C1) scf done: -647.065384

C	1.735360	-0.149578	-0.371202
C	1.160618	1.017321	0.163159
C	0.932266	-1.111522	-0.966122
O	2.050131	1.882430	0.722875
C	-0.201147	1.214894	0.102451
C	-0.443680	-0.911241	-1.033861
H	-0.654267	2.105289	0.520168
H	-1.079531	-1.655810	-1.496494
C	-1.009151	0.245722	-0.502079
C	-2.471423	0.427642	-0.559033
O	3.067568	-0.333921	-0.303308
O	-3.050163	1.402940	-0.141169
H	-3.023006	-0.403927	-1.025403
O	-2.150178	-1.630222	1.877231
O	-0.856939	-1.749402	2.005377
H	-0.473220	-1.432900	1.162583
H	3.469543	0.424672	0.138641
H	1.603511	2.658780	1.077082
H	1.393704	-2.001166	-1.370895

19

TS1-C1 scf done: -647.029261

C	1.032378	0.846878	0.283418
C	0.877575	2.256675	0.359919
C	0.102025	0.073358	-0.418053
O	1.897100	2.884765	1.008766
C	-0.190440	2.872804	-0.210731
C	-0.989115	0.677895	-0.985753
H	-0.302048	3.948524	-0.182800
H	-1.715154	0.099808	-1.542033
C	-1.240953	2.077952	-0.777972
C	-2.146039	2.732165	-1.780731
O	2.094805	0.261001	0.851754
O	-2.069841	3.890639	-2.093469
H	-2.910988	2.066617	-2.211128
O	-2.540222	2.065023	0.469151
O	-2.007778	1.525987	1.631164
H	-2.121859	0.572657	1.518222
H	2.630487	0.935391	1.290849
H	1.700580	3.819602	1.133036

H	0.278953	-0.989157	-0.514455
19			
1A(C1)	scf done:	-647.037832	
C	1.710756	-0.271041	-0.517724
C	1.213495	0.579278	0.518702
C	0.816134	-0.959661	-1.348861
O	2.204695	1.206021	1.214359
C	-0.106851	0.731717	0.737130
C	-0.527495	-0.849873	-1.157774
H	-0.471697	1.399541	1.506774
H	-1.225322	-1.373936	-1.798039
C	-1.107342	-0.026534	-0.054236
C	-2.172835	0.876505	-0.688889
O	3.035045	-0.394375	-0.706670
O	-2.091071	2.072160	-0.736444
H	-3.015352	0.329534	-1.141559
O	-1.953717	-0.860798	0.805644
O	-1.153641	-1.850171	1.426307
H	-1.125407	-2.550962	0.760037
H	3.496042	0.153536	-0.057900
H	1.836338	1.750268	1.918344
H	1.219738	-1.573032	-2.143314
19			
Complejo 1(C2)	scf done:	-647.073075	
C	-2.107859	0.629952	-0.157150
C	-1.324735	-0.538762	-0.140120
C	-1.506185	1.876521	-0.073361
O	-2.035987	-1.697771	-0.233050
C	0.043210	-0.458786	-0.037596
C	-0.125851	1.960978	0.028237
H	0.644586	-1.359297	-0.029359
H	0.353702	2.929040	0.093956
C	0.649428	0.802582	0.048089
C	2.095373	0.937246	0.156397
O	-3.446026	0.535853	-0.256183
O	2.892177	0.013573	0.206284
H	2.470328	1.969090	0.193489
O	2.230312	-3.241669	0.069361
O	3.323715	-2.612251	0.403076
H	3.121251	-1.644977	0.331548
H	-3.694663	-0.396129	-0.304068
H	-1.453968	-2.464863	-0.210396
H	-2.128806	2.759673	-0.089152
19			
TS1-C2	scf done:	-647.032282	
C	0.705677	0.867211	0.504477
C	0.746618	2.258991	0.398538
C	-0.281193	0.151548	-0.154444
O	1.745787	2.877568	1.060682
C	-0.268150	2.980608	-0.283141
C	-1.232108	0.830480	-0.926135
H	-0.025013	3.964017	-0.665401
H	-1.985771	0.266568	-1.461070
C	-1.217326	2.204622	-1.026760
C	-2.227290	2.892630	-1.815648
O	1.641967	0.214121	1.225476
O	-2.367862	4.102290	-1.831384
H	-2.888160	2.243688	-2.410713
O	-1.117262	3.684324	1.198160

O	-2.486891	3.646402	1.073307
H	-2.684698	4.356914	0.445602
H	2.216775	0.855440	1.660406
H	1.635159	3.835625	1.044338
H	-0.296198	-0.924950	-0.064933

19

1A(C2) scf done: -647.057552

C	-2.019749	0.332566	-0.006362
C	-1.082040	-0.660800	-0.145849
C	-1.617975	1.669836	0.091327
O	-1.501628	-1.937575	-0.203560
C	0.377120	-0.399083	-0.292498
C	-0.252373	1.992726	0.076492
H	0.694653	-0.726525	-1.291412
H	0.040630	3.027895	0.201962
C	0.727048	1.042786	-0.073705
C	2.109937	1.438469	-0.041228
O	-3.339855	0.037530	0.067912
O	3.060876	0.668145	-0.140792
H	2.292307	2.514319	0.089457
O	1.028613	-1.293051	0.639032
O	2.169461	-1.875765	0.027321
H	2.762611	-1.097725	-0.027313
H	-3.453971	-0.920046	0.044661
H	-0.757955	-2.525169	-0.006771
H	-2.369823	2.433971	0.221049

19

Complejo 1(C3) scf done: -647.069181

C	0.497212	-0.938096	0.555552
C	0.406802	0.424033	0.232389
C	-0.160998	-1.869661	-0.240142
O	1.079536	1.300436	1.066348
C	-0.317502	0.847067	-0.857277
C	-0.886725	-1.449517	-1.343040
H	-0.386317	1.900103	-1.100275
H	-1.395222	-2.175004	-1.965148
C	-0.965471	-0.095289	-1.659132
C	-1.737611	0.334356	-2.833964
O	1.211065	-1.371687	1.607695
O	-1.857465	1.484996	-3.190483
H	-2.220861	-0.481952	-3.395073
O	1.814845	0.397074	3.811783
O	1.165368	1.525299	3.765778
H	0.919352	1.636832	2.819655
H	1.569433	-0.638706	2.131825
H	1.346850	2.085301	0.572518
H	-0.082291	-2.915588	0.020993

19

TS1-C3 scf done: -647.033251

C	0.470921	0.963399	0.555648
C	0.338833	2.394185	0.431411
C	-0.439881	0.122986	-0.049100
O	1.461157	3.082169	0.778899
C	-0.562016	2.900543	-0.548627
C	-1.412174	0.663925	-0.883605
H	-0.572450	3.960874	-0.761699
H	-2.127865	0.010989	-1.365883
C	-1.461620	2.044932	-1.145489
C	-2.462333	2.558196	-2.100147

O	1.453783	0.484360	1.320951
O	-2.565390	3.719934	-2.417771
H	-3.133017	1.794454	-2.526240
O	-0.710005	2.667487	1.979531
O	-0.280817	3.874728	2.528056
H	0.263691	3.600477	3.278881
H	1.998630	1.226392	1.619776
H	1.189117	3.915676	1.197571
H	-0.366017	-0.942202	0.115851

19

1A(C3) scf done: -647.048732

C	1.130019	1.159712	0.042529
C	0.820011	-0.297606	0.232988
C	0.177799	2.063030	-0.323929
O	1.552623	-0.739572	1.342065
C	-0.638212	-0.580965	0.322065
C	-1.167898	1.671083	-0.405785
H	-0.949218	-1.573090	0.619278
H	-1.922271	2.387199	-0.700284
C	-1.556718	0.363451	-0.042358
C	-2.999910	0.036779	-0.022746
O	2.411484	1.515301	0.208112
O	-3.451348	-1.024761	0.335546
H	-3.664639	0.847656	-0.362076
O	1.374661	-0.904767	-0.965137
O	1.247218	-2.316830	-0.820020
H	2.173513	-2.588186	-0.773271
H	2.899854	0.771114	0.584354
H	1.323608	-1.659125	1.520765
H	0.471504	3.086565	-0.509873

19

Complejo 1(C4) scf done: -647.065039

C	1.254764	-0.804121	0.310874
C	1.156543	0.599596	0.313619
C	0.336173	-1.564521	-0.401549
O	2.110612	1.230958	1.049431
C	0.153485	1.228307	-0.388623
C	-0.672479	-0.927416	-1.121368
H	0.067079	2.308069	-0.386524
H	-1.387443	-1.513125	-1.684692
C	-0.767540	0.460207	-1.111551
C	-1.847633	1.113035	-1.870032
O	2.238468	-1.410321	0.998531
O	-2.018804	2.309259	-1.920973
H	-2.516404	0.423508	-2.410293
O	-0.605357	-0.432951	2.982289
O	-1.533362	-0.792275	2.137249
H	-1.073962	-1.020335	1.303805
H	2.732578	-0.744017	1.493054
H	1.940382	2.177574	1.100889
H	0.432900	-2.641431	-0.394139

19

TS1-C4 scf done: -647.037049

C	0.474784	0.798986	0.643368
C	0.476383	2.233927	0.491779
C	-0.353733	0.030815	-0.226732
O	1.438912	2.853794	1.204524
C	-0.481052	2.853094	-0.260982
C	-1.318707	0.661920	-0.962651

H	-0.532305	3.932594	-0.324908
H	-2.008260	0.088335	-1.569234
C	-1.402551	2.069811	-0.972989
C	-2.442508	2.711766	-1.783100
O	1.568368	0.201277	1.150525
O	-2.588963	3.911466	-1.879372
H	-3.106338	2.017591	-2.322588
O	-0.545128	0.731027	2.217153
O	-1.797852	1.271116	2.083295
H	-2.342500	0.533492	1.774466
H	2.032937	0.828880	1.719134
H	1.328550	3.811145	1.175074
H	-0.243329	-1.044052	-0.210615

19

1A(C4) scf done: -647.055180

C	1.287300	-0.254998	-0.384242
C	0.448918	0.975542	-0.151718
C	0.472805	-1.489238	-0.584534
O	1.208800	2.078855	-0.088833
C	-0.901658	0.942911	-0.033162
C	-0.866156	-1.491464	-0.437841
H	-1.467564	1.848568	0.146170
H	-1.427537	-2.409927	-0.557063
C	-1.582083	-0.287734	-0.148733
C	-3.029187	-0.339620	-0.006682
O	2.155024	-0.091946	-1.454075
O	-3.723815	0.629004	0.243173
H	-3.480509	-1.334701	-0.140282
O	2.182365	-0.435952	0.750387
O	1.409020	-0.462002	1.936294
H	1.219259	-1.404287	2.046030
H	2.631444	0.739309	-1.330070
H	0.665489	2.865190	0.045702
H	1.033054	-2.382987	-0.825174

19

Complejo 1(C5) scf done: -647.065013

C	1.474950	-0.648174	0.420179
C	1.198079	0.718387	0.602911
C	0.703012	-1.403994	-0.453050
O	2.019141	1.348653	1.486432
C	0.164605	1.317858	-0.082224
C	-0.337298	-0.796815	-1.151647
H	-0.058668	2.368584	0.057843
H	-0.941214	-1.377894	-1.836928
C	-0.607753	0.556176	-0.965831
C	-1.723406	1.174824	-1.702615
O	2.486617	-1.225508	1.094797
O	-2.029349	2.341700	-1.619185
H	-2.282355	0.488100	-2.358540
O	-2.854988	-1.629344	1.095908
O	-1.758666	-1.289359	1.717637
H	-1.070838	-1.200692	1.028052
H	2.906507	-0.566083	1.661804
H	1.777807	2.276088	1.585022
H	0.933814	-2.452507	-0.580565

19

TS1-C5 scf done: -647.027759

C	0.823950	0.857117	0.451830
C	0.741263	2.255522	0.449262

C	-0.209298	0.068414	-0.128020
O	1.736369	2.881963	1.141357
C	-0.257257	2.892438	-0.246539
C	-1.135987	0.750047	-0.980989
H	-0.326151	3.972367	-0.265704
H	-1.845160	0.174344	-1.560412
C	-1.184426	2.120100	-0.986270
C	-2.207688	2.790935	-1.808398
O	1.841545	0.233490	1.053875
O	-2.339685	3.990284	-1.884707
H	-2.868347	2.110773	-2.369414
O	-1.300137	-0.288645	1.293317
O	-0.597558	-1.025753	2.235064
H	-0.715695	-1.941772	1.950941
H	2.409238	0.889781	1.480130
H	1.658065	3.838471	1.064514
H	0.035576	-0.964140	-0.338544

19

1A(C5) scf done: -647.040604

C	-1.037765	0.659142	0.307814
C	0.030473	1.446503	-0.079505
C	-0.922857	-0.813547	0.482607
O	-0.278059	2.763471	-0.297254
C	1.307179	0.922250	-0.195289
C	0.495226	-1.271865	0.487419
H	2.144867	1.536436	-0.494872
H	0.682427	-2.308902	0.732591
C	1.514129	-0.449261	0.125886
C	2.880097	-1.010246	0.087110
O	-2.254639	1.186724	0.502600
O	3.863476	-0.376275	-0.214782
H	2.951183	-2.076214	0.355714
O	-1.529104	-1.525370	-0.640005
O	-2.942141	-1.534298	-0.471192
H	-3.101114	-2.449277	-0.205756
H	-2.212340	2.137158	0.329188
H	0.521747	3.282442	-0.426215
H	-1.461935	-1.133503	1.378161

19

Complejo 1(C6) scf done: -647.065013

C	1.474950	-0.648174	0.420179
C	1.198079	0.718387	0.602911
C	0.703012	-1.403994	-0.453050
O	2.019141	1.348653	1.486432
C	0.164605	1.317858	-0.082224
C	-0.337298	-0.796815	-1.151647
H	-0.058668	2.368584	0.057843
H	-0.941214	-1.377894	-1.836928
C	-0.607753	0.556176	-0.965831
C	-1.723406	1.174824	-1.702615
O	2.486617	-1.225508	1.094797
O	-2.029349	2.341700	-1.619185
H	-2.282355	0.488100	-2.358540
O	-2.854988	-1.629344	1.095908
O	-1.758666	-1.289359	1.717637
H	-1.070838	-1.200692	1.028052
H	2.906507	-0.566083	1.661804
H	1.777807	2.276088	1.585022
H	0.933814	-2.452507	-0.580565

19

TS1-C6 scf done: -647.034756
C 0.985877 0.823895 0.303671
C 0.725258 2.211780 0.489152
C 0.189493 0.081522 -0.520420
O 1.575150 2.832824 1.337145
C -0.301231 2.840126 -0.193257
C -0.973987 0.674641 -1.094527
H -0.467961 3.904773 -0.083618
H -1.452363 0.159427 -1.917552
C -1.111066 2.095801 -1.033332
C -2.202942 2.731170 -1.777357
O 2.043921 0.265382 0.930778
O -2.431858 3.921419 -1.764211
H -2.823031 2.044290 -2.374626
O -2.348616 0.165728 0.050708
O -2.073331 0.626578 1.315755
H -1.480565 -0.041549 1.688623
H 2.513834 0.943130 1.431317
H 1.370354 3.772221 1.412186
H 0.400277 -0.968464 -0.665490

19

1A(C6) scf done: -647.050141
C 1.690556 -0.288064 -0.345648
C 1.206765 0.983194 0.141835
C 0.828452 -1.217921 -0.793689
O 2.174816 1.811323 0.580297
C -0.140199 1.298530 0.111441
C -0.646144 -1.013464 -0.720310
H -0.482577 2.274124 0.436513
H -1.123730 -1.314385 -1.657131
C -1.056314 0.376419 -0.345655
C -2.469997 0.712336 -0.408773
O 3.027270 -0.497658 -0.357814
O -2.933860 1.783825 -0.059757
H -3.127585 -0.075225 -0.807565
O -1.250495 -1.974307 0.196264
O -0.798710 -1.693527 1.510779
H 0.016258 -2.210942 1.568406
H 3.478741 0.289487 -0.032146
H 1.809441 2.654844 0.874126
H 1.199758 -2.159766 -1.174937

15

2 scf done: -495.645849
C 0.237076 0.147601 -0.009714
C -0.461379 1.383517 -0.015578
C -1.823308 1.381390 -0.044704
C -2.607913 0.159967 -0.069409
C -1.873388 -1.055820 -0.063054
C -0.490359 -1.048720 -0.033820
O -3.869462 0.275536 -0.094450
H -2.427389 -1.985543 -0.081459
C 1.675743 0.091400 0.020293
O 2.442785 1.046139 0.043273
O -2.570677 2.517878 -0.052630
H 0.092586 2.313434 0.002864
H 0.052652 -1.988191 -0.029220
H 2.088844 -0.934712 0.021672
H -3.482303 2.168956 -0.072779

18

Complejo 2(H) scf done: -646.604643

C	-0.220054	0.121351	-0.050786
C	0.644658	-1.010595	-0.005072
C	1.988861	-0.821073	0.007843
C	2.595636	0.503903	-0.025320
C	1.698327	1.612067	-0.073296
C	0.338002	1.414773	-0.084911
O	3.851766	0.571157	-0.007866
H	2.122814	2.606826	-0.099646
C	-1.627177	-0.011751	-0.062043
O	-2.253273	-1.092491	-0.033859
O	-5.004760	0.124605	0.642264
O	-4.747671	-0.949895	-0.055532
O	2.884789	-1.840318	0.053206
H	0.224776	-2.007540	0.021613
H	-0.331601	2.267178	-0.120250
H	-2.198237	0.925578	-0.100684
H	-3.710499	-1.034476	-0.059895
H	3.743646	-1.379300	0.054239

18

TS2-H scf done: -646.564561

C	0.134633	-4.071020	1.789816
C	0.875852	-3.465726	2.844760
C	1.947494	-4.121463	3.362971
C	2.376452	-5.427073	2.884182
C	1.608314	-5.996392	1.828242
C	0.522212	-5.331232	1.304311
O	3.383541	-5.948203	3.434423
H	1.903899	-6.966836	1.451488
C	-0.991139	-3.414813	1.213038
O	-1.498639	-2.347245	1.457719
O	-2.335670	-4.241112	-0.775523
O	-3.421083	-3.457156	-0.447800
O	2.709792	-3.619395	4.368655
H	0.584625	-2.495534	3.226451
H	-0.051126	-5.781208	0.502143
H	-1.530389	-4.036352	0.275151
H	-3.136260	-2.556622	-0.653640
H	3.377302	-4.317297	4.504774

14

2R(H) scf done: -494.993833

C	-2.383188	-0.383851	0.124046
C	-1.561563	0.811492	0.048759
C	-1.723427	-1.617749	-0.131877
O	-2.236448	1.964911	0.300569
H	-2.309417	-2.526229	-0.083182
C	-0.233798	0.774432	-0.248242
C	-0.376512	-1.654952	-0.433241
H	0.346663	1.687188	-0.295398
H	0.114872	-2.601306	-0.626318
C	0.389338	-0.482496	-0.498102
C	1.783740	-0.565419	-0.814127
O	-3.606364	-0.234537	0.407932
O	2.627293	0.275512	-0.925778
H	-3.142900	1.646757	0.472575

18

Complejo 2(H2) scf done: -646.598123

C	1.784362	-0.050206	-0.014328
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C	1.687226	-1.448707	0.199195
C	0.536485	0.639710	-0.250366
H	-0.234252	3.091545	0.322484
O	0.717621	1.989682	-0.447339
C	0.454812	-2.077260	0.179223
C	-0.677047	0.027139	-0.273526
C	-0.732957	-1.371885	-0.052714
C	-1.986999	-2.085844	-0.058311
O	2.840317	0.652393	-0.021539
H	-1.892273	-3.171600	0.127068
O	-3.094328	-1.600964	-0.242612
O	-0.814663	3.770732	0.765204
O	-1.693521	4.138780	-0.127922
H	2.597497	-2.005177	0.379432
H	0.397583	-3.147589	0.346768
H	1.698117	2.066865	-0.372239
H	-1.587981	0.582387	-0.458478

18

TS2-H2 scf done: -646.539110

C	2.038487	-0.297066	0.001094
C	1.785331	-1.685627	0.166893
C	0.861825	0.548554	-0.163633
H	-0.375865	2.879320	0.380019
O	1.144412	1.874409	-0.321114
C	0.496102	-2.183134	0.170290
C	-0.378201	0.014864	-0.141587
C	-0.631832	-1.359315	0.013062
C	-1.949200	-1.946348	-0.010413
O	3.160399	0.279300	-0.018921
H	-1.953101	-3.040584	0.145201
O	-3.001041	-1.353870	-0.187755
O	-1.281493	2.749447	0.705749
O	-1.869719	1.999890	-0.314844
H	2.634285	-2.344794	0.289789
H	0.331780	-3.248682	0.293019
H	2.121333	1.891873	-0.265817
H	-1.384668	0.981272	-0.236526

14

2R(H2) scf done: -494.955325

C	1.609128	0.468624	0.000071
C	0.946751	-0.837332	0.000019
C	0.757080	1.610352	0.000008
O	1.792516	-1.900559	0.000047
C	-0.397050	-0.881752	0.000008
C	-0.617555	1.483845	0.000000
H	-1.241060	2.372364	-0.000033
C	-1.254971	0.227033	0.000017
C	-2.693497	0.154391	0.000012
O	2.870048	0.470885	-0.000078
O	-3.375955	-0.860113	-0.000026
H	-3.187504	1.143861	-0.000016
H	2.668768	-1.471932	0.000134
H	1.224853	2.585798	-0.000044

18

Complejo 2(H3) scf done: -646.598178

C	1.622683	0.198878	0.020662
C	0.509271	-0.648182	-0.206211
C	-0.711569	-0.081276	-0.395860
C	-0.949469	1.344617	-0.386929

C	0.190139	2.158751	-0.159163
C	1.434115	1.586898	0.038984
O	-2.140620	1.731838	-0.582189
O	-1.862002	-0.803457	-0.619093
C	2.945811	-0.337129	0.228163
O	3.254382	-1.520524	0.229847
O	-3.775604	-2.728468	1.084808
O	-2.492542	-2.877199	0.889452
H	0.059353	3.232791	-0.141772
H	0.643482	-1.722442	-0.227221
H	2.294684	2.224062	0.213244
H	3.724723	0.428672	0.397801
H	-2.531733	-0.086842	-0.712893
H	-2.215104	-2.100990	0.328369

18

TS2-H3 scf done: -646.566625

C	1.742602	0.192322	0.054774
C	0.786898	-0.644244	-0.532639
C	-0.507439	-0.204096	-0.736251
C	-0.923079	1.153818	-0.363611
C	0.088142	1.955172	0.285023
C	1.361280	1.493106	0.467087
O	-2.073518	1.556276	-0.603221
O	-1.411553	-0.997821	-1.322047
C	3.106224	-0.245780	0.262680
O	3.566269	-1.335135	-0.044924
O	-2.865896	-1.351514	0.672126
O	-1.875452	-0.888378	1.474082
H	-0.198521	2.952856	0.591537
H	1.059349	-1.646379	-0.839290
H	2.106759	2.127541	0.934853
H	3.757581	0.503210	0.748474
H	-2.227994	-1.025186	-0.719775
H	-1.227858	-1.608007	1.525063

14

2R(H3) scf done: -495.006777

C	-0.817785	-0.001856	-2.466816
C	-1.961019	-0.331733	-1.763303
C	0.381154	0.333819	-1.770638
H	-2.869216	-0.585781	-2.295375
H	1.262189	0.588334	-2.350059
C	-1.997863	-0.352439	-0.333817
C	0.430061	0.337842	-0.409697
O	-3.026826	-0.649243	0.304492
H	1.338869	0.592307	0.121033
C	-0.723737	0.003530	0.398069
O	-0.684992	0.005315	1.633928
C	-0.798535	0.014059	-3.922814
H	0.174611	0.293985	-4.365032
O	-1.739169	-0.248138	-4.651991

18

Complejo 2(H5) scf done: -646.594673

C	-0.633293	1.544046	-0.553515
C	0.554517	1.526435	0.284466
C	-0.985544	0.304290	-1.161408
O	0.842153	2.718865	0.865198
C	1.316177	0.409955	0.459152
C	-0.190144	-0.824068	-0.996340
H	2.194619	0.433707	1.091190

H	-0.468284	-1.752480	-1.483388
C	0.950699	-0.797928	-0.190984
C	1.722999	-2.008598	-0.029476
O	-1.263477	2.633578	-0.658628
O	2.736294	-2.133604	0.641688
H	1.323496	-2.878251	-0.582664
O	-2.623197	-1.790568	1.250421
O	-2.100070	-0.636708	1.559230
H	-1.632632	-0.320766	0.748883
H	0.121495	3.294419	0.547063
H	-1.865808	0.277676	-1.790888

18

TS2-H5 scf done: -646.538265

C	0.512827	1.386025	0.064990
C	-0.937641	1.501390	-0.048988
C	0.936644	0.041317	0.155324
O	-1.376238	2.783826	-0.142888
C	-1.779438	0.427732	-0.060304
C	0.128975	-1.063185	0.153988
H	-2.848185	0.574579	-0.146667
H	0.546543	-2.061371	0.232967
C	-1.259326	-0.885868	0.042850
C	-2.110906	-2.052085	0.035393
O	1.199469	2.440725	0.067787
O	-3.329288	-2.054357	-0.061273
H	-1.568221	-3.010532	0.126684
O	3.376982	-0.543636	0.180744
O	3.281965	-1.880854	-0.220780
H	3.365832	-1.828850	-1.181433
H	-0.553302	3.304442	-0.098865
H	2.298072	-0.190056	0.213654

14

2R(H5) scf done: -494.955494

C	1.659450	0.551811	0.000424
C	0.971404	-0.735082	0.000032
C	0.755147	1.630102	0.000050
O	1.814980	-1.801517	-0.000047
C	-0.388625	-0.864103	-0.000024
C	-0.606102	1.560397	0.000112
H	-0.843749	-1.845831	-0.000122
H	-1.227555	2.450389	0.000050
C	-1.211736	0.287877	0.000121
C	-2.651531	0.202556	0.000157
O	2.922151	0.551767	-0.000652
O	-3.317580	-0.823616	0.000116
H	-3.162805	1.182890	0.000297
H	2.695265	-1.380675	0.000428

18

Complejo 2(H6) scf done: -646.594623

C	1.399518	-1.048321	-0.063074
C	0.226684	-1.270547	-0.841234
C	1.548623	0.285935	0.494794
H	-1.550845	-0.428207	-1.696170
O	2.665142	0.450929	1.248291
C	-0.673388	-0.239701	-1.086976
C	0.649973	1.284714	0.267460
C	-0.489389	1.032678	-0.541123
C	-1.472280	2.058166	-0.806380
O	2.295555	-1.899105	0.198406

H	-2.312905	1.725917	-1.442617
H	3.083284	-0.429719	1.211889
O	-1.442084	3.209554	-0.398210
O	-2.529132	-1.979293	1.288843
O	-1.419803	-1.481614	1.760768
H	-0.853208	-1.284615	0.976658
H	0.078829	-2.252955	-1.271134
H	0.795427	2.266181	0.699806

18

TS2-H6 scf done: -646.538780

C	2.316005	-6.582903	2.961535
C	1.555759	-5.599270	3.672094
C	2.026882	-6.709329	1.542176
H	-0.047081	-3.923639	3.692412
O	2.779391	-7.646685	0.905980
C	0.628599	-4.877142	2.973775
C	1.088507	-5.958049	0.902459
C	0.328152	-4.992991	1.624258
C	-0.695183	-4.190909	0.996705
O	3.203519	-7.327092	3.456032
H	-1.210054	-3.488835	1.671946
H	3.341901	-7.998182	1.619788
O	-1.011155	-4.242503	-0.183320
O	-0.517062	-3.089406	4.321944
O	-0.083065	-1.904179	3.724571
H	0.740538	-1.707320	4.189157
H	1.746217	-5.453681	4.727139
H	0.901800	-6.086825	-0.156429

14

2R(H6) scf done: -494.959190

C	1.626668	0.482519	0.000049
C	0.899619	-0.779998	0.000046
C	0.825094	1.672358	-0.000065
O	1.704840	-1.878216	0.000086
C	-0.458769	-0.860434	0.000034
C	-0.526209	1.513931	-0.000070
H	-0.958105	-1.821714	0.000062
C	-1.247169	0.332057	-0.000009
C	-2.686463	0.312547	-0.000010
O	2.885568	0.440278	-0.000087
O	-3.390317	-0.689434	0.000090
H	-3.155126	1.311873	-0.000009
H	2.599681	-1.492265	0.000151
H	1.320860	2.634425	-0.000141

18

Complejo 2(C) scf done: -646.594495

C	1.878441	-0.592412	0.011815
C	0.932871	-1.377914	-0.704172
C	1.450919	0.747922	0.381558
H	1.217295	-2.383063	-0.987286
O	2.382896	1.457008	1.065918
C	-0.310376	-0.869966	-1.030788
C	0.223262	1.244997	0.059824
H	-1.020085	-1.485652	-1.572846
H	-0.065221	2.247645	0.349000
C	-0.695267	0.428096	-0.657966
C	-2.010432	0.908202	-1.016152
O	3.039506	-0.949219	0.356423
H	-2.625094	0.177021	-1.571491

O	-2.467024	2.011593	-0.756246
O	-2.604202	-1.217847	1.669596
O	-1.432246	-0.781734	2.039994
H	-1.022028	-0.392592	1.233778
H	3.126783	0.827913	1.129041

18

TS2-C	scf done:	-646.565905	
C	2.062038	-0.673525	-0.082367
C	1.085825	-1.596108	-0.587645
C	1.610783	0.693400	0.167679
H	1.409741	-2.607344	-0.794881
O	2.559041	1.528999	0.626104
C	-0.200980	-1.191520	-0.801958
C	0.323309	1.086029	-0.061944
H	-0.938329	-1.887489	-1.180889
H	0.002633	2.102331	0.120648
C	-0.607307	0.142181	-0.535851
C	-2.009255	0.545261	-0.784058
O	3.260971	-0.949945	0.153671
H	-2.628202	-0.254653	-1.217186
O	-2.364605	1.725100	-0.832910
O	-2.308299	-0.176514	1.025243
O	-2.677190	-1.537415	0.957673
H	-1.915715	-1.985345	1.341691
H	3.361472	0.981466	0.687192

18

2A(C)	scf done:	-646.575371	
C	2.207967	-0.403994	0.162009
C	1.460441	-1.600748	0.426663
C	1.448283	0.773593	-0.248971
H	2.011693	-2.479985	0.732517
O	2.175189	1.873476	-0.481936
C	0.101671	-1.603809	0.296247
C	0.081826	0.747302	-0.375921
H	-0.465408	-2.505294	0.494514
H	-0.462018	1.626296	-0.696305
C	-0.607911	-0.436512	-0.088457
C	-2.106569	-0.528239	-0.343058
O	3.451448	-0.295319	0.261243
H	-2.542390	-1.295249	0.328583
O	-2.324844	-0.656741	-1.617887
O	-2.724981	0.752192	0.143696
O	-2.516025	0.841088	1.553870
H	-1.639309	1.242224	1.611720
H	3.096880	1.608883	-0.313993

18

Complejo 2(C1)	scf done:	-646.594496	
C	1.930074	-0.127969	-0.373736
C	1.313550	0.989703	0.323848
C	1.049712	-0.977749	-1.099442
O	2.190535	1.768665	1.004965
C	-0.027139	1.232534	0.286862
C	-0.309061	-0.727469	-1.136502
H	-0.455730	2.074014	0.816366
H	-0.965414	-1.389492	-1.691038
C	-0.875447	0.359391	-0.450849
C	-2.303385	0.572133	-0.515243
O	3.182365	-0.256042	-0.276372
O	-2.919627	1.476024	0.029500

H	-2.847102	-0.175806	-1.120057
O	-1.956344	-2.062328	1.725334
O	-0.849392	-1.435320	2.012377
H	-0.679420	-0.827834	1.256257
H	3.045641	1.330947	0.830973
H	1.476183	-1.823402	-1.623244

18

scf done: -646.562413

C	1.080594	0.806494	0.318895
C	0.876252	2.250991	0.400644
C	0.092824	0.069520	-0.397798
O	1.880361	2.913761	1.020984
C	-0.199242	2.876321	-0.131956
C	-1.006128	0.691704	-0.934248
H	-0.304467	3.951060	-0.079089
H	-1.740016	0.126756	-1.497480
C	-1.269169	2.092937	-0.701613
C	-2.108951	2.727672	-1.758866
O	2.125488	0.326626	0.846380
O	-2.021941	3.877375	-2.119592
H	-2.851845	2.049790	-2.212170
O	-2.607764	2.096047	0.469065
O	-2.136184	1.455306	1.633028
H	-1.939851	0.558953	1.326091
H	2.494760	2.201986	1.277066
H	0.259547	-0.990911	-0.541053

18

TS2-C1 scf done: -646.562413

C	1.080594	0.806494	0.318895
C	0.876252	2.250991	0.400644
C	0.092824	0.069520	-0.397798
O	1.880361	2.913761	1.020984
C	-0.199242	2.876321	-0.131956
C	-1.006128	0.691704	-0.934248
H	-0.304467	3.951060	-0.079089
H	-1.740016	0.126756	-1.497480
C	-1.269169	2.092937	-0.701613
C	-2.108951	2.727672	-1.758866
O	2.125488	0.326626	0.846380
O	-2.021941	3.877375	-2.119592
H	-2.851845	2.049790	-2.212170
O	-2.607764	2.096047	0.469065
O	-2.136184	1.455306	1.633028
H	-1.939851	0.558953	1.326091
H	2.494760	2.201986	1.277066
H	0.259547	-0.990911	-0.541053

18

2A(C1) scf done: -646.565653

C	1.799848	-0.235957	-0.534746
C	1.226519	0.663562	0.474954
C	0.871765	-0.938148	-1.343538
O	2.161055	1.357441	1.167201
C	-0.095864	0.818553	0.672461
C	-0.486522	-0.828678	-1.157040
H	-0.470703	1.523968	1.401917
H	-1.180512	-1.362533	-1.795749
C	-1.069703	-0.024480	-0.051702
C	-2.245725	0.737271	-0.639530
O	3.068152	-0.280651	-0.627773

O	-2.375987	1.935798	-0.619774
H	-2.981747	0.092611	-1.149995
O	-1.818449	-0.934428	0.889112
O	-0.921969	-1.904462	1.412582
H	-0.532491	-2.282947	0.607467
H	2.999016	1.038341	0.780977
H	1.266376	-1.557213	-2.140674

18

Complejo 2(C2) scf done: -646.602085

C	-2.272910	0.590794	-0.273205
C	-1.468374	-0.616900	-0.144979
C	-1.567788	1.828718	-0.222854
O	-2.183476	-1.768706	-0.205890
C	-0.120295	-0.586831	0.020712
C	-0.202447	1.853456	-0.056605
H	0.434012	-1.511752	0.104497
H	0.317951	2.804338	-0.018896
C	0.550562	0.669314	0.070229
C	1.951316	0.785863	0.256422
O	-3.515052	0.452020	-0.420329
O	2.775404	-0.132751	0.416756
H	2.337597	1.814839	0.258848
O	2.690735	-3.169839	-0.468695
O	2.793537	-2.655036	0.727174
H	2.716601	-1.645875	0.606477
H	-3.097703	-1.453840	-0.329970
H	-2.139671	2.742188	-0.319693

18

TS2-C2 scf done: -646.564107

C	0.672575	0.796508	0.581494
C	0.738233	2.240501	0.406754
C	-0.366703	0.122977	-0.117889
O	1.760911	2.835895	1.021782
C	-0.233835	2.989253	-0.284507
C	-1.239385	0.839535	-0.910394
H	0.022131	3.985529	-0.615126
H	-2.009418	0.307768	-1.460151
C	-1.186592	2.236227	-1.049505
C	-2.181894	2.906585	-1.814683
O	1.565044	0.273730	1.298764
O	-2.363050	4.128535	-1.854117
H	-2.844611	2.245419	-2.400339
O	-1.130077	3.721300	1.237309
O	-2.501883	3.589136	1.061125
H	-2.678984	4.143639	0.286858
H	2.209950	2.095075	1.478797
H	-0.437608	-0.952164	-0.027378

18

2A(C2) scf done: -646.585191

C	-2.091588	0.344258	0.063375
C	-1.103310	-0.666877	-0.222354
C	-1.615294	1.677430	0.251218
O	-1.582202	-1.888837	-0.452147
C	0.364200	-0.468764	-0.287615
C	-0.268232	1.942507	0.130166
H	0.748332	-0.896659	-1.219848
H	0.069348	2.967159	0.256232
C	0.719695	0.983742	-0.144587
C	2.066476	1.372478	-0.183738

O	-3.292696	-0.032758	0.100610
O	3.054957	0.612815	-0.306451
H	2.252360	2.453733	-0.087908
O	0.962644	-1.282863	0.767216
O	2.192267	-1.823401	0.290505
H	2.696368	-0.996602	0.085815
H	-2.549137	-1.774567	-0.340492
H	-2.329759	2.458173	0.469160

18

Complejo 2(C3) scf done: -646.593365

C	-1.587962	0.691499	-0.399144
C	-0.949196	-0.497554	-0.946934
C	-0.725160	1.628229	0.232465
O	-1.803423	-1.360524	-1.547221
C	0.398271	-0.711804	-0.871738
C	0.639687	1.409760	0.296701
H	0.840746	-1.607820	-1.288432
H	1.278729	2.139663	0.782015
C	1.226505	0.256947	-0.241315
C	2.654013	0.074031	-0.136443
O	-2.840755	0.787236	-0.522310
O	3.293053	-0.878765	-0.559075
H	3.179732	0.897820	0.379906
O	-1.341147	-2.071251	2.173173
H	-0.166747	-0.998382	1.243066
O	-0.257574	-1.344389	2.157977
H	-2.671106	-0.934925	-1.408931
H	-1.167664	2.520226	0.656245

18

TS2-C3 scf done: -646.569419

C	0.548054	0.701123	0.514100
C	0.256614	2.151242	0.598774
C	-0.250221	-0.055310	-0.393965
O	1.180215	2.851086	1.289111
C	-0.518142	2.776929	-0.390298
C	-1.140355	0.574709	-1.225621
H	-0.583396	3.856070	-0.422820
H	-1.739834	-0.010112	-1.915030
C	-1.287023	1.986327	-1.243151
C	-2.207391	2.572682	-2.197257
O	1.461880	0.256099	1.239245
O	-2.434890	3.764606	-2.338012
H	-2.731673	1.838984	-2.835898
O	-1.010823	2.038593	2.058019
H	-2.669879	2.193176	1.208224
O	-2.235046	1.481964	1.694460
H	1.692826	2.161702	1.748588
H	-0.107208	-1.127229	-0.425966

18

2A(C3) scf done: -646.582250

C	-1.369337	0.865535	-0.213799
C	-0.852461	-0.571333	-0.378082
C	-0.455531	1.876833	0.181180
O	-1.513894	-1.183851	-1.432514
C	0.615638	-0.693773	-0.476132
C	0.897192	1.619950	0.253237
H	1.027301	-1.641161	-0.796535
H	1.581596	2.408839	0.544187
C	1.438370	0.352913	-0.088071

C	2.886209	0.220692	-0.078262
O	-2.578066	1.035408	-0.456939
O	3.516709	-0.783923	-0.368378
H	3.426247	1.135719	0.224972
O	-1.346813	-1.366550	0.779253
H	0.130618	-1.028534	1.896250
O	-0.813199	-0.825589	1.976765
H	-2.390314	-0.767599	-1.432203
H	-0.853822	2.863870	0.377405

18

Complejo 2(C4) scf done: -646.593399

C	1.500043	0.235504	-0.743817
C	0.771482	1.305697	-0.080678
C	0.735970	-0.917801	-1.084585
O	1.538628	2.371612	0.257897
C	-0.569112	1.247900	0.157144
C	-0.635359	-0.959625	-0.858470
H	-1.078448	2.067898	0.646622
H	-1.201521	-1.837132	-1.151697
C	-1.303149	0.099625	-0.239252
C	-2.727097	-0.001551	-0.016500
O	2.734595	0.402394	-0.948355
O	-3.437527	0.847362	0.500613
H	-3.175254	-0.950635	-0.363559
O	1.754749	-1.223833	2.558094
O	0.717260	-1.721074	1.942424
H	0.702030	-1.330199	1.038325
H	2.427254	2.102752	-0.041984
H	1.245455	-1.738896	-1.572223

18

TS2-C4 scf done: -646.562853

C	1.226551	-0.100972	-0.532263
C	0.516170	1.067610	0.052611
C	0.355683	-1.117299	-1.130616
O	1.342294	2.051439	0.401918
C	-0.839599	1.114986	0.203424
C	-0.989098	-1.063191	-0.954673
H	-1.326164	1.965382	0.661000
H	-1.629123	-1.840491	-1.357524
C	-1.606811	0.034140	-0.275354
C	-3.047052	0.026962	-0.137385
O	2.420679	0.105403	-0.890638
O	-3.714276	0.901768	0.398045
H	-3.548216	-0.857713	-0.566382
O	1.461072	-0.965923	1.115670
O	0.308338	-1.325866	1.836615
H	-0.054369	-2.057360	1.321919
H	2.210895	1.717390	0.082379
H	0.837534	-1.928930	-1.659940

18

2A(C4) scf done: -646.591271

C	1.342684	-0.169836	-0.360526
C	0.533148	1.099604	-0.053238
C	0.538368	-1.328708	-0.835815
O	1.205047	2.150902	0.039656
C	-0.864027	0.995963	0.076254
C	-0.801859	-1.338094	-0.699464
H	-1.424242	1.877202	0.359851
H	-1.368904	-2.215179	-0.994036

C	-1.535750	-0.194907	-0.210384
C	-2.964254	-0.307550	-0.099347
O	2.375066	0.140332	-1.229541
O	-3.735368	0.570149	0.285259
H	-3.371247	-1.291089	-0.397519
O	2.067231	-0.571655	0.859189
O	1.130811	-0.815357	1.895058
H	0.648203	-1.590372	1.569635
H	2.596800	1.059443	-1.007073
H	1.087242	-2.173804	-1.232701

18

Complejo 2(C5) scf done: -646.594673

C	1.633667	-0.244009	0.560852
C	0.988269	-1.173318	-0.352016
C	0.762088	0.558826	1.352282
O	1.851137	-1.901282	-1.105273
C	-0.365631	-1.306312	-0.432409
C	-0.617349	0.400505	1.280409
H	-0.811716	-2.008809	-1.124654
H	-1.260649	1.010351	1.905522
C	-1.199499	-0.511671	0.397297
C	-2.640000	-0.612177	0.341512
O	2.896105	-0.205069	0.566066
O	-3.283483	-1.359624	-0.379671
H	-3.169003	0.068943	1.032990
O	-0.502689	3.266082	-0.637073
O	0.236778	2.313912	-1.134036
H	0.360348	1.654753	-0.409408
H	2.722740	-1.573230	-0.814509
H	1.206231	1.264759	2.042383

18

TS2-C5 scf done: -646.564679

C	1.209268	0.923912	0.428864
C	0.866526	2.334156	0.439278
C	0.204223	0.002175	-0.076968
O	1.788166	3.137107	1.029730
C	-0.267092	2.812865	-0.139838
C	-0.870704	0.545334	-0.828826
H	-0.495176	3.870136	-0.132817
H	-1.528840	-0.119761	-1.374144
C	-1.141512	1.902794	-0.803728
C	-2.311670	2.389228	-1.515293
O	2.310786	0.571606	0.909922
O	-2.673900	3.551541	-1.583092
H	-2.895687	1.601994	-2.024861
O	-0.514970	-0.478218	1.590234
O	-1.703723	-1.190409	1.348357
H	-2.365036	-0.492109	1.281742
H	2.477582	2.519343	1.327587
H	0.548773	-0.997953	-0.298874

18

2A(C5) scf done: -646.573163

C	1.318592	-0.690392	0.354709
C	0.286190	-1.527610	-0.169011
C	1.014965	0.770490	0.553568
O	0.671993	-2.800582	-0.475717
C	-1.016441	-1.115245	-0.303303
C	-0.434215	1.050938	0.685647
H	-1.777221	-1.775843	-0.693824

H	-0.753441	1.982234	1.137284
C	-1.371268	0.173301	0.181180
C	-2.773378	0.577539	0.224260
O	2.466054	-1.161844	0.568207
O	-3.716204	-0.069959	-0.192488
H	-2.947585	1.567491	0.682502
O	1.573894	1.401488	-0.676262
O	1.448355	2.814328	-0.541758
H	0.549375	2.967824	-0.859893
H	1.617649	-2.816708	-0.256653
H	1.611818	1.173415	1.372427

18

Complejo 2(C6) scf done: -646.594673

C	-1.724874	0.045579	-0.337900
C	-1.157147	-1.138381	0.286124
C	-0.795261	0.929677	-0.958179
O	-2.071135	-1.941728	0.887062
C	0.176233	-1.418509	0.257483
C	0.560509	0.624735	-1.002604
H	0.563931	-2.309964	0.733607
H	1.247309	1.304035	-1.495930
C	1.066365	-0.529203	-0.399788
C	2.488589	-0.780390	-0.449161
O	-2.975324	0.207571	-0.264211
O	3.068438	-1.741577	0.033281
H	3.067564	-0.004863	-0.983255
O	0.812408	2.926634	1.554587
O	-0.010697	1.958202	1.846220
H	-0.225962	1.513193	0.991542
H	-2.910350	-1.468736	0.732625
H	-1.180596	1.823728	-1.431501

18

TS2-C6 scf done: -646.563955

C	1.004280	0.776551	0.347031
C	0.721458	2.220726	0.482476
C	0.156252	0.053546	-0.495868
O	1.569554	2.849048	1.301626
C	-0.292709	2.857818	-0.189910
C	-0.974149	0.671744	-1.082074
H	-0.449542	3.922997	-0.084238
H	-1.467367	0.165171	-1.902616
C	-1.116522	2.101801	-1.025378
C	-2.204814	2.711868	-1.762917
O	2.009877	0.363411	0.999052
O	-2.462156	3.905040	-1.783395
H	-2.821815	2.004883	-2.342306
O	-2.477466	0.269946	0.028993
O	-2.086576	0.539534	1.331444
H	-1.290682	-0.004755	1.440497
H	2.163474	2.114593	1.581043
H	0.335997	-1.003434	-0.641317

18

2A(C6) scf done: -646.577694

C	-1.754758	0.280549	-0.364959
C	-1.213381	-1.005624	0.163509
C	-0.846132	1.195611	-0.828541
O	-2.180506	-1.805562	0.586232
C	0.124724	-1.329756	0.165658
C	0.622406	0.977302	-0.730660

H	0.463094	-2.297232	0.513152
H	1.134466	1.257467	-1.656451
C	1.043380	-0.403262	-0.312879
C	2.445747	-0.715737	-0.372286
O	-3.033441	0.327166	-0.326667
O	2.954869	-1.773163	-0.007997
H	3.084509	0.079863	-0.790246
O	1.235718	1.968821	0.177009
O	0.676782	1.804759	1.471953
H	-0.274722	1.886360	1.288200
H	-2.974936	-1.225191	0.379520
H	-1.191704	2.128067	-1.257468

14

3	scf done:	-495.089471	
C	-0.804856	0.029505	-2.472971
C	-1.970137	-0.210590	-1.683265
C	0.410991	0.294390	-1.825524
H	-2.904230	-0.414257	-2.196155
H	1.302123	0.478077	-2.418925
C	-1.986296	-0.200333	-0.281316
C	0.469886	0.320449	-0.443129
O	-3.025137	-0.414374	0.427211
H	1.406258	0.524562	0.066670
C	-0.670711	0.086132	0.396308
O	-0.582916	0.117122	1.650094
C	-0.803197	0.015921	-3.898825
H	0.191201	0.222880	-4.344702
O	-1.757248	-0.194565	-4.658804

14

TS3-Ha	scf done:	-495.058476	
C	-1.513555	-0.318611	-0.018212
C	-0.777094	0.871447	-0.235032
C	-0.847248	-1.520073	0.124280
H	-1.304335	1.815263	-0.348465
H	-1.395252	-2.446361	0.264012
C	0.637068	0.923681	-0.297605
C	0.565476	-1.523159	0.082233
O	1.272111	2.014371	-0.489952
H	1.100303	-2.460818	0.212079
C	1.364376	-0.371409	-0.117549
O	2.641951	-0.414577	-0.148678
C	-2.991145	-0.266969	-0.095900
O	-3.747028	-0.028394	0.822835
H	-3.433979	-0.451957	-1.094464

14

3a	scf done:	-495.087059	
C	-0.742684	0.042647	-2.476476
C	-1.925480	-0.201347	-1.707339
C	0.454826	0.303980	-1.797616
H	-2.852434	-0.403703	-2.240056
H	1.358251	0.490524	-2.366948
C	-1.988428	-0.201011	-0.307964
C	0.463819	0.319443	-0.414357
O	-3.057660	-0.421835	0.362761
H	1.384285	0.520487	0.126321
C	-0.697078	0.080536	0.399033
O	-0.630184	0.107078	1.657038
C	-0.801148	0.016234	-3.902884
O	0.120106	0.204275	-4.708457

H	-1.810462	-0.202388	-4.306392
17			
Complejo 3(H)b	scf done:	-646.045126	
C	0.585460	0.684863	-0.498252
C	0.083610	-0.612969	-0.866300
C	-1.214452	-1.078467	-0.579222
C	-2.065149	-0.163199	0.265426
C	-1.494555	1.097532	0.647366
C	-0.226644	1.515013	0.278713
O	-3.227243	-0.492300	0.605188
H	-2.125246	1.735993	1.258073
C	1.906999	1.075703	-0.877646
O	2.475049	2.149093	-0.645886
O	2.150112	-2.150376	1.273887
O	0.965956	-1.746149	1.634971
O	-1.666019	-2.206095	-0.955058
H	0.705515	-1.250788	-1.490841
H	0.153666	2.481512	0.588509
H	2.457499	0.302262	-1.448936
H	0.535443	-1.341626	0.810007
17			
TS3-Hb	scf done:	-646.011933	
C	0.507549	0.718381	-0.281865
C	-0.066481	-0.577824	-0.529964
C	-1.424183	-0.883440	-0.366797
C	-2.287080	0.226248	0.176687
C	-1.663569	1.505360	0.404001
C	-0.324980	1.749152	0.191026
O	-3.503997	0.046798	0.407261
H	-2.311805	2.290885	0.778833
C	1.905100	0.948592	-0.377440
O	2.567868	1.971849	-0.342733
O	2.888812	-1.428275	-0.055898
O	2.242930	-1.598230	1.152572
O	-1.945210	-2.011702	-0.643406
H	0.556937	-1.344920	-0.981875
H	0.106300	2.720824	0.400458
H	2.513000	-0.108852	-0.419988
H	1.299443	-1.616848	0.903418
13			
3R(H)b	scf done:	-494.436857	
C	-0.748692	0.041593	-2.449222
C	-1.931479	-0.202393	-1.679306
C	0.457608	0.304757	-1.775486
H	-2.855227	-0.404102	-2.213924
H	1.359736	0.491003	-2.347137
C	-1.985135	-0.200059	-0.280020
C	0.470458	0.321055	-0.394461
O	-3.048615	-0.419572	0.397859
H	1.392542	0.522434	0.142851
C	-0.689624	0.082358	0.421745
O	-0.617697	0.109986	1.677589
C	-0.781422	0.020713	-3.868785
O	0.055106	0.190234	-4.723767
17			
Complejo 3(H2)	scf done:	-646.041224	
C	1.493786	-1.618834	-0.034750
C	2.557673	-0.645464	0.039487
C	0.086821	-1.085802	-0.147982

H	-2.674388	-1.022602	0.154068
O	-0.868745	-1.886910	-0.236053
C	2.301562	0.692540	0.026539
C	-0.107555	0.335957	-0.144515
C	0.971105	1.201527	-0.062439
C	0.828160	2.653207	-0.060912
O	1.712673	-2.838778	-0.008496
O	-0.206704	3.288762	-0.120482
H	1.791739	3.195069	0.001475
O	-3.491796	-0.593672	0.432147
O	-3.529477	0.589021	-0.443352
H	3.568742	-1.027272	0.110723
H	-1.134167	0.698020	-0.221563
H	3.120635	1.401545	0.085688

17

TS3-H2 scf done: -645.995567

C	-0.790746	-1.904405	-0.130875
C	-2.119864	-1.345459	0.020759
C	0.348238	-0.937511	0.188513
H	2.688691	-0.559402	0.069701
O	1.495157	-1.419684	0.509161
C	-2.347038	0.007684	0.154109
C	0.029689	0.408469	0.070097
C	-1.274867	0.941309	0.156614
C	-1.635975	2.320370	-0.013222
O	-0.593607	-3.120622	-0.393150
O	-0.936890	3.325513	-0.236083
H	-2.740050	2.469854	0.076850
O	3.416844	0.042521	-0.325706
O	3.001944	1.357469	0.090131
H	-2.940976	-2.048607	-0.058173
H	2.034899	1.326156	-0.071977
H	-3.366766	0.387683	0.152815

13

3R(H2) scf done: -494.404004

C	2.354916	-0.609330	0.060875
C	1.892548	0.829120	0.155046
C	1.362452	-1.576810	-0.325220
O	2.791429	1.700991	0.318999
H	1.687418	-2.604461	-0.447557
C	0.491599	1.185918	0.057537
C	0.057581	-1.211057	-0.504939
H	-0.673825	-1.967429	-0.783284
C	-0.376442	0.138862	-0.308919
C	-1.808268	0.324744	-0.482016
O	3.540957	-0.940921	0.279706
O	-2.484294	1.337513	-0.356520
H	-2.336567	-0.609785	-0.773596

17

Complejo 3(H5) scf done: -646.051949

C	2.162365	-0.818067	-0.176405
C	0.909472	-1.452865	-0.516844
C	2.125354	0.657947	0.131718
H	-1.214221	-1.243736	-0.821478
O	3.176728	1.270387	0.422867
C	-0.269069	-0.765291	-0.559899
C	0.850735	1.306266	0.072180
C	-0.304667	0.631488	-0.263880
C	-1.606856	1.306635	-0.336198

O	3.233322	-1.446167	-0.136598
O	-1.772410	2.499220	-0.121688
H	-2.447172	0.647346	-0.604877
O	-3.375450	-1.407112	-0.662934
O	-3.269101	-1.125584	0.772088
H	-2.376279	-1.416889	0.977750
H	0.949803	-2.512986	-0.739288
H	0.812697	2.365588	0.296698

17

TS3-H5 scf done: -645.992758

C	-0.769234	0.757794	-0.001793
C	0.511263	1.561030	-0.040724
C	-0.768511	-0.695759	-0.148524
O	0.486424	2.813797	-0.056292
C	1.729423	0.820913	-0.019738
C	0.468725	-1.278188	-0.123526
H	2.663358	1.363835	0.023683
H	0.555981	-2.365458	-0.174162
C	1.722408	-0.562546	-0.062097
C	2.950054	-1.325630	0.053449
O	-1.835512	1.388709	0.158194
O	4.087050	-0.874776	0.103145
H	2.800785	-2.419429	0.109786
O	-3.265319	-1.766132	0.074578
O	-3.965339	-0.454857	-0.030569
H	-3.260920	0.199314	0.178902
H	-1.882412	-1.297867	-0.072929

13

3R(H5) scf done: -494.404811

C	1.303855	1.341852	0.754408
C	1.199382	2.829087	0.421942
C	0.197929	0.588092	0.291577
O	2.144381	3.591456	0.793359
C	0.055580	3.249720	-0.275836
C	-0.909688	1.008706	-0.387062
H	-0.023343	4.304895	-0.513190
H	-1.701896	0.331574	-0.692913
C	-0.998934	2.385321	-0.688859
C	-2.157224	2.822596	-1.397921
O	2.293829	0.891932	1.375754
O	-2.435815	3.971642	-1.761015
H	-2.868626	2.005536	-1.634047

17

Complejo 3(H6) scf done: -646.051949

C	1.661029	-1.671540	0.539674
C	0.851770	-0.777242	1.335863
C	1.354183	-1.749470	-0.934954
H	-0.763702	0.648464	1.397748
O	2.010264	-2.512241	-1.678568
C	-0.150005	-0.023485	0.795674
C	0.293834	-0.923244	-1.426433
C	-0.437603	-0.093988	-0.601489
C	-1.532927	0.741130	-1.111003
O	2.572947	-2.355542	1.033272
O	-1.889976	0.762946	-2.280501
H	-2.024432	1.363389	-0.346649
O	-1.951632	2.454158	1.625009
O	-0.972662	3.174744	0.805085
H	-0.169781	2.662899	0.938063

H	1.079911	-0.732703	2.394590
H	0.068782	-0.968277	-2.485379
17			
TS3-H6	scf done:	-645.991409	
C	1.875319	-1.065113	-0.037925
C	0.494587	-1.468320	-0.208663
C	2.143566	0.418071	0.104466
H	-1.884285	-1.050155	-0.455683
O	3.319878	0.844834	0.254063
C	-0.573754	-0.608043	-0.241578
C	1.009496	1.277101	0.060408
C	-0.284298	0.798549	-0.111595
C	-1.414065	1.706212	-0.171203
O	2.816029	-1.882501	-0.002678
O	-1.382359	2.937123	-0.095388
H	-2.379411	1.187448	-0.289644
O	-3.010058	-1.458496	-0.528510
O	-3.488577	-1.047058	0.767834
H	-2.814138	-1.437771	1.356442
H	0.349367	-2.543742	-0.304183
H	1.184058	2.342260	0.167043
13			
3R(H6)	scf done:	-494.405714	
C	1.271918	1.341243	0.733311
C	1.188458	2.818959	0.418416
C	0.174043	0.498002	0.288127
O	2.139644	3.582379	0.796184
C	0.054751	3.250252	-0.276554
C	-0.870226	1.055467	-0.381190
H	-0.021727	4.306789	-0.510712
C	-1.023157	2.396344	-0.706978
C	-2.175660	2.843539	-1.412026
O	2.244497	0.860520	1.350537
O	-2.437802	4.001496	-1.763490
H	-2.892412	2.035791	-1.654729
H	0.244456	-0.559514	0.516896
17			
Complejo 3(C)	scf done:	-646.053958	
C	-2.622283	-0.196183	0.070314
C	-1.406178	-1.086931	-0.065085
C	-2.411818	1.231561	0.128565
O	-1.568572	-2.345779	-0.130644
C	-0.168399	-0.436145	-0.104097
C	-1.166341	1.799916	0.071930
H	0.711869	-1.061927	-0.199814
H	-1.049862	2.878219	0.115784
C	-0.011220	0.988530	-0.047609
C	1.210589	1.667384	-0.104688
O	-3.770269	-0.677910	0.126685
O	2.382615	1.193276	-0.210594
H	1.141074	2.762528	-0.055179
O	4.471008	-0.877932	0.474177
O	3.371899	-1.055536	-0.206366
H	2.858982	-0.120773	-0.203849
H	-3.303019	1.843096	0.223793
17			
TS3-C	scf done:	-646.035973	
C	-2.170854	-0.471066	0.139446
C	-1.597904	0.844423	0.155899

C	-1.446994	-1.526358	-0.459798
O	-2.387032	1.827795	0.533372
H	-1.937883	-2.495774	-0.561298
C	-0.273627	1.023116	-0.272753
C	-0.145108	-1.328103	-0.871317
H	0.189919	2.002864	-0.216765
H	0.422473	-2.149923	-1.292535
C	0.458074	-0.064529	-0.735530
C	1.918507	0.062201	-0.985037
O	-3.413932	-0.650158	0.521119
O	2.488639	1.172878	-1.132614
H	2.374551	-0.835413	-1.427766
O	1.944400	-0.121347	1.108712
O	3.213841	-0.705872	1.454312
H	3.731056	0.053779	1.793701

17

3A(C) scf done: -646.073245

C	2.428562	-0.484172	0.058276
C	1.830893	0.886841	0.109208
C	1.522837	-1.579113	-0.171566
O	2.549845	1.892833	0.317947
H	1.961975	-2.570263	-0.201908
C	0.408592	0.992217	-0.094907
C	0.177579	-1.396382	-0.354869
H	-0.038876	1.978096	-0.074524
H	-0.472917	-2.245431	-0.532860
C	-0.394782	-0.093181	-0.313143
C	-1.887479	0.067236	-0.539713
O	3.661980	-0.664447	0.205321
O	-2.389530	1.283802	-0.569586
H	-2.176369	-0.557267	-1.414143
O	-2.486076	-0.699111	0.629473
O	-3.849839	-0.266687	0.641626
H	-3.663581	0.632929	0.226038

17

Complejo 3(C1) scf done: -646.053958

C	-2.622439	-0.196204	0.069837
C	-1.406285	-1.086926	-0.064786
C	-2.412022	1.231555	0.128056
O	-1.568580	-2.345795	-0.129965
C	-0.168528	-0.436153	-0.103833
C	-1.166500	1.799892	0.071744
H	0.711700	-1.061950	-0.199848
H	-1.049986	2.878180	0.115957
C	-0.011363	0.988501	-0.047500
C	1.210448	1.667428	-0.104708
O	-3.770412	-0.678072	0.125999
O	2.382405	1.193263	-0.210744
H	1.140944	2.762549	-0.054850
O	4.471523	-0.877944	0.474100
O	3.372656	-1.055474	-0.206840
H	2.859460	-0.121099	-0.204303
H	-3.303189	1.843046	0.223849

17

TS3-C1 scf done: -646.014263

C	1.978756	-0.403671	-0.139651
C	1.168448	-1.573235	-0.296838
C	1.314031	0.921975	-0.196447
H	-0.747061	-2.393059	-0.599918

O	2.026365	1.997980	-0.092122
C	-0.190456	-1.487896	-0.470155
C	-0.068091	0.933906	-0.344127
C	-0.860351	-0.264705	-0.480091
C	-2.271746	-0.252966	-0.725842
O	3.234147	-0.493233	0.040991
O	-2.973427	0.760371	-0.826799
H	-2.734917	-1.245384	-0.836006
O	-0.560767	-0.012648	1.368221
O	-1.939400	-0.183067	1.607281
H	-2.312924	0.696999	1.452637
H	1.674104	-2.531783	-0.251877
H	-0.578735	1.890150	-0.349753

17

3A(C1) scf done: -646.014256

C	2.071396	-0.494434	-0.144089
C	1.558410	0.879790	0.223873
C	1.111565	-1.423552	-0.637457
O	2.378854	1.775905	0.571554
H	1.514661	-2.362905	-1.008594
C	0.168582	1.097840	0.134464
C	-0.244826	-1.185660	-0.721317
H	-0.209539	2.069930	0.432668
H	-0.903524	-1.900276	-1.202089
C	-0.830194	0.041099	-0.112996
C	-1.866428	0.679278	-1.009477
O	3.307660	-0.782697	-0.065323
O	-2.832155	1.319123	-0.658550
H	-1.615310	0.587487	-2.083248
O	-1.475531	-0.261483	1.205494
O	-2.465631	-1.288101	1.019260
H	-1.902892	-2.062388	0.883777

17

Complejo 3(C2) scf done: -646.053957

C	-2.592585	0.283177	-0.111996
C	-1.722416	-0.947468	-0.249541
C	-1.937788	1.557452	0.070999
O	-2.276685	-2.077865	-0.423900
C	-0.341812	-0.736845	-0.167427
C	-0.575089	1.688827	0.129401
H	0.293989	-1.609916	-0.263100
H	-0.120647	2.665193	0.265146
C	0.261862	0.552080	0.010821
C	1.638016	0.795205	0.076440
O	-3.835337	0.201555	-0.158126
O	2.598461	-0.029940	-0.000601
H	1.922058	1.848074	0.208787
O	3.846743	-2.706376	0.635690
O	2.805893	-2.476257	-0.116873
H	2.623777	-1.427604	-0.070126
H	-2.588440	2.420712	0.164407

17

TS3-C2 scf done: -646.034913

C	0.790206	0.762491	0.497946
C	0.894327	2.265946	0.395397
C	-0.274952	0.119461	-0.230335
O	1.863122	2.864212	0.938128
C	-0.133607	2.922918	-0.320306
C	-1.191513	0.821697	-0.973085

H	-0.066026	3.997379	-0.411819
H	-1.980108	0.299201	-1.506820
C	-1.142204	2.233047	-1.040550
C	-2.189959	2.896305	-1.729111
O	1.616896	0.106081	1.165048
O	-2.419450	4.123645	-1.751023
H	-2.868043	2.227444	-2.289775
O	-1.486703	3.925514	1.608259
O	-2.728165	3.794561	1.053954
H	-2.631157	4.175562	0.162656
H	-0.322916	-0.962041	-0.164128

17

3A(C2) scf done: -646.059616

C	-2.131801	0.226274	0.056033
C	-1.168867	-0.800704	-0.300497
C	-1.624267	1.571738	0.321828
O	-1.501513	-1.966407	-0.638815
C	0.327772	-0.490734	-0.269729
C	-0.314837	1.910438	0.192116
H	0.769424	-0.946415	-1.160516
H	-0.005010	2.939147	0.358707
C	0.695783	0.962630	-0.158614
C	2.014899	1.363347	-0.269077
O	-3.379387	0.003517	0.098601
O	3.034752	0.619631	-0.448538
H	2.192185	2.448871	-0.182608
O	0.885518	-1.261944	0.843270
O	2.209921	-1.690524	0.495853
H	2.627649	-0.849844	0.155255
H	-2.366461	2.313613	0.594333

17

Complejo 3(C3) scf done: -646.050299

C	-1.755827	-1.611093	0.036811
C	-0.989556	-1.236002	1.280687
C	-1.186938	-1.215381	-1.232030
O	-1.434445	-1.532804	2.410355
C	0.246831	-0.537466	1.102302
C	-0.002698	-0.544740	-1.316335
H	0.808521	-0.271213	1.989460
H	0.404253	-0.262451	-2.281138
C	0.732006	-0.198186	-0.144347
C	1.998207	0.519860	-0.309232
O	-2.826622	-2.232689	0.115572
O	2.709010	0.874513	0.622044
H	2.320328	0.734482	-1.344088
O	3.957631	1.397816	-2.620601
H	3.924733	2.003873	-0.798224
O	4.133646	2.461237	-1.617952
H	-1.747512	-1.480902	-2.120256

17

TS3-C3 scf done: -646.025708

C	-1.493600	0.790111	-0.277511
C	-0.916328	-0.598293	-0.634015
C	-0.576713	1.806053	0.200207
O	-1.550663	-1.313576	-1.466357
C	0.564465	-0.655480	-0.633291
C	0.773626	1.601547	0.267854
H	1.006460	-1.575525	-0.993352
H	1.423167	2.394357	0.627985

C	1.376197	0.373645	-0.138519
C	2.806828	0.287531	-0.069105
O	-2.695344	1.030821	-0.418429
O	3.513445	-0.671160	-0.394879
H	3.295317	1.198576	0.328651
O	-1.263415	-1.390598	0.932920
H	0.363208	-0.798881	1.692425
O	-0.529462	-0.870568	2.055990
H	-1.013434	2.756748	0.484841

17

3A(C3) scf done: -646.027179

C	-1.373103	0.901250	-0.064825
C	-0.877771	-0.481087	-0.579203
C	-0.382942	1.911374	0.240836
O	-1.213523	-0.704315	-1.823333
C	0.594673	-0.704874	-0.306526
C	0.959971	1.635352	0.272155
H	0.980800	-1.673922	-0.599150
H	1.664315	2.426100	0.515131
C	1.479373	0.337873	0.003006
C	2.901682	0.180940	0.074037
O	-2.580496	1.149296	-0.007287
O	3.551273	-0.854029	-0.113965
H	3.445861	1.111213	0.331263
O	-1.611849	-1.522043	0.274087
H	-0.282815	-1.321850	1.592753
O	-1.252978	-1.335178	1.651325
H	-0.755388	2.904262	0.468411

17

Complejo 3(C4) scf done: -646.053958

C	-2.622283	-0.196183	0.070314
C	-1.406178	-1.086931	-0.065085
C	-2.411818	1.231561	0.128565
O	-1.568572	-2.345779	-0.130644
C	-0.168399	-0.436145	-0.104097
C	-1.166341	1.799916	0.071930
H	0.711869	-1.061927	-0.199814
H	-1.049862	2.878219	0.115784
C	-0.011220	0.988530	-0.047609
C	1.210589	1.667384	-0.104688
O	-3.770269	-0.677910	0.126685
O	2.382615	1.193276	-0.210594
H	1.141074	2.762528	-0.055179
O	4.471008	-0.877932	0.474177
O	3.371899	-1.055536	-0.206366
H	2.858982	-0.120773	-0.203849
H	-3.303019	1.843096	0.223793

17

TS3-C4 scf done: -646.030820

C	1.431937	0.105676	-0.509758
C	0.558938	1.249216	0.065487
C	0.635028	-1.017991	-1.106714
O	1.084907	2.328783	0.377706
C	-0.843560	1.009572	0.226277
C	-0.699649	-1.122357	-0.990824
H	-1.434389	1.786935	0.696093
H	-1.231004	-1.950118	-1.452986
C	-1.482339	-0.131713	-0.272651
C	-2.885865	-0.349006	-0.153202

O	2.515784	0.406807	-1.087482
O	-3.714523	0.384718	0.415325
H	-3.242502	-1.282025	-0.630713
O	1.792502	-0.500333	1.110333
O	1.347983	-1.835621	1.387208
H	0.406272	-1.787014	1.183710
H	1.216374	-1.752436	-1.652343

17

3A(C4) scf done: -646.033191

C	1.331677	0.139319	-0.441613
C	0.347590	1.282775	-0.030239
C	0.598775	-1.121173	-0.864164
O	0.789063	2.431173	0.142614
C	-1.033862	0.968635	0.151147
C	-0.722994	-1.308081	-0.719974
H	-1.686444	1.763457	0.493381
H	-1.193530	-2.222574	-1.072487
C	-1.581729	-0.283655	-0.150406
C	-2.963621	-0.583420	0.018153
O	2.318162	0.449650	-1.199692
O	-3.847119	0.167060	0.473694
H	-3.250075	-1.604151	-0.300808
O	1.763595	-0.172371	1.084852
O	2.401212	-1.449366	1.169606
H	1.649824	-2.048219	1.087592
H	1.222535	-1.862567	-1.351369

17

3A(C5) scf done: -646.053958

C	-2.622299	-0.196016	0.070263
C	-1.406275	-1.086850	-0.065059
C	-2.411742	1.231741	0.128345
O	-1.568778	-2.345675	-0.130480
C	-0.168445	-0.436210	-0.104119
C	-1.166208	1.799953	0.071704
H	0.711720	-1.062089	-0.200188
H	-1.049595	2.878232	0.115783
C	-0.011129	0.988442	-0.047621
C	1.210665	1.667301	-0.104780
O	-3.770316	-0.677708	0.126402
O	2.382731	1.193168	-0.210482
H	1.141191	2.762427	-0.055233
O	4.471444	-0.877978	0.473558
O	3.371689	-1.055688	-0.205906
H	2.858869	-0.120696	-0.203491
H	-3.302856	1.843320	0.224084

17

TS3-C5 scf done: -646.029441

C	-1.157471	0.506950	0.405278
C	-0.135042	1.440953	-0.163535
C	-0.792498	-0.890294	0.694109
O	-0.478841	2.611509	-0.506348
C	1.179849	0.936826	-0.253894
C	0.576810	-1.247584	0.704065
H	1.953684	1.578391	-0.656210
H	0.883613	-2.225495	1.055846
C	1.522966	-0.362071	0.177804
C	2.897236	-0.824251	0.135112
O	-2.352121	0.860484	0.563909
O	3.873396	-0.200006	-0.265986

H	3.038957	-1.854460	0.513595
O	-1.598087	-1.659700	-0.754126
O	-3.007087	-1.594856	-0.503075
H	-3.105611	-0.665062	-0.223130
H	-1.469220	-1.387575	1.381836

17

3A(C5) scf done: -646.032918

C	-1.100562	0.654848	0.324544
C	-0.006437	1.567813	-0.046549
C	-0.884867	-0.828936	0.498515
O	-0.246954	2.802638	-0.244356
C	1.283340	0.987459	-0.157034
C	0.512222	-1.267592	0.477626
H	2.115761	1.618763	-0.440224
H	0.748777	-2.297421	0.717480
C	1.515459	-0.378701	0.106506
C	2.863537	-0.925396	0.041962
O	-2.306283	1.045422	0.421192
O	3.891018	-0.326535	-0.247935
H	2.922910	-2.003097	0.287112
O	-1.608761	-1.505148	-0.647607
O	-3.025586	-1.341399	-0.435971
H	-3.053029	-0.390501	-0.164704
H	-1.458040	-1.184538	1.364320

17

Complejo 3(C6) scf done: -646.050299

C	2.654846	0.670926	-0.035567
C	2.255835	-0.783053	0.007221
C	1.588212	1.646713	-0.053242
O	3.128411	-1.677915	0.006983
C	0.855646	-1.076821	0.047173
C	0.274445	1.283272	-0.018338
H	0.559439	-2.118043	0.086570
H	-0.506757	2.035436	-0.028978
C	-0.108399	-0.089351	0.034393
C	-1.537877	-0.407429	0.072607
O	3.851065	0.999408	-0.054150
O	-1.983661	-1.546744	0.111730
H	-2.240046	0.445615	0.078075
O	-4.303611	1.078834	0.379720
H	-3.982972	-0.724255	-0.199508
O	-4.643293	-0.077683	-0.465404
H	1.882810	2.688512	-0.092669

17

TS3-C6 scf done: -646.037420

C	-1.813300	0.081926	-0.399168
C	-1.253767	-1.173082	0.256782
C	-0.873935	0.964646	-1.014956
O	-2.029367	-2.006554	0.781558
C	0.157273	-1.347590	0.228443
C	0.505141	0.767360	-0.962102
H	0.563231	-2.235387	0.699786
H	1.150334	1.323553	-1.627796
C	1.018387	-0.448773	-0.385952
C	2.444636	-0.640136	-0.394243
O	-3.044539	0.277267	-0.406756
O	3.062086	-1.587205	0.090415
H	3.005275	0.168065	-0.895915
O	1.275147	2.124462	0.447246

O	0.250818	2.161698	1.439467
H	-0.523545	1.869612	0.926078
H	-1.281241	1.830772	-1.524839

17

3A(C6) scf done: -646.050587

C	-1.819440	0.100365	-0.412482
C	-1.215622	-1.155198	0.242785
C	-0.919905	1.071179	-0.849026
O	-1.966422	-2.016950	0.747709
C	0.199306	-1.306212	0.207367
C	0.549213	1.005827	-0.692768
H	0.608073	-2.240291	0.578392
H	1.079481	1.378368	-1.574703
C	1.069532	-0.342546	-0.295201
C	2.465956	-0.562922	-0.405832
O	-3.073262	0.165893	-0.531659
O	3.096900	-1.592259	-0.086597
H	3.030003	0.288875	-0.831406
O	1.024023	2.057306	0.273770
O	0.321113	1.894360	1.500577
H	-0.575508	1.694091	1.161987
H	-1.333741	1.950212	-1.334092