Neutral complexes

Compound 8:

```
 35
SCF Done:  E(RB+HF-LYP) =  -1920.41955190     A.U. after   23 cycles
 C                     2.33134   0.19607   0.05072
 C                     2.28474   0.0674    1.45508
 C                     1.11813  -0.69192   2.05459
 C                    -0.1224   -0.09063   1.42624
 C                    -0.147     0.02703   0.02088
 C                     1.09748   0.15399  -0.70112
 Mn                    0.96863   1.77172   0.73926
 C                    -0.3802    2.82684   0.15933
 O                    -1.24776   3.50311  -0.21007
 C                     1.09238   0.12631  -2.21585
 C                     2.15252   3.01052   0.16082
 O                     2.91009   3.8089   -0.20683
 C                     0.92597   2.3615    2.43797
 O                     0.90373   2.69605   3.5496
 H                     1.19188  -1.78667   1.90375
 H                     1.09493  -0.52865   3.13681
 C                     3.50589   0.20861   2.33653
 C                     3.64479   0.40761  -0.67835
 C                    -1.44819   0.04081  -0.75706
 C                    -1.37521  -0.10851   2.27256
 H                    -2.1586    0.55799   1.90553
 H                    -1.79391  -1.12497   2.32873
 H                    -1.14133   0.19703   3.29714
 H                    -1.4718    0.80011  -1.54116
 H                    -1.57966  -0.93489  -1.24299
 H                    -2.31136   0.20075  -0.11194
 H                     2.05961   0.39721  -2.63745
 H                     0.85146  -0.88264  -2.57855
 H                     0.35219   0.80762  -2.64112
 H                     3.58537   1.16787  -1.4595
 H                     4.44504   0.69704   0.0016
 H                     3.94684  -0.53465  -1.15347
 H                     4.20231   0.97956   2.00048
 H                     3.20611   0.46342   3.35773
 H                     4.05655  -0.74285   2.39293
```

Compound 7:

```
 32
SCF Done:  E(RB+HF-LYP) =  -1881.10802034     A.U. after   22 cycles
 C                     0.67546  -2.55053   0.56617
 C                     0.17509  -1.44846  -0.15203
 C                     1.17716  -0.55427  -0.86052
 C                     2.27114  -0.24269   0.14566
 C                     2.81787  -1.31677   0.87219
 C                     2.01294  -2.48383   1.0731
 Mn                    0.93753  -0.8256    1.90418
 C                     1.90016  -0.29433   3.34227
 O                     2.51149   0.05268   4.26458
 C                    -1.2501   -1.38223  -0.64609
 C                     3.00457   1.06326  -0.04444
```

C	4.19811	-1.28107	1.49256
C	-0.14581	-3.78526	0.87017
C	-0.2809	-1.55133	3.02863
O	-1.06435	-2.00949	3.75052
C	0.06948	0.73632	1.69754
O	-0.48018	1.74125	1.50935
H	1.57077	-1.00811	-1.79154
H	0.6838	0.37724	-1.15811
H	3.65325	1.32199	0.7952
H	3.62978	1.02194	-0.9496
H	2.29639	1.88618	-0.18463
H	4.2962	-2.03204	2.28094
H	4.94771	-1.49909	0.72149
H	4.44707	-0.30899	1.92229
H	0.27844	-4.345	1.70788
H	-1.18585	-3.55739	1.11084
H	-0.15066	-4.44182	-0.00901
H	-1.95856	-1.89531	0.00781
H	-1.57644	-0.34137	-0.73918
H	-1.33052	-1.83363	-1.64689
H	2.4157	-3.32208	1.63061

Compound 9:

20
SCF Done: E(RB+HF-LYP) = -1723.82889781 A.U. after 19 cycles

6	1.15303	-0.80109	2.09193
6	-0.08568	-0.23167	1.42699
6	-0.11764	-0.07403	0.0386
6	1.09631	0.0892	-0.69607
6	2.31114	0.12999	0.05421
6	2.2881	-0.03283	1.44206
1	1.2454	-1.8943	1.96704
1	1.12971	-0.60354	3.1671
1	3.20162	0.14886	2.00058
1	3.22642	0.43359	-0.44645
1	1.09164	0.22585	-1.77023
1	-1.06433	0.0727	-0.47411
1	-1.02374	-0.20573	1.97366
25	0.95442	1.66865	0.76673
6	0.89995	2.27216	2.46803
8	0.86956	2.61953	3.57277
6	-0.41401	2.70395	0.17982
8	-1.29028	3.35745	-0.20188
6	2.13319	2.91894	0.18673
8	2.88927	3.71025	-0.19114

Deprotonated compounds

Compound 8 in position C7 :

34
SCF Done: E(RB+HF-LYP) = -1919.86151723 A.U. after 22 cycles

C	2.15822	0.25016	0.00561
C	2.23182	0.13211	1.42577
C	1.04885	-0.41212	2.05019
C	0.41694	-1.62606	1.38384

C	0.28217	-1.43162	-0.11077
C	0.92765	-0.21265	-0.62716
Mn	0.61152	1.37142	0.89356
C	-1.15867	1.18559	1.06292
O	-2.31266	1.02973	1.19102
C	3.47459	0.52143	2.20105
C	0.93181	-0.46017	3.56286
C	-0.41745	-2.31884	-0.85812
C	0.70663	0.06413	-2.10398
C	3.33984	0.73163	-0.81128
C	0.66313	2.71356	-0.29249
O	0.69973	3.59807	-1.0647
C	0.86288	2.5284	2.22974
O	1.03359	3.29022	3.10833
H	1.00459	-2.5399	1.59939
H	-0.57845	-1.80037	1.81455
H	-0.54227	-2.21792	-1.93091
H	-0.91429	-3.16557	-0.38907
H	1.06601	1.05063	-2.40335
H	1.202	-0.68484	-2.74576
H	-0.36285	0.02926	-2.3382
H	3.94653	1.46371	-0.27205
H	3.99422	-0.11538	-1.07257
H	3.02798	1.19587	-1.74876
H	3.96467	1.41132	1.79655
H	3.24328	0.72752	3.24829
H	4.20976	-0.299	2.18664
H	1.28248	0.45193	4.05315
H	-0.11737	-0.59595	3.85296
H	1.49382	-1.31015	3.99247

Compound 8 in position C9

34

SCF Done: E(RB+HF-LYP) = -1919.84204396 A.U. after 23 cycles

C	2.22836	0.32123	0.01358
C	2.24432	0.10288	1.43003
C	1.19235	-0.62222	2.05778
C	0.4013	-1.58866	1.19698
C	0.09772	-0.79643	-0.06778
C	1.31922	-0.48347	-0.83682
Mn	0.37943	1.11248	0.96331
C	-1.20986	0.94492	1.75457
O	-2.25063	0.79187	2.27213
C	3.36948	0.69573	2.26119
C	1.15312	-0.87813	3.55029
C	-1.11126	-1.27068	-0.84253
C	1.50478	-0.70033	-2.16953
C	3.34777	1.07446	-0.67296
C	-0.15456	2.09154	-0.44607
O	-0.50438	2.71193	-1.37303
C	0.87907	2.55995	1.91038
O	1.15483	3.52126	2.52481
H	0.92755	-2.55682	1.0214
H	-0.53876	-1.83685	1.70684
H	-1.35635	-0.59409	-1.66959
H	-0.95108	-2.27536	-1.27948
H	-1.99062	-1.33865	-0.18981
H	2.36912	-0.3209	-2.70544
H	0.7545	-1.21291	-2.76266

H	3.75837	1.87725	-0.05732
H	4.17959	0.40325	-0.94424
H	2.98477	1.52578	-1.60107
H	3.65856	1.69668	1.93532
H	3.10918	0.76196	3.318
H	4.2583	0.05325	2.17971
H	1.46788	-0.02187	4.15348
H	0.13069	-1.12623	3.85682
H	1.78868	-1.7366	3.83177

Compound 8 in position C11

34

SCF Done: E(RB+HF-LYP) = -1919.83487512 A.U. after 22 cycles

C	2.50099	0.04529	0.01453
C	2.23902	0.20888	1.45693
C	1.20603	-0.55587	2.05368
C	0.61565	-1.66475	1.20228
C	0.22007	-0.94969	-0.07607
C	1.23859	-0.19201	-0.7097
Mn	0.25388	1.04408	0.8616
C	-1.29125	0.68713	1.65786
O	-2.32213	0.47531	2.18274
C	3.27652	0.94376	2.27538
C	1.05311	-0.68805	3.55239
C	-0.96787	-1.50528	-0.82908
C	1.21832	0.10807	-2.19161
C	3.71058	0.2702	-0.58529
C	-0.35763	2.08682	-0.4577
O	-0.77897	2.7632	-1.32147
C	0.69629	2.52122	1.77028
O	0.97093	3.48577	2.38321
H	1.31145	-2.51856	1.03842
H	-0.27927	-2.06848	1.69096
H	-1.35214	-0.82042	-1.58962
H	-0.70666	-2.45232	-1.33447
H	-1.79177	-1.72182	-0.14024
H	1.72313	1.05425	-2.4084
H	1.75096	-0.68324	-2.74356
H	0.2052	0.16627	-2.59436
H	4.58621	0.55177	-0.01099
H	3.82319	0.24573	-1.6635
H	3.63139	1.83542	1.75018
H	2.89792	1.25454	3.25117
H	4.14914	0.29332	2.44796
H	1.25577	0.24388	4.08625
H	0.033	-0.99464	3.80807
H	1.73618	-1.45848	3.95264

Compound 7 in position C7

31

SCF Done: E(RB+HF-LYP) = -1880.54829483 A.U. after 23 cycles

6	-0.43546	-0.60068	-0.20024
6	0.40297	0.04192	-1.3006
6	1.64495	0.71632	-0.74919
6	1.92311	0.41884	0.66105
6	1.48952	-0.8433	1.20713

6	0.2663	-1.40628	0.76781
6	2.39102	1.53666	-1.52787
25	-0.07775	0.47525	1.66409
6	-1.58424	-0.02731	2.47498
8	-2.57429	-0.36652	3.01022
6	3.15101	1.05763	1.27816
6	-0.20367	-2.74514	1.29184
6	-1.81451	-1.01386	-0.67644
6	-0.66415	2.03004	1.00665
8	-1.05609	3.0308	0.54048
6	0.59511	1.04235	3.2275
8	1.02778	1.41651	4.2528
1	2.0692	-1.33355	1.98716
1	0.68929	-0.71126	-2.06129
1	-0.20592	0.7868	-1.83029
1	3.28367	2.0361	-1.16528
1	2.09046	1.75654	-2.54989
1	3.26337	0.76635	2.32674
1	4.06879	0.76121	0.74299
1	3.09758	2.1519	1.2443
1	0.29338	-2.98719	2.23836
1	-1.28254	-2.77081	1.46808
1	0.02887	-3.54674	0.57389
1	-2.43895	-1.42075	0.12386
1	-2.34729	-0.151	-1.09492
1	-1.75997	-1.77487	-1.47689

Compound 7 in position C9

31

SCF Done: E(RB+HF-LYP) = -1880.52845498 A.U. after 23 cycles

6	1.28524	-1.58395	-0.2983
6	1.13359	-0.17282	-0.83999
6	2.22437	0.63507	-0.13968
6	3.58575	0.20397	-0.51712
6	3.71282	-1.22666	-0.20731
6	2.6032	-2.11007	-0.25107
25	2.34172	-0.83171	1.49156
6	2.46607	-2.24159	2.6044
8	2.52906	-3.12788	3.37077
6	1.96579	2.12172	-0.04973
6	4.63828	0.9913	-0.87443
6	2.87331	-3.60037	-0.17218
6	0.06721	-2.47711	-0.36807
6	0.83141	-0.20197	2.19672
8	-0.17666	0.22425	2.61679
6	3.4861	0.15681	2.46636
8	4.22162	0.81462	3.0917
1	4.7082	-1.66244	-0.14849
1	1.16872	-0.1262	-1.95441
1	0.15037	0.21901	-0.5478
1	2.70808	2.62404	0.58186
1	2.00407	2.60629	-1.04458
1	0.97267	2.32383	0.37063
1	5.63908	0.57566	-0.97223
1	4.53636	2.06543	-0.99082
1	3.88293	-3.79288	0.20404
1	2.17058	-4.12748	0.47796
1	2.79509	-4.04568	-1.17422
1	0.17504	-3.40133	0.20743

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 1                    -0.81349  -1.95184   0.01927
 1                    -0.16257  -2.7603   -1.41087
```

Compound 7 in position C3

```
 31
SCF Done:  E(RB+HF-LYP) =  -1880.48988271     A.U. after   23 cycles
 6                     0.17213  -1.4325   -0.11733
 6                     1.16462  -0.5493   -0.84491
 6                     2.244    -0.24785   0.17471
 6                     2.78118  -1.3543    0.88747
 6                     2.0546   -2.58394   1.09466
 6                     0.70397  -2.54637   0.58971
 25                    0.91239  -0.79542   1.89635
 6                    -0.29729  -1.5317    3.00126
 8                    -1.09631  -1.98539   3.72358
 6                     3.00299   1.0451   -0.0344
 6                     4.17837  -1.27324   1.48702
 6                    -0.16407  -3.76811   0.85837
 6                    -1.25109  -1.3866   -0.63102
 6                     0.07383   0.7538    1.66735
 8                    -0.47376   1.77472   1.48429
 6                     1.88455  -0.30886   3.32676
 8                     2.49885   0.02943   4.2617
 1                     1.56257  -1.01377  -1.77659
 1                     0.67436   0.38433  -1.15185
 1                     3.63471   1.31415   0.81599
 1                     3.6559    0.97235  -0.92209
 1                     2.31258   1.87825  -0.21424
 1                     4.29383  -2.07315   2.22142
 1                     4.9235   -1.42967   0.69225
 1                     4.40869  -0.31394   1.96215
 1                     0.31253  -4.37498   1.6312
 1                    -1.1884   -3.53409   1.16699
 1                    -0.23132  -4.37355  -0.05838
 1                    -1.96341  -1.87504   0.03899
 1                    -1.58131  -0.34976  -0.76964
 1                    -1.32692  -1.88261  -1.61482
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Lithiated compounds

Compound 8 in position C7 in conformation trans

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 59
SCF Done:  E(RB+HF-LYP) =  -2275.15913681     A.U. after   23 cycles
 6                     0.26048  -0.51635   1.11704
 6                    -0.23857  -0.67096  -0.30625
 6                     0.55941   0.1937   -1.26271
 6                     1.82415   0.68373  -0.77982
 6                     2.49865   0.04908   0.36097
 6                     1.6837   -0.61167   1.32673
```

6	0.03675	0.42516	-2.52743
25	1.17779	1.44389	1.22876
6	1.08277	1.61639	3.009
8	1.02873	1.71186	4.17079
6	2.61123	1.56426	-1.73386
6	2.29035	-1.34771	2.50575
6	-0.71938	-1.04877	2.14534
6	-0.36501	2.29679	0.88212
8	-1.38877	2.79878	0.63962
6	2.29708	2.85565	1.14302
8	3.02583	3.76502	1.08917
3	0.67863	-1.61355	-2.89004
7	-0.41522	-3.04777	-3.93534
6	-0.50752	-2.60082	-5.33813
6	0.44076	-4.24762	-3.79802
6	1.93196	-3.90452	-3.88281
7	2.32583	-2.8792	-2.89022
6	3.59873	-2.23874	-3.27366
6	-1.76822	-3.30107	-3.40624
6	2.45409	-3.45638	-1.5357
6	4.01179	-0.01603	0.43629
1	-0.22343	-1.74319	-0.62621
1	-1.29442	-0.37832	-0.36236
1	0.51414	1.10456	-3.2267
1	-1.02613	0.25067	-2.69487
1	3.44326	2.07471	-1.24837
1	3.02257	0.99546	-2.58519
1	1.96818	2.34319	-2.15525
1	3.14464	-0.82474	2.94194
1	1.56103	-1.49692	3.30301
1	2.63744	-2.34524	2.19677
1	-0.43681	-0.81012	3.17322
1	-1.71162	-0.61357	1.97954
1	-0.83506	-2.14502	2.07756
1	0.19745	-5.00421	-4.56324
1	0.22012	-4.70243	-2.82739
1	2.16668	-3.51242	-4.8776
1	2.52375	-4.82746	-3.76114
1	-2.36924	-2.39241	-3.49421
1	-2.27905	-4.11198	-3.95073
1	-1.71002	-3.57107	-2.34825
1	-1.10479	-1.68691	-5.38905
1	0.48395	-2.37732	-5.74014
1	-0.97682	-3.36532	-5.9792
1	2.67407	-2.66061	-0.82058
1	1.51983	-3.93275	-1.22825
1	3.25793	-4.20946	-1.49376
1	3.85262	-1.46815	-2.54246
1	4.42606	-2.96555	-3.31941
1	3.49714	-1.76378	-4.25368
1	4.3688	-0.03556	1.46746
1	4.39556	-0.92476	-0.05486
1	4.4878	0.83528	-0.05188

Compound 8 in position C7 in conformation cis

59
SCF Done: E(RB+HF-LYP) = -2275.17906943 A.U. after 24 cycles

6	1.76552	-0.76476	1.32098
6	0.35476	-0.4816	1.24372

6	-0.26446	-0.55334	-0.14512
6	0.51397	0.29077	-1.12695
6	1.85999	0.65235	-0.69795
6	2.55556	-0.1642	0.29775
25	1.53159	1.34565	1.37662
6	2.88232	2.5437	1.31697
8	3.73805	3.335	1.26242
6	-0.59391	-0.94079	2.33483
6	-0.08132	0.69573	-2.29472
6	2.67221	1.4667	-1.68947
6	4.03887	-0.44162	0.17178
6	2.37075	-1.64683	2.39384
6	1.4806	1.44531	3.17942
8	1.43157	1.50923	4.34136
6	0.17718	2.35684	0.97328
8	-0.75652	2.95091	0.51986
3	-1.02765	2.64248	-1.41125
7	-3.10851	2.92437	-1.81963
6	-3.76826	3.25741	-0.54231
6	-3.0737	4.09024	-2.7295
6	-1.97956	5.09329	-2.352
7	-0.62892	4.49114	-2.37352
6	0.31902	5.31704	-1.60088
6	-0.13324	4.32581	-3.75059
6	-3.8054	1.79208	-2.45203
1	-0.3125	-1.59605	-0.50988
1	-1.30541	-0.2067	-0.10437
1	0.47662	1.17014	-3.09653
1	-1.0684	0.31253	-2.54802
1	3.59906	1.84949	-1.26168
1	2.93146	0.88128	-2.58503
1	2.10192	2.33771	-2.03151
1	3.3435	-1.28995	2.74018
1	1.72048	-1.71475	3.2674
1	2.50703	-2.66866	2.01148
1	-0.19888	-0.79489	3.34274
1	-1.5344	-0.38032	2.27672
1	-0.84972	-2.00818	2.22733
1	-2.03848	5.96348	-3.0292
1	-2.1577	5.4709	-1.34059
1	-2.89876	3.71722	-3.74353
1	-4.04798	4.60884	-2.74907
1	1.30425	4.84397	-1.6057
1	0.4161	6.33169	-2.0217
1	-0.01508	5.38924	-0.56365
1	0.8548	3.85962	-3.72789
1	-0.79598	3.67637	-4.3277
1	-0.05095	5.29414	-4.27315
1	-3.74354	2.3871	0.11745
1	-3.24012	4.06518	-0.03365
1	-4.81874	3.55646	-0.69747
1	-3.79148	0.93189	-1.77725
1	-4.85648	2.03109	-2.68685
1	-3.29672	1.50965	-3.37786
1	4.48328	-0.73696	1.12349
1	4.209	-1.26136	-0.5411
1	4.59735	0.42254	-0.19191

Compound 8 in position C9 in conformation trans

```
 59
SCF Done:  E(RB+HF-LYP) =  -2275.15126249     A.U. after   25 cycles
 6                     1.1556   -1.44501   1.24835
 6                     1.36664  -1.59685  -0.24401
 6                     1.19805  -0.20097  -0.81663
 6                     2.09215   0.81062  -0.2981
 6                     2.24405   0.77797   1.15769
 6                     1.82695  -0.38505   1.90383
 25                    0.08023   0.49612   0.95269
 6                    -0.61567   0.88461   2.57361
 8                    -1.09115   1.1306    3.60845
 6                     0.75321  -0.13262  -2.25921
 6                     2.68087   1.83103  -1.09645
 6                     2.07868  -0.43526   3.40185
 6                     0.63858  -2.66955   1.97304
 6                    -1.3715   -0.37517   0.36413
 8                    -2.28228  -0.97606  -0.04375
 6                    -0.39226   2.12088   0.31921
 8                    -0.67779   3.16766  -0.09755
 3                     4.42529   0.74116  -1.58394
 7                     6.07234  -0.18968  -0.65021
 6                     6.71805   0.55152   0.44787
 6                     7.01948  -0.3872   -1.76928
 6                     6.31002  -0.73697  -3.08077
 7                     5.27793   0.25742  -3.44426
 6                     5.87405   1.51139  -3.94122
 6                     4.36092  -0.2895   -4.46013
 6                     5.55578  -1.47554  -0.14001
 6                     3.01636   1.90481   1.81206
 1                     2.33621  -2.08755  -0.4996
 1                     0.58824  -2.25096  -0.65303
 1                     0.41661   0.86878  -2.54513
 1                     1.5621   -0.41665  -2.95788
 1                    -0.07627  -0.82528  -2.43843
 1                     2.96912   2.76504  -0.61643
 1                     2.25163   1.98814  -2.08554
 1                     1.84403   0.50316   3.90752
 1                     1.49725  -1.2186    3.88639
 1                     3.13879  -0.65523   3.58836
 1                     0.22031  -2.45346   2.95875
 1                    -0.15413  -3.14424   1.38576
 1                     1.43309  -3.42241   2.10447
 1                     7.06407  -0.84526  -3.87986
 1                     5.81331  -1.7078   -2.98672
 1                     7.58717   0.54064  -1.89102
 1                     7.75498  -1.17628  -1.53642
 1                     3.58152   0.44386  -4.68019
 1                     4.88641  -0.53754  -5.3973
 1                     3.87917  -1.19402  -4.07959
 1                     5.07777   2.22402  -4.17088
 1                     6.52001   1.96274  -3.18356
 1                     6.47238   1.3465   -4.85299
 1                     4.81931  -1.28619   0.64456
 1                     5.05683  -2.03582  -0.93463
 1                     6.36403  -2.10236   0.27217
 1                     6.00132   0.70053   1.25845
 1                     7.5926    0.01278   0.8489
 1                     7.04504   1.5336    0.09435
 1                     3.03128   1.8336    2.89943
 1                     4.06233   1.9199    1.4689
 1                     2.5951    2.88066   1.55229
```

Compound 8 in position C9 in conformation cis

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 59
SCF Done:  E(RB+HF-LYP) =  -2275.16205746     A.U. after   23 cycles
 6                     1.64686  -1.04522   0.95462
 6                     0.59499  -1.50718  -0.03303
 6                    -0.11333  -0.2364   -0.47403
 6                     0.73774   0.73342  -1.15112
 6                     1.96225   1.01042  -0.38739
 6                     2.44595   0.0611    0.58168
 25                    0.55361   0.87629   1.30542
 6                     1.40212   1.67213   2.69811
 8                     1.90855   2.20334   3.60163
 6                    -1.527    -0.42457  -0.97296
 6                     0.33538   1.49126  -2.259
 6                     2.83952   2.15189  -0.85361
 6                     3.80787   0.28588   1.21547
 6                     2.07322  -2.05362   2.00022
 6                    -0.67294   0.01213   2.29796
 8                    -1.48231  -0.56864   2.89934
 6                    -0.38818   2.29485   0.89385
 8                    -1.00126   3.20553   0.44159
 3                    -0.8763    3.23276  -1.58684
 7                    -0.3662    5.25321  -2.05114
 6                    -1.7095    5.84789  -2.21304
 6                    -2.65796   4.94242  -3.00374
 7                    -2.83827   3.62153  -2.36498
 1                     1.01846  -2.10531  -0.86762
 1                    -0.12189  -2.15846   0.47957
 1                    -2.05658   0.52927  -1.07885
 1                    -1.54956  -0.92002  -1.95934
 1                    -2.103    -1.04992  -0.28224
 1                     1.07715   2.08528  -2.78806
 1                    -0.461     1.08549  -2.88046
 1                     3.57836   2.45133  -0.10991
 1                     3.38317   1.88034  -1.77115
 1                     2.23776   3.03453  -1.09129
 1                     3.96117   1.31297   1.55285
 1                     3.97216  -0.36754   2.07137
 1                     4.58894   0.06093   0.47755
 1                     2.57255  -1.60628   2.86298
 1                     1.19863  -2.59258   2.37835
 1                     2.75267  -2.80718   1.57129
 6                    -3.77747   3.69432  -1.23037
 6                    -3.31878   2.63137  -3.34329
 6                     0.36678   5.91869  -0.95983
 6                     0.41779   5.32981  -3.29511
 1                    -1.65358   6.83326  -2.70894
 1                    -2.11584   6.02276  -1.21207
 1                    -3.62514   5.45872  -3.1338
 1                    -2.25734   4.77602  -4.00858
 1                    -3.85048   2.71341  -0.75483
 1                    -3.4186    4.3976   -0.4766
 1                    -4.78422   4.00532  -1.5578
 1                    -3.42465   1.65855  -2.85677
 1                    -4.29474   2.91433  -3.77319
 1                    -2.5942    2.5282   -4.15578
 1                     1.34642   5.44864  -0.83924
 1                     0.51831   6.99295  -1.16008
 1                    -0.18127   5.80334  -0.02204
 1                     1.39073   4.85707  -3.14025
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 1                    -0.08474    4.79644   -4.10541
 1                     0.58109    6.37427   -3.61223
```

Compound 8 in position C11 in conformation trans

```
 59
SCF Done:  E(RB+HF-LYP) =  -2275.14556017     A.U. after   24 cycles
 6                     0.7057   -0.80911    1.78258
 6                     1.34533  -1.56483    0.6355
 6                     1.49405  -0.52179   -0.45325
 6                     2.15238   0.68605   -0.10184
 6                     2.23116   1.09792    1.29067
 6                     1.34019   0.3917     2.19744
 25                    0.04115   0.86213    0.48623
 6                    -0.9782    1.84111    1.60517
 8                    -1.64432   2.46105    2.33265
 6                     1.41229  -1.01938   -1.88001
 6                     2.86692   1.53251   -1.13364
 6                     1.19048   0.92685    3.6054
 6                    -0.2029   -1.60631    2.69305
 6                    -1.27579  -0.18493   -0.11431
 8                    -2.11915  -0.89001   -0.50288
 6                    -0.13662   2.14858   -0.76385
 8                    -0.25252   2.96978   -1.5821
 3                     4.92565   1.18035    2.22775
 7                     5.63559  -0.76611    2.52615
 6                     4.75303  -1.61567    3.34622
 6                     6.93679  -0.5471     3.1917
 6                     7.67417   0.67539    2.63215
 7                     6.84455   1.89826    2.68399
 6                     6.76934   2.45325    4.04751
 6                     7.34962   2.92489    1.75626
 6                     5.79771  -1.36504    1.18809
 1                     2.30228  -2.06767    0.90687
 1                     0.67048  -2.35757    0.29485
 1                     1.24175  -0.22199   -2.60711
 1                     2.33618  -1.54653   -2.17079
 1                     0.59008  -1.73416   -1.98546
 1                     2.68231   2.60042   -0.99444
 1                     3.95335   1.3798    -1.04286
 1                     2.5847    1.2706    -2.15336
 1                     1.05715   2.01114    3.62366
 1                     0.35258   0.47384    4.13538
 1                     2.10272   0.70588    4.18052
 1                    -0.85172  -0.98162    3.31126
 1                    -0.85199  -2.26042    2.10243
 1                     0.37918  -2.25615    3.36768
 1                     8.62357   0.80773    3.17921
 1                     7.94006   0.49967    1.58498
 1                     6.7438   -0.40575    4.25984
 1                     7.58935  -1.43312    3.1056
 1                     6.68736   3.79409    1.78071
 1                     8.36995   3.25292    2.01625
 1                     7.35912   2.53236    0.73554
 1                     6.10731   3.32299    4.04923
 1                     6.35828   1.71733    4.74347
 1                     7.76076   2.76398    4.41796
 1                     4.81731  -1.47043    0.71704
 1                     6.41371  -0.7261     0.54953
 1                     6.27132  -2.3597     1.24141
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 1                     3.7816   -1.70949   2.85481
 1                     5.17247  -2.62446   3.49542
 1                     4.59887  -1.15464   4.32602
 6                     3.13683   2.13477   1.7419
 1                     2.8323    2.64936   2.65533
 1                     3.41467   2.86834   0.9827
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Compound 8 in position C11 in conformation cis

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 59
SCF Done:  E(RB+HF-LYP) =  -2275.15319007     A.U. after   23 cycles
 6                     1.28976   0.49189   2.1692
 6                     0.74545  -0.74018   1.75707
 6                     1.52296  -1.53232   0.72683
 6                     1.77513  -0.53632  -0.38566
 6                     2.3752    0.69668  -0.0225
 6                     2.33427   1.14533   1.36829
 25                    0.18739   0.86419   0.27277
 6                     0.14067   1.86145  -1.21216
 8                     0.13294   2.47028  -2.21158
 6                    -0.24634  -1.51241   2.59871
 6                     1.88322  -1.10554  -1.78316
 6                     3.2317    1.48003  -0.99056
 6                     3.09599   2.22777   1.8528
 6                     0.96329   1.07665   3.5239
 6                    -0.92326   1.97857   1.12516
 8                    -1.69277   2.68678   1.66234
 6                    -1.05542  -0.29503  -0.28808
 8                    -1.87529  -1.03241  -0.66404
 3                     1.35695   3.51193   1.37892
 7                     1.24141   5.26047   0.10982
 6                    -0.09828   5.41514  -0.49675
 6                     2.26113   5.30553  -0.95432
 6                     1.50616   6.33464   1.08933
 6                     0.64563   6.21862   2.34584
 7                     0.8823    4.96657   3.09492
 6                    -0.26208   4.70499   3.98775
 6                     2.11537   5.06647   3.89598
 1                     2.44982  -1.98256   1.13532
 1                     0.90636  -2.35585   0.35212
 1                     1.80024  -0.35001  -2.56784
 1                     2.84491  -1.6255   -1.91869
 1                     1.09215  -1.84205  -1.95469
 1                     3.13223   2.55805  -0.84578
 1                     4.28955   1.23101  -0.82333
 1                     3.00047   1.25425  -2.0317
 1                     0.97537   2.16803   3.51263
 1                    -0.01053   0.75432   3.89312
 1                     1.72055   0.75597   4.25371
 1                    -0.97954  -0.87641   3.0997
 1                    -0.79939  -2.22399   1.97885
 1                     0.27779  -2.09596   3.37165
 1                     0.82978   7.09904   2.98666
 1                    -0.41229   6.25147   2.07157
 1                     2.56759   6.28912   1.35556
 1                     1.33479   7.32668   0.63347
 1                    -0.07299   3.80412   4.57586
 1                    -0.43268   5.5417    4.6869
 1                    -1.16464   4.5384    3.3963
 1                     2.27396   4.13463   4.44318
 1                     2.98379   5.22215   3.25211
```

1	2.05831	5.89553	4.6229
1	-0.22364	4.67486	-1.28675
1	-0.88376	5.25009	0.24327
1	-0.22553	6.42122	-0.93189
1	2.06375	4.51725	-1.68354
1	2.25799	6.27536	-1.48084
1	3.25393	5.14709	-0.52344
1	3.17542	2.36388	2.92659
1	3.96009	2.55608	1.28395

Compound 7 in position C7 in conformation trans

56

SCF Done: E(RB+HF-LYP) = -2235.84736648 A.U. after 23 cycles

C	-0.28054	-0.68995	-0.23615
C	0.47901	0.16629	-1.23704
C	1.77585	0.62549	-0.82701
C	2.45968	0.01178	0.29725
C	1.71607	-0.63237	1.31494
C	0.28778	-0.55276	1.16663
C	-0.09221	0.40429	-2.48026
Mn	1.20361	1.42872	1.20044
C	-0.35815	2.27016	0.92546
O	-1.39547	2.76516	0.73214
C	2.59518	1.44358	-1.80347
C	2.42226	-1.30232	2.47341
C	-0.63025	-1.09605	2.24279
C	2.30885	2.84547	1.02354
O	3.02152	3.76107	0.91097
C	1.20137	1.63868	2.97875
O	1.20369	1.75691	4.13941
Li	0.62839	-1.60461	-2.90025
H	3.544	0.06399	0.35746
H	-0.29915	-1.7586	-0.56476
H	-1.33331	-0.38173	-0.23447
H	0.36554	1.09357	-3.18467
H	-1.16287	0.24668	-2.60684
H	3.53935	1.76388	-1.35492
H	2.8348	0.87419	-2.71714
H	2.06292	2.34493	-2.1255
H	3.45332	-0.94454	2.56005
H	1.92687	-1.12002	3.42989
H	2.45198	-2.39206	2.3295
H	-0.26589	-0.89575	3.25321
H	-1.62532	-0.64356	2.1627
H	-0.76641	-2.18786	2.1502
N	-0.3853	-3.02927	-4.03119
N	2.2758	-2.87677	-2.79193
C	1.95346	-3.88594	-3.82574
C	0.46047	-4.23104	-3.85238
C	-1.77049	-3.28739	-3.59697
C	-0.38341	-2.56323	-5.43075
H	0.27343	-4.97529	-4.64505
H	0.17206	-4.70165	-2.90745
H	2.25722	-3.47815	-4.79525
H	2.53621	-4.81087	-3.67728
C	2.29905	-3.47323	-1.43977
C	3.57983	-2.24277	-3.06632
H	-2.3627	-2.37586	-3.7111
H	-2.24484	-4.08909	-4.18632

H	-1.78307	-3.57364	-2.54165
H	-0.97254	-1.64583	-5.50822
H	0.63343	-2.3397	-5.76367
H	-0.81254	-3.31684	-6.11165
H	2.50107	-2.69236	-0.70317
H	1.33186	-3.92076	-1.19735
H	3.07348	-4.25369	-1.35855
H	3.77807	-1.48193	-2.30829
H	4.4027	-2.97601	-3.05365
H	3.56073	-1.75752	-4.04648

Compound 7 in position C7 in conformation cis

56

SCF Done: E(RB+HF-LYP) = -2235.86602637 A.U. after 23 cycles

6	1.62854	-0.98052	0.95938
6	0.65831	-1.4958	0.06917
6	-0.15436	-0.49257	-0.56224
6	0.56674	0.76747	-1.03053
6	1.41904	1.36004	0.07243
6	1.74479	0.44683	1.15619
25	-0.27397	-0.37586	1.62482
6	-1.11956	1.1409	1.56868
8	-1.53768	2.25369	1.44326
6	0.52984	-2.98461	-0.15942
6	-1.31348	-0.89255	-1.45267
6	1.79773	2.67814	0.01657
6	2.70164	0.92866	2.22811
1	2.26716	-1.6529	1.52566
6	0.08881	-0.49101	3.39188
8	0.31542	-0.52128	4.53588
6	-1.67002	-1.50817	1.79549
8	-2.57825	-2.23029	1.89407
3	-0.05171	3.53834	1.14605
7	0.22273	4.58907	2.97641
6	1.60602	5.05997	3.16184
6	-0.70997	5.71754	2.76708
6	-0.61184	6.30498	1.35642
7	-0.90967	5.30465	0.30784
6	-0.35747	5.72996	-0.98896
6	-2.36183	5.07935	0.17486
6	-0.18823	3.78812	4.14621
1	1.20288	0.56148	-1.91151
1	-0.17046	1.50852	-1.36542
1	2.53459	3.0923	0.69968
1	1.57062	3.26345	-0.87252
1	2.8713	0.15737	2.98381
1	3.67656	1.20144	1.79719
1	2.32202	1.81448	2.75053
1	0.98783	-3.54696	0.66055
1	-0.51017	-3.30795	-0.24673
1	1.03804	-3.27013	-1.09089
1	-1.87556	-1.74409	-1.06165
1	-2.01857	-0.06044	-1.56287
1	-0.969	-1.15762	-2.46606
1	-0.5359	6.52035	3.50501
1	-1.72384	5.34513	2.94233
1	0.40128	6.68062	1.18176
1	-1.28683	7.17503	1.27936
1	0.49022	2.94021	4.26744

1	-0.17466	4.383	5.07458
1	-1.19475	3.39455	3.98907
1	2.26687	4.20079	3.29895
1	1.95176	5.61051	2.28349
1	1.69842	5.7159	4.04427
1	-2.54204	4.30045	-0.56958
1	-2.78693	4.73212	1.1178
1	-2.88496	5.99897	-0.13749
1	-0.56705	4.96672	-1.74331
1	-0.79296	6.68379	-1.33206
1	0.72695	5.8484	-0.91353

Compound 7 in position C9 in conformation trans

56

SCF Done: E(RB+HF-LYP) = -2235.84007733 A.U. after 23 cycles

C	1.25695	-1.60724	-0.30732
C	1.13202	-0.19777	-0.87027
C	2.081	0.7762	-0.38673
C	2.31302	0.67734	1.04393
C	1.90476	-0.45393	1.81541
C	1.14837	-1.47472	1.2003
Mn	0.14397	0.52468	0.9878
C	-1.37947	-0.27393	0.48358
O	-2.33783	-0.83293	0.12976
C	0.62192	-0.09553	-2.28836
C	2.65657	1.82838	-1.15185
C	2.26168	-0.47542	3.28891
C	0.65646	-2.68697	1.95657
C	-0.29954	2.18008	0.40777
O	-0.57694	3.24065	0.02431
C	-0.43088	0.92414	2.65301
O	-0.82801	1.18037	3.71728
Li	4.36778	0.72074	-1.66053
H	2.8795	1.46433	1.53466
H	2.18037	-2.14689	-0.62587
H	0.42096	-2.21344	-0.67472
H	0.32785	0.92544	-2.55101
H	1.3833	-0.41453	-3.02463
H	-0.25036	-0.74167	-2.43511
H	2.98845	2.70741	-0.59322
H	2.17665	2.08613	-2.0954
H	2.51809	0.52646	3.64486
H	1.45194	-0.85284	3.91636
H	3.12998	-1.12786	3.45319
H	0.42024	-2.4766	3.00248
H	-0.24873	-3.09004	1.49006
H	1.40866	-3.4928	1.94168
N	5.3418	0.22754	-3.44818
N	5.9521	-0.13961	-0.60396
C	6.99319	-0.28817	-1.64315
C	6.40243	-0.69915	-2.99697
C	4.49195	-0.4	-4.47582
C	5.90123	1.48833	-3.96971
H	7.21536	-0.77288	-3.7398
H	5.9592	-1.69671	-2.91908
H	7.50696	0.6737	-1.73958
H	7.75889	-1.02456	-1.34447
C	5.48758	-1.44732	-0.10202
C	6.43735	0.67819	0.52184

H	3.68934	0.28764	-4.75409
H	5.06308	-0.65893	-5.38289
H	4.03693	-1.3113	-4.07813
H	5.0849	2.1615	-4.24385
H	6.50745	1.98793	-3.2095
H	6.53161	1.31807	-4.85861
H	4.68064	-1.2925	0.61787
H	5.09261	-2.05815	-0.91792
H	6.3027	-2.00685	0.38667
H	5.63247	0.80419	1.25007
H	7.30044	0.21466	1.02795
H	6.73373	1.66806	0.16298

Compound 7 in position C9 in conformation cis

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SCF Done: E(RB+HF-LYP) = -2235.84932393 A.U. after 23 cycles

6	1.63664	-0.98365	0.99891
6	0.71186	-1.48033	0.05499
6	-0.18679	-0.46388	-0.62422
6	-0.71058	0.4373	0.48867
6	0.31291	1.16289	1.22819
6	1.38262	0.26358	1.64227
25	-0.28685	-1.09681	2.02864
6	-1.03677	-0.16852	3.3104
8	-1.49591	0.59892	4.09006
6	0.90577	-2.80282	-0.64985
6	-2.01847	1.136	0.19996
6	0.20321	2.4708	1.71613
1	2.1176	0.62487	2.35693
6	2.88229	-1.7473	1.39928
6	0.36369	-2.36357	3.15416
8	0.74322	-3.1704	3.90186
6	-1.7279	-2.03703	1.50156
8	-2.66667	-2.61338	1.12789
3	-0.87494	2.47916	3.6493
7	0.06186	3.16579	5.43853
6	1.12342	4.13997	5.13608
6	-1.0823	3.79896	6.12707
6	-1.9586	4.61504	5.17165
7	-2.50679	3.79386	4.07132
6	-2.90656	4.63935	2.93413
6	0.61342	2.06495	6.24756
6	-3.65783	2.98957	4.52075
1	0.32851	0.08249	-1.44245
1	-1.03288	-0.98341	-1.08852
1	-2.43917	1.60652	1.09655
1	-1.8968	1.93104	-0.55609
1	-2.76217	0.43085	-0.18694
1	1.10211	2.92382	2.13591
1	-0.47483	3.15521	1.20933
1	3.26044	-1.40763	2.36776
1	2.71834	-2.8248	1.46238
1	3.6684	-1.5787	0.65188
1	1.38363	-3.56086	-0.02413
1	-0.0574	-3.20644	-0.97887
1	1.52573	-2.67664	-1.55171
1	-0.74226	4.45096	6.95121
1	-1.67692	3.0012	6.58261
1	-2.76527	5.10133	5.74768

1	-1.36685	5.42015	4.72502
1	-4.00774	2.36226	3.69756
1	-3.36901	2.32561	5.33737
1	-4.49087	3.62921	4.85881
1	-3.28037	4.00732	2.12445
1	-3.6974	5.3577	3.20958
1	-2.04198	5.19485	2.56059
1	1.4377	1.59249	5.70664
1	0.9931	2.41866	7.2212
1	-0.1563	1.30895	6.41847
1	1.93049	3.64048	4.59453
1	0.7446	4.94335	4.49984
1	1.53998	4.58856	6.05459

Compound 7 in position C3

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SCF Done: E(RB+HF-LYP) = -2235.83540556 A.U. after 25 cycles

C	0.19828	-1.46407	-0.13478
C	1.1534	-0.52642	-0.84328
C	2.27911	-0.07553	-0.11193
C	2.28029	0.00452	1.33172
C	1.02387	-0.35956	1.95214
C	-0.08606	-0.81617	1.20392
Mn	0.62266	1.22094	0.49156
C	-0.92894	1.35204	-0.39367
O	-1.93762	1.40115	-0.97316
C	1.10902	-0.55902	-2.3547
C	3.53004	0.3742	-0.85015
C	0.90477	-0.21115	3.46106
C	-1.42391	-1.14767	1.8264
C	1.4304	2.59642	-0.33332
O	1.95184	3.49713	-0.86061
C	0.18952	2.32202	1.84199
O	-0.07606	3.04884	2.7159
Li	3.77699	0.89881	2.39796
H	0.59699	-2.49555	-0.03817
H	-0.73172	-1.5467	-0.70926
H	1.64395	0.27029	-2.82317
H	1.54834	-1.49583	-2.73404
H	0.07324	-0.52708	-2.70941
H	4.16673	0.98104	-0.19872
H	4.10982	-0.50649	-1.15927
H	3.32804	0.95793	-1.75176
H	1.69998	0.43106	3.85278
H	-0.04877	0.20944	3.78984
H	1.00563	-1.196	3.93758
H	-1.68494	-0.50204	2.66804
H	-2.22519	-1.06448	1.08436
H	-1.43206	-2.18821	2.18926
N	4.4943	2.83294	2.88971
N	5.3362	0.11242	3.59366
C	5.82533	1.29012	4.33926
C	5.81974	2.5605	3.4815
C	4.60732	3.77214	1.75885
C	3.55104	3.37389	3.88704
H	6.17038	3.40964	4.09429
H	6.53491	2.45488	2.65941
H	5.17205	1.42721	5.20648
H	6.84295	1.12469	4.73489
C	6.3438	-0.40162	2.65073

C	4.91735	-0.96279	4.50693
H	3.62449	3.92681	1.30986
H	5.00975	4.74923	2.07507
H	5.2684	3.35563	0.99333
H	2.57672	3.53496	3.42065
H	3.4146	2.6704	4.71284
H	3.90696	4.33122	4.3042
H	5.91618	-1.23174	2.08253
H	6.64134	0.37384	1.94021
H	7.24842	-0.75829	3.17255
H	4.50716	-1.79218	3.92507
H	5.75631	-1.33963	5.11652
H	4.13507	-0.59829	5.17854