Supplementary Material (ESI) for Organic and Biomolecular Chemistry

SUPPORTING INFORMATION

Reaction of [60]Fullerene with *trans*-Epoxides: A Theoretical Study

Guan-Wu Wang,*[†,‡] Ping Wu,[†] and Hai-Tao Yang[†]

[†] *Hefei National Laboratory for Physical Sciences at Microscale and Department of Chemistry, University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China*

[‡] *State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou, Gansu 730000, People's Republic of China*

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1. Computational details: General

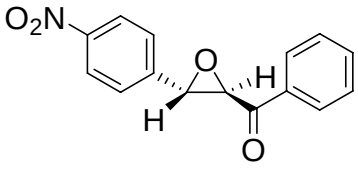
All calculations were done with the help of Gaussian 03, Revision B.03. All structures were checked by a vibrational analysis. All transition-state structures were found by using the route of "# AM1 opt = (calcfc, ts, noeigentest) freq=noraman", or "# PM3 opt = (calcfc, ts, noeigentest) freq=noraman", "# B3LYP/6-31G* opt = (calcfc, ts, noeigentest) freq=noraman".

For the reaction of C_{60} with **1a** at the AM1 level, the starting point for the TS (TS1) searching for the ring opening of epoxide **1a** was the highest energy point in the potential energy scan (by increasing the bond length of the cleaving C–C bond of epoxide **1a**). For the TS (TS2) of isomerization of INT1 to INT2, the starting point was also the highest energy point in the potential energy scan (by rotation of the C–O bond in the Ar–CH=O–CH–COAr' system). For each TS (TS3 or TS4) of the cycloaddition to C_{60}, the bond-forming lengths of the starting point were obtained from the corresponding bond lengths of the TS for the reaction of **1a** with ethylene. The starting points of other TSs for the reaction of C_{60} with **1b**, **1b** and **3a-c** were obtained in the same way as for the reaction of C_{60} with **1a**. The start points of transition states calculated at the levels of PM3 and B3LYP/6-31G* were got from the AM1 results.

All transition states have been analyzed by IRC. The first and last points in IRC were read out and optimized to the expected structures. Computational total energies were given in a.u.

2. Results for the reaction of **1a** with C_{60}

2.1 IRCs calculated at the AM1 level



trans-**1a**

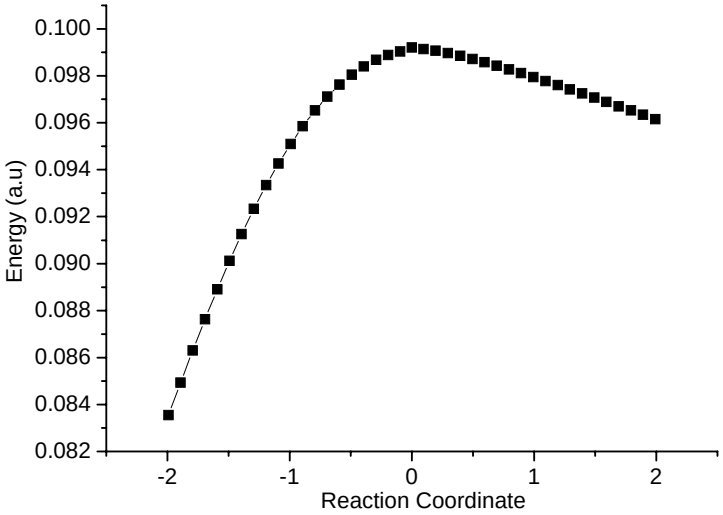


Figure S1. IRC for TS1 of the reaction of C_{60} with **1a** at the AM1 level.

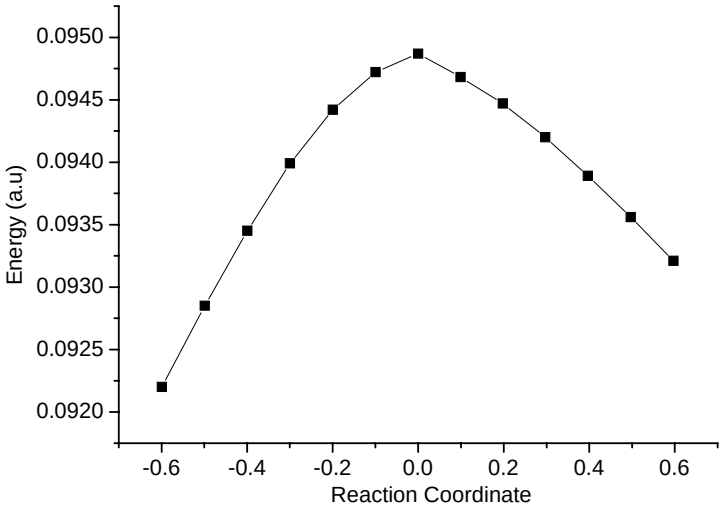


Figure S2. IRC for TS2 of reaction of C_{60} with **1a** at the AM1 level.

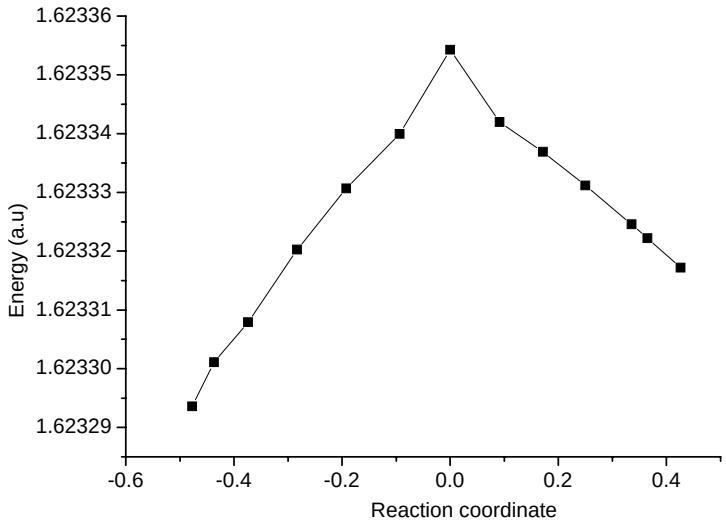


Figure S3. IRC for TS3 of the reaction of C_{60} with **1a** at the AM1 level.

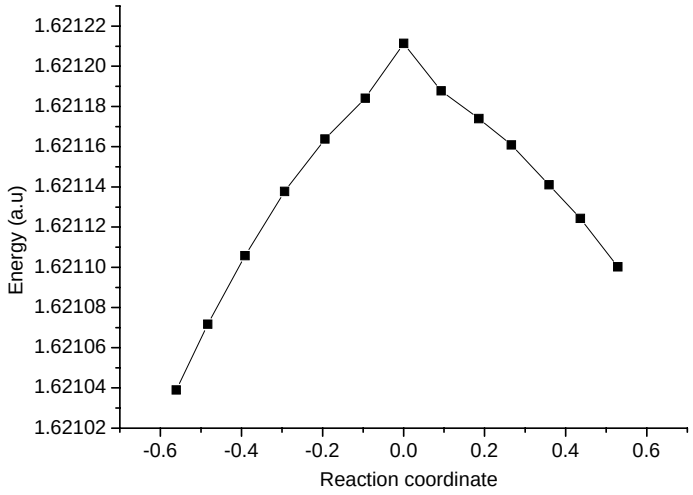


Figure S4. IRC for TS4 of the reaction of C_{60} with **1a** at the AM1 level.

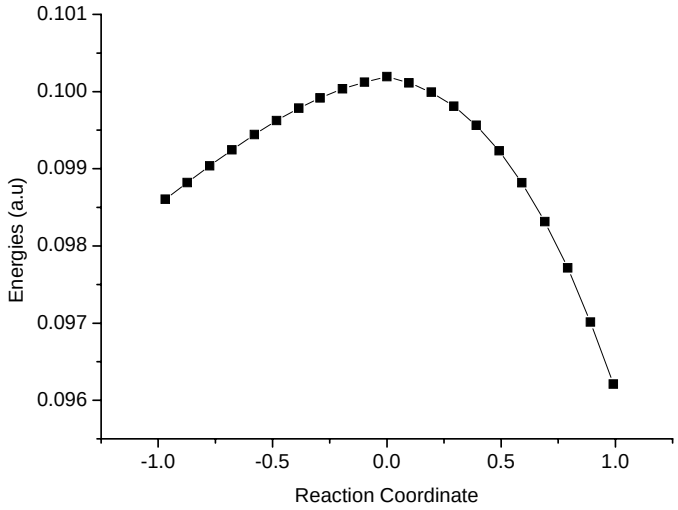


Figure S5. IRC for TS1' of the reaction of C_{60} with **1a** at the AM1 level.

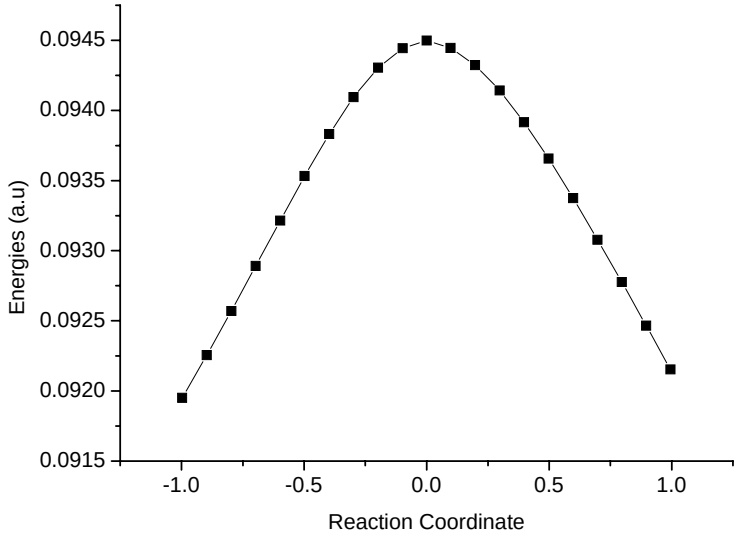


Figure S6. IRC for TS2' of the reaction of C_{60} with **1a** at the AM1 level.

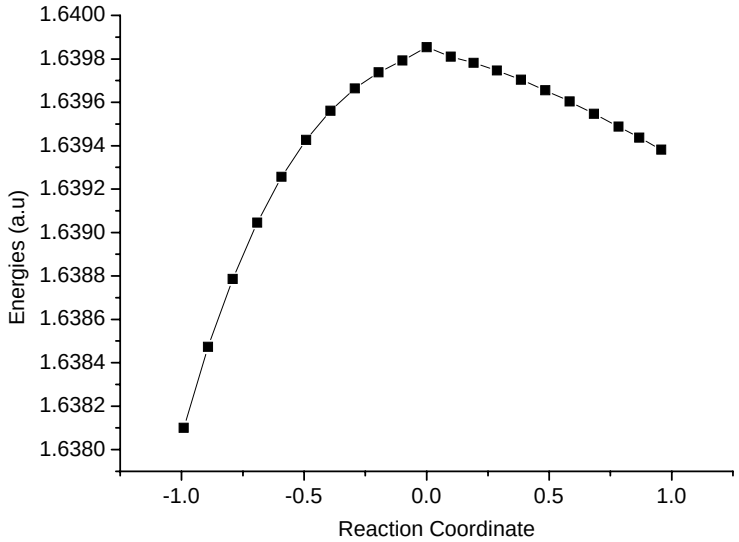


Figure S7. IRC for TS3’ of the reaction of C_{60} with **1a** at the AM1 level.

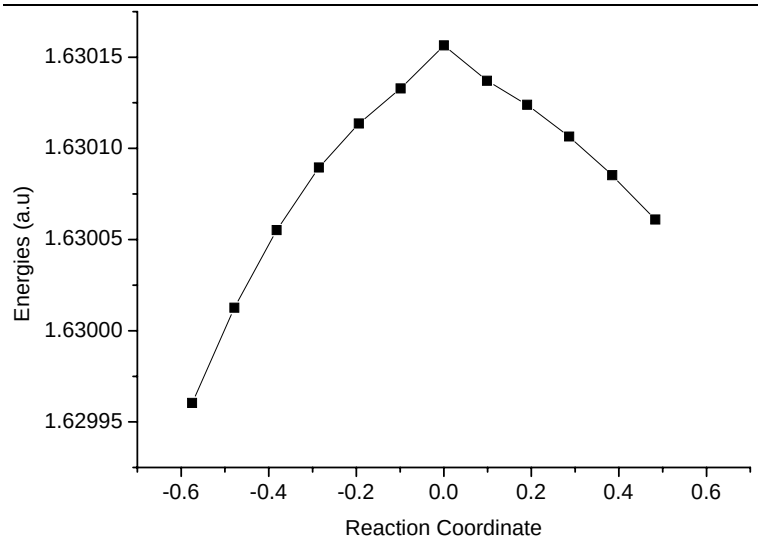


Figure S8. IRC for TS4' of the reaction of C_{60} with **1a** at the AM1 level.

2.2 IRCs calculated at the PM3 level

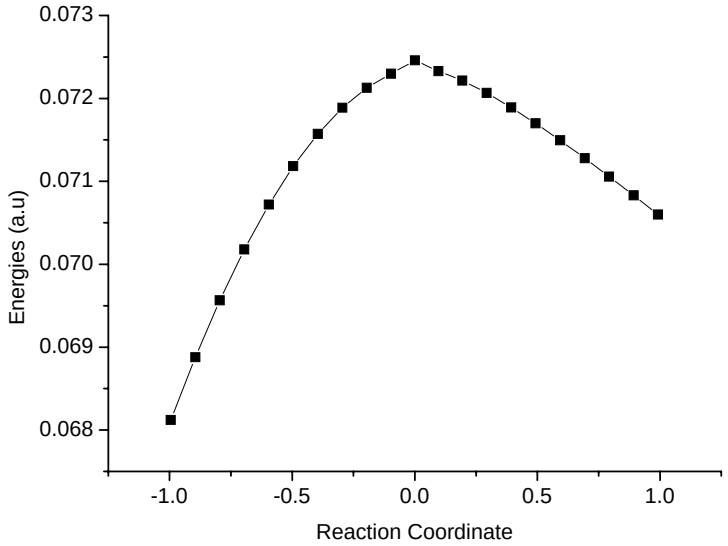


Figure S9. IRC for TS1 of the reaction of C_{60} with **1a** at the PM3 level.

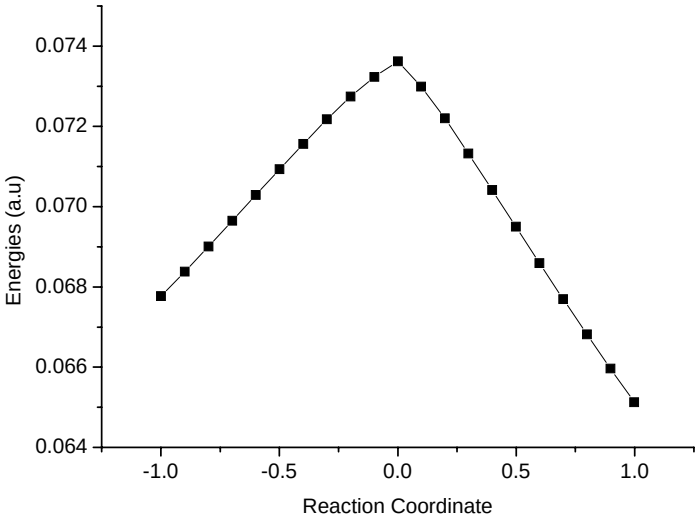


Figure S10. IRC for TS2 of reaction of C_{60} with **1a** at the PM3 level.

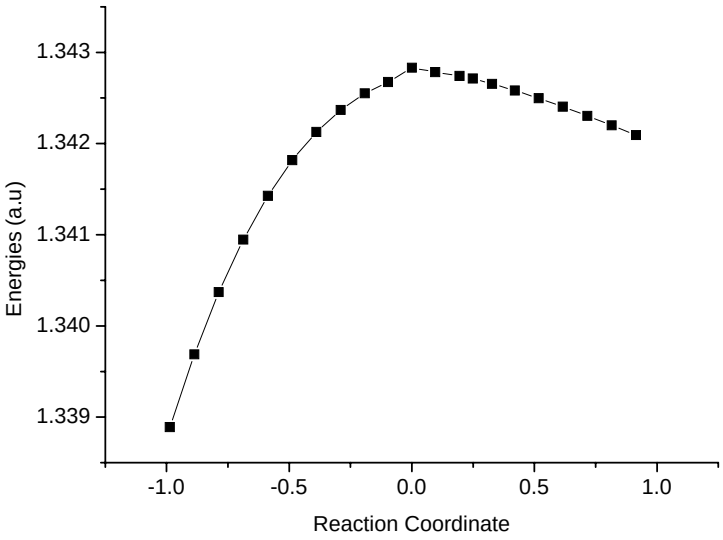


Figure S11. IRC for TS3 of reaction of C_{60} with **1a** at the PM3 level.

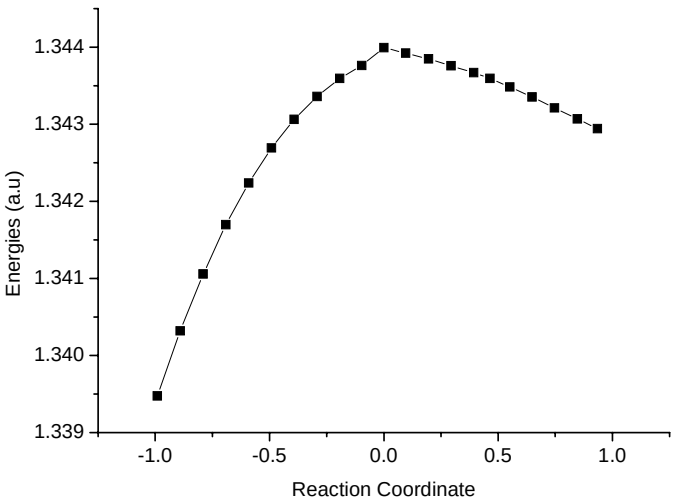


Figure S12. IRC for TS4 of reaction of C_{60} with **1a** at the PM3 level.

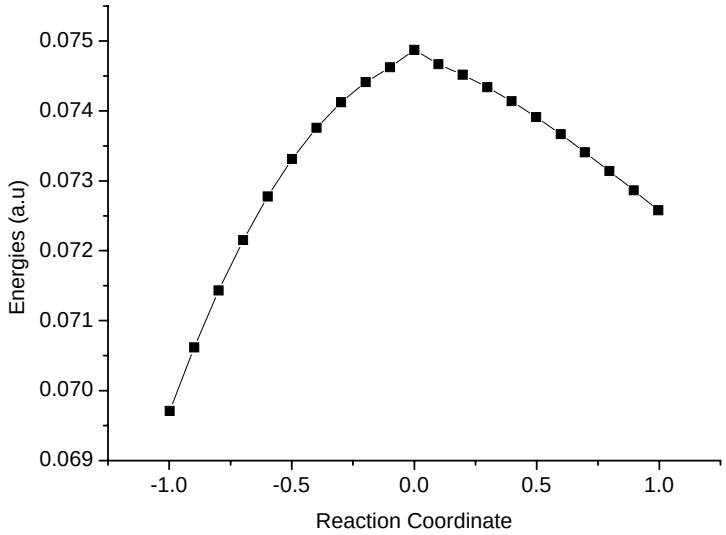


Figure S13. IRC for TS1' of the reaction of C_{60} with **1a** at the PM3 level.

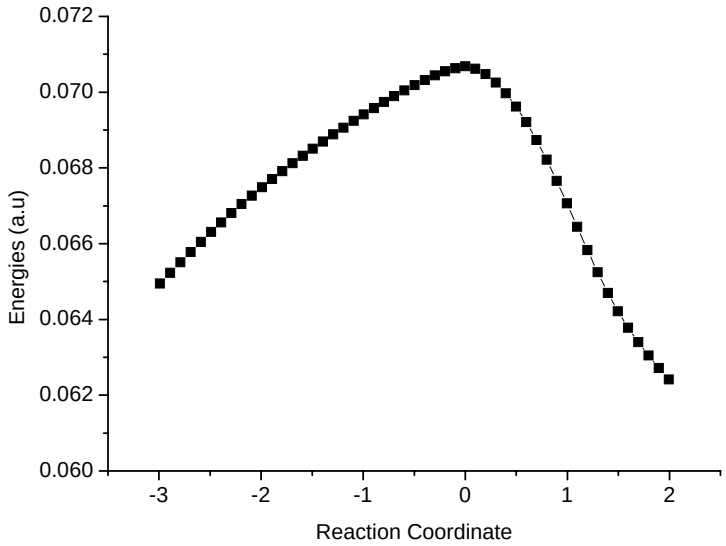


Figure S14. IRC for TS2' of the reaction of C_{60} with **1a** at the PM3 level.

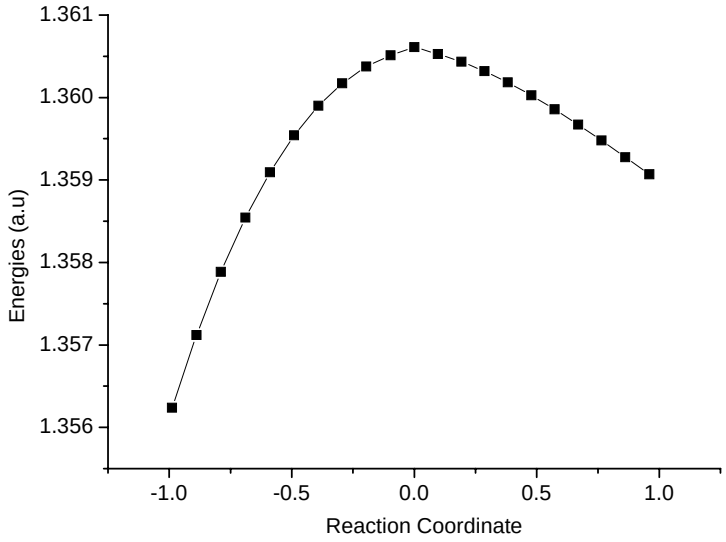


Figure S15. IRC for TS3' of the reaction of C_{60} with **1a** at the PM3 level.

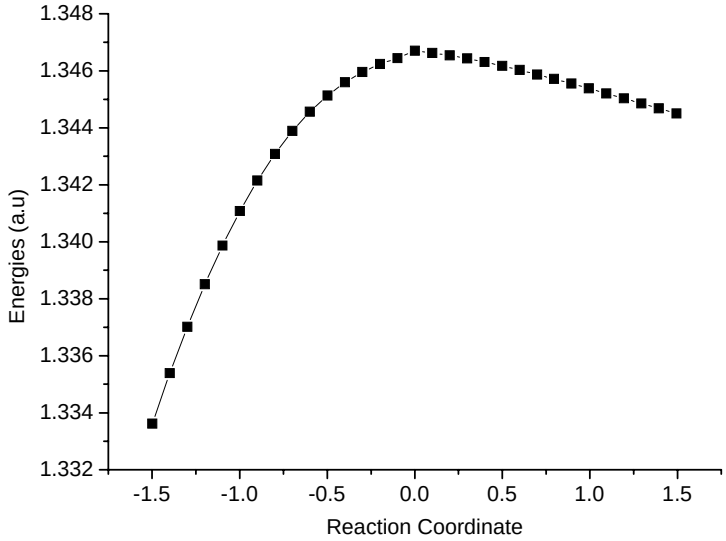


Figure S16. IRC for TS4' of the reaction of C_{60} with **1a** at the PM3 level.

2.3 IRCs calculated at the B3LYP/6-31G* level

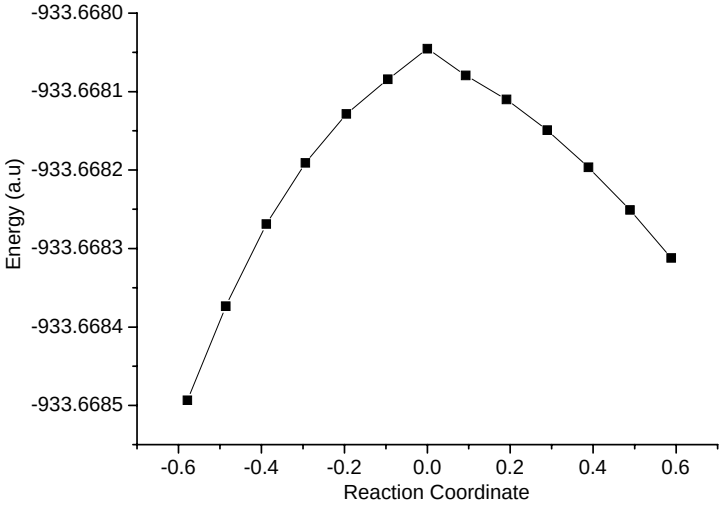


Figure S17. IRC for TS1 of **1a** at the B3LYP/6-31G* level.

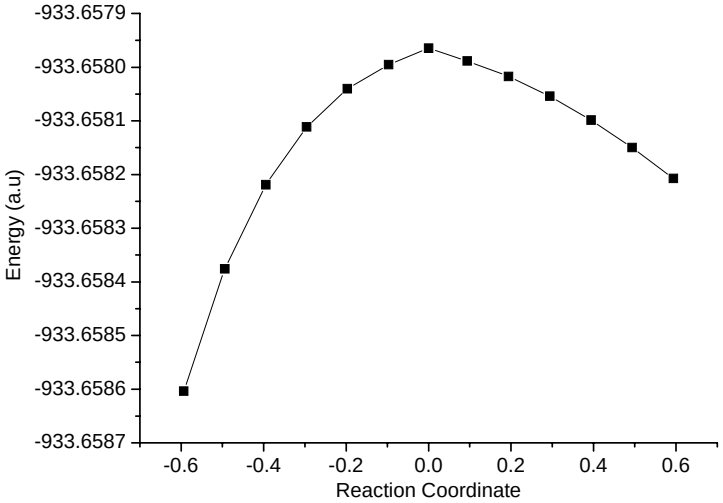


Figure S18. IRC for TS2 of **1a** at the B3LYP/6-31G* level.

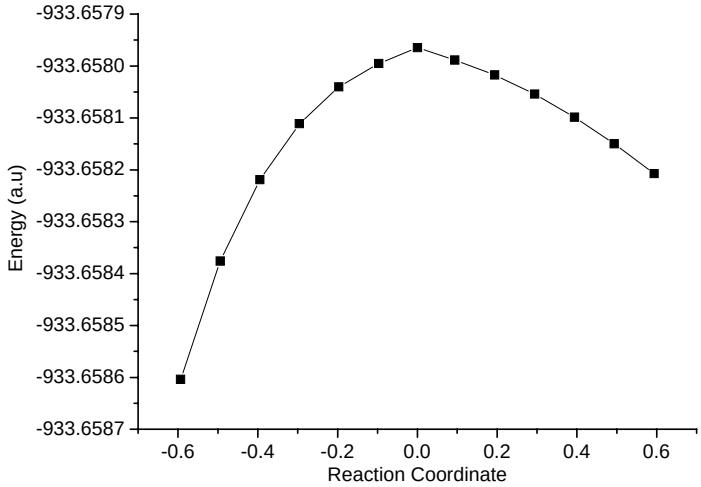


Figure S19. IRC for TS1' of **1a** at the B3LYP/6-31G* level.

2.4 FMO for C_{60} and carbonyl ylide generated from **1a** at the B3LYP/6-31G*//PM3 level

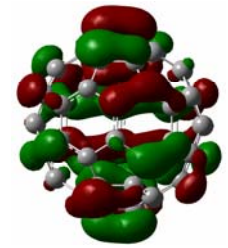
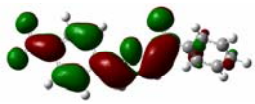
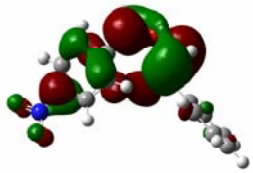
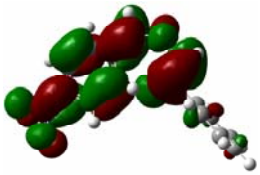
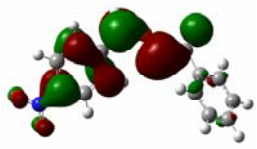
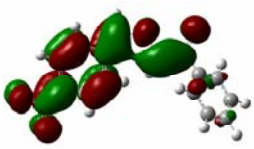
HOMO	LUMO	HOMO	LUMO
			
C_{60}	C_{60}	INT1	INT1
			
INT2	INT2	INT1'	INT1'
			
INT2'	INT2'		

Figure S20. FMO orbital for C_{60} and carbonyl ylide generated from **1a** at the B3LYP/6-31G*//PM3 level.

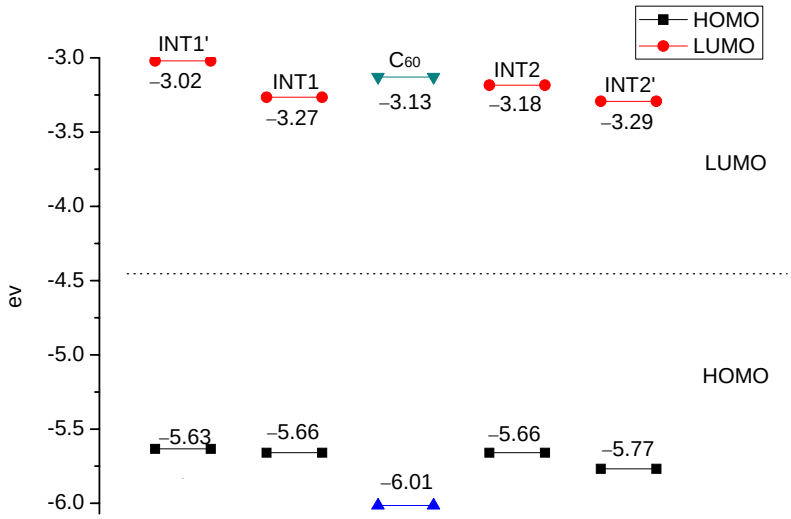


Figure S21. FMO orbital scheme for C_{60} and carbonyl ylide generated from **1a** at the B3LYP/6-31G*//PM3 level.

2.5 Cartesian coordinates for the reaction of **1a** with C_{60} at the AM1 level

C_{60}

-AM1-

C	0.373809	1.522199	-3.192788
C	-0.144826	2.630694	-2.389527
C	0.645432	3.202519	-1.406751
C	1.999493	2.698572	-1.171029
C	2.490034	1.650065	-1.930836
C	1.654576	1.045517	-2.969838
C	-0.724649	0.584747	-3.432735
C	-1.922137	1.113849	-2.777760
C	-1.563802	2.378321	-2.133006
C	-2.115766	2.711379	-0.907571
C	0.061884	3.554619	-0.111196
C	2.252788	2.739223	0.270209
C	2.982972	1.729213	0.873592
C	3.501633	0.620773	0.070265
C	3.262038	0.582333	-1.292975
C	2.903713	-0.682119	-1.937779
C	1.910299	-0.395817	-2.974173
C	0.871328	-1.282567	-3.201171
C	-0.482883	-0.77865	-3.436745
C	-2.813062	0.250925	-2.162201
C	-2.557473	-1.19045	-2.166399
C	-1.424772	-1.690927	-2.785938
C	-0.652844	-2.75871	-2.147996
C	0.766327	-2.506354	-2.404764

C	1.705985	-2.777171	-1.424446
C	2.804379	-1.839677	-1.184451
C	3.057688	-1.799026	0.256803
C	3.396620	-0.603015	0.866721
C	1.055314	3.268279	0.925228
C	0.724595	-0.584773	3.432787
C	0.482798	0.778609	3.436850
C	-0.871256	1.282539	3.201114
C	-1.910234	0.395784	2.974130
C	-1.654604	-1.045591	2.969896
C	0.144802	-2.630678	2.389468
C	1.563784	-2.378285	2.132965
C	1.922129	-1.113852	2.777765
C	2.813049	-0.250901	2.162238
C	2.557429	1.190531	2.166504
C	1.424743	1.690979	2.786098
C	-0.766226	2.506291	2.404661
C	-1.705844	2.777119	1.424339
C	-2.804306	1.839658	1.184359
C	-2.903654	0.682113	1.937722
C	-3.262029	-0.582309	1.292963
C	-2.490093	-1.650095	1.930846
C	-1.999534	-2.698562	1.170990
C	-0.645406	-3.202448	1.406647
C	2.115764	-2.711335	0.907512
C	1.280336	-3.315829	-0.131538
C	-0.061845	-3.554560	0.111085
C	-1.055397	-3.268231	-0.925031
C	-2.252851	-2.739222	-0.270240
C	-2.983015	-1.729219	-0.873609
C	-3.501666	-0.620770	-0.070283
C	-3.396632	0.602977	-0.866706
C	-3.057644	1.798990	-0.256822
C	0.652804	2.758712	2.148200
C	-1.280276	3.315854	0.131470
C	-0.373817	-1.522237	3.192877

Energy = 1.549591029779
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -2286.18057840

trans-epoxide (**1a**)
-AM1-

C	5.962140	-1.202552	-0.652405

C	4.831342	-1.869919	-0.179295
C	3.659688	-1.162642	0.081905
C	3.616336	0.221934	-0.127042
C	4.757841	0.890497	-0.591392
C	5.924733	0.176856	-0.857458
C	2.392273	0.993080	0.149129
O	2.387421	2.217133	0.314546
C	1.109847	0.213195	0.167917
O	0.765557	-0.425271	1.406839
C	-0.052379	0.681533	0.983169
C	-1.440397	0.382625	0.589200
C	-1.979429	-0.899349	0.746330
C	-3.297342	-1.160686	0.381916
C	-4.078783	-0.121429	-0.147802
C	-3.549733	1.169929	-0.307329
C	-2.231460	1.413838	0.065780
H	0.065947	1.592502	1.610444
H	-1.353057	-1.703238	1.167364
H	-1.810091	2.424785	-0.052164
H	-3.723150	-2.171063	0.508025
H	-4.173188	1.980597	-0.722444
H	0.955563	-0.418796	-0.730432
H	2.771611	-1.689041	0.468019
H	4.720977	1.982233	-0.737838
H	4.864035	-2.956380	-0.009477
H	6.817352	0.704231	-1.225481
H	6.884858	-1.764951	-0.860888
N	-5.486452	-0.390821	-0.544066
O	-5.926724	-1.500761	-0.407331
O	-6.146723	0.508075	-0.991853

Energy = 0.034458273169
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -933.719323724

TS1
-AM1-

C	-2.548177	-1.188428	1.000632
C	-1.688274	-0.740121	-0.020196
C	-2.162665	0.183010	-0.968308
C	-3.469671	0.654330	-0.904763
C	-4.313536	0.198267	0.120378
C	-3.856140	-0.727415	1.074597
C	-0.345938	-1.247030	-0.077006

O	0.465384	-0.875711	-1.116884
C	1.484036	-0.326111	-0.358950
C	2.803400	-0.930055	-0.450651
O	2.966040	-2.112220	-0.794443
N	-5.711330	0.700356	0.198893
O	-6.424416	0.297018	1.078066
C	3.935060	-0.058269	-0.067615
C	3.869475	1.331056	-0.226159
C	4.954282	2.126742	0.138207
C	6.107438	1.541912	0.662758
C	6.180057	0.157145	0.814610
C	5.100475	-0.643230	0.445718
O	-6.088812	1.496865	-0.617773
H	0.043133	-1.975071	0.648006
H	-1.491260	0.525982	-1.772869
H	-2.183911	-1.915074	1.743844
H	-3.840476	1.377417	-1.652216
H	-4.530873	-1.081154	1.873682
H	1.262935	0.584544	0.203183
H	2.968391	1.797005	-0.653519
H	5.153440	-1.739419	0.544953
H	4.900950	3.217748	0.008540
H	7.091532	-0.305934	1.220723
H	6.960959	2.173033	0.952169

Energy = 0.099198161008
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -933.660962908

INT1
-AM1-

C	-2.673461	1.374727	0.664426
C	-1.786597	0.526930	-0.020167
C	-2.272182	-0.606697	-0.688835
C	-3.636060	-0.894029	-0.684058
C	-4.511108	-0.035916	-0.002150
C	-4.036842	1.099324	0.676600
C	-0.366189	0.832659	0.000662
O	0.446374	0.086433	-0.693876
C	1.798339	0.415705	-0.695296
C	2.588713	-0.259416	0.262097
O	2.083145	-0.934603	1.193296
C	4.060207	-0.136943	0.116174
C	4.656243	0.997794	-0.443582

C	6.043516	1.073085	-0.564502
C	6.843332	0.016869	-0.129396
C	6.254296	-1.114617	0.435404
C	4.868878	-1.191130	0.562548
H	0.010724	1.700818	0.578500
H	-1.567348	-1.276171	-1.213751
H	-2.293174	2.261003	1.198541
H	-4.020850	-1.787276	-1.208427
H	-4.738439	1.762368	1.213733
H	2.076378	1.147697	-1.443865
H	4.033045	1.837768	-0.783655
H	4.391607	-2.072184	1.020630
H	6.506659	1.968161	-1.004079
H	6.883290	-1.946570	0.783903
H	7.936732	0.077083	-0.228975
N	-5.974857	-0.333188	0.005223
O	-6.709156	0.409940	0.596064
O	-6.368005	-1.303076	-0.581568

Energy = 0.067884117679
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -933.682404283

TS2
-AM1-

C	-2.673461	1.374727	0.664426
C	-1.786597	0.526930	-0.020167
C	-2.272182	-0.606697	-0.688835
C	-3.636060	-0.894029	-0.684058
C	-4.511108	-0.035916	-0.002150
C	-4.036842	1.099324	0.676600
C	-0.366189	0.832659	0.000662
O	0.446374	0.086433	-0.693876
C	1.798339	0.415705	-0.695296
C	2.588713	-0.259416	0.262097
O	2.083145	-0.934603	1.193296
C	4.060207	-0.136943	0.116174
C	4.656243	0.997794	-0.443582
C	6.043516	1.073085	-0.564502
C	6.843332	0.016869	-0.129396
C	6.254296	-1.114617	0.435404
C	4.868878	-1.191130	0.562548
H	0.010724	1.700818	0.578500
H	-1.567348	-1.276171	-1.213751

H	-2.293174	2.261003	1.198541
H	-4.020850	-1.787276	-1.208427
H	-4.738439	1.762368	1.213733
H	2.076378	1.147697	-1.443865
H	4.033045	1.837768	-0.783655
H	4.391607	-2.072184	1.020630
H	6.506659	1.968161	-1.004079
H	6.883290	-1.946570	0.783903
H	7.936732	0.077083	-0.228975
N	-5.974857	-0.333188	0.005223
O	-6.709156	0.409940	0.596064
O	-6.368005	-1.303076	-0.581568

Energy = 0.094868123519
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -933.645017927

INT2
-AM1-

C	0.315689	0.388330	0.059454
C	-1.749459	-0.707944	-0.154194
O	-0.410905	-0.692528	-0.156791
H	-0.143736	1.369460	0.254082
C	1.748973	0.208826	0.030656
C	2.347597	-1.037643	-0.214733
C	2.560708	1.335904	0.257761
C	3.732043	-1.165872	-0.234522
H	1.714583	-1.921279	-0.393456
C	3.945044	1.221723	0.240753
H	2.096444	2.316219	0.450343
C	4.529287	-0.032693	-0.005984
H	4.200178	-2.146790	-0.427643
H	4.581411	2.106161	0.418899
H	-2.101840	-1.725783	-0.373743
C	-2.621327	0.415402	0.050768
O	-2.207868	1.582704	0.215777
C	-4.069789	0.110088	0.029623
C	-4.568752	-1.106015	0.510374
C	-4.956018	1.074772	-0.468215
C	-5.939298	-1.358543	0.479832
H	-3.884184	-1.859632	0.928149
C	-6.324693	0.814769	-0.502796
H	-4.557846	2.039160	-0.822092
C	-6.817241	-0.401977	-0.030740

H	-6.328211	-2.313919	0.861772
H	-7.016193	1.572984	-0.899030
H	-7.898007	-0.605960	-0.056902
N	6.009821	-0.160940	-0.025224
O	6.680753	0.816629	0.171423
O	6.497028	-1.239155	-0.236913

Energy = 0.062380906394
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -933.692079044

TS1'
-AM1-

C	2.085631	1.098398	1.179992
C	1.342495	1.305847	0.002869
C	1.726654	0.645153	-1.178437
C	2.831555	-0.195763	-1.194063
C	3.561853	-0.391824	-0.009267
C	3.189839	0.253694	1.181045
C	0.256051	2.251251	0.036197
O	-0.645496	2.381205	-0.984322
C	-1.270916	1.148243	-0.847949
C	-2.084682	0.901272	0.325912
O	-1.863201	1.465824	1.415460
N	4.742633	-1.295217	-0.016904
O	5.362679	-1.449481	1.000886
C	-3.180715	-0.074828	0.155856
C	-3.800950	-0.267440	-1.084386
C	-4.834114	-1.194534	-1.210418
C	-5.252603	-1.932805	-0.102875
C	-4.643049	-1.737367	1.136570
C	-3.613607	-0.807524	1.269544
O	5.045323	-1.846642	-1.040955
H	0.130698	2.966530	0.863637
H	1.142629	0.803652	-2.099528
H	1.786383	1.604911	2.111768
H	3.133864	-0.706240	-2.125082
H	3.767541	0.090009	2.107615
H	-1.248814	0.521748	-1.740654
H	-3.485319	0.322513	-1.958542
H	-3.135974	-0.633319	2.247081
H	-5.321434	-1.341413	-2.185584
H	-4.976816	-2.313635	2.012163
H	-6.066290	-2.666129	-0.206634

Energy = 0.1001932
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -933.6501776

INT1'
-AM1-

C	2.643066	1.703834	0.614649
C	1.413536	1.602103	-0.071943
C	1.123912	0.428605	-0.783259
C	2.033495	-0.628039	-0.815002
C	3.244541	-0.511012	-0.121160
C	3.552508	0.658150	0.600438
C	0.558171	2.753718	-0.086349
O	-0.731553	2.880614	-0.295103
C	-1.671577	1.929888	-0.331161
C	-1.656598	0.665582	0.347784
O	-0.712060	0.292084	1.073818
N	4.218596	-1.633638	-0.143891
O	5.247364	-1.523885	0.468310
C	-2.876702	-0.157902	0.185951
C	-3.627092	-0.130210	-0.995237
C	-4.766174	-0.924290	-1.117114
C	-5.163031	-1.747187	-0.062605
C	-4.414110	-1.782815	1.113695
C	-3.271127	-0.995189	1.238166
O	3.955362	-2.620247	-0.777951
H	0.998484	3.758694	0.082398
H	0.172463	0.337159	-1.330573
H	2.877880	2.620063	1.178461
H	1.795276	-1.548763	-1.375240
H	4.506507	0.735591	1.149790
H	-2.575585	2.339864	-0.807651
H	-3.313922	0.508101	-1.835251
H	-2.663080	-1.026774	2.156592
H	-5.351590	-0.902332	-2.048032
H	-4.722051	-2.435742	1.943734
H	-6.064360	-2.370326	-0.160696

Energy = 0.0758585
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -933.6749156

TS2'
-AM1-

C	2.847413	1.717964	-0.621479
C	1.563315	1.562682	-0.069161
C	1.211061	0.365301	0.565069
C	2.130320	-0.683591	0.640292
C	3.398694	-0.523773	0.068807
C	3.765250	0.677198	-0.565494
C	0.636872	2.677240	-0.137804
O	-0.635505	2.662221	-0.379592
C	-1.349980	1.509812	-0.657920
C	-2.047100	0.919381	0.418562
O	-1.800118	1.204223	1.619297
N	4.384644	-1.642414	0.134818
O	5.466186	-1.486388	-0.363283
C	-3.093448	-0.073059	0.070744
C	-3.011704	-0.864664	-1.079545
C	-4.019105	-1.784167	-1.369947
C	-5.113913	-1.917435	-0.516470
C	-5.197660	-1.134059	0.634826
C	-4.190367	-0.218152	0.931276
O	4.066307	-2.661389	0.682657
H	1.035271	3.709378	-0.004098
H	0.207736	0.255285	1.025018
H	3.129025	2.663556	-1.111722
H	1.852657	-1.627643	1.143242
H	4.770762	0.789821	-1.007774
H	-1.338444	1.232361	-1.707015
H	-2.149742	-0.769804	-1.756113
H	-4.237036	0.396601	1.844474
H	-3.948890	-2.404957	-2.274805
H	-6.057920	-1.240417	1.311596
H	-5.908763	-2.640681	-0.749686

Energy = 0.0944975
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -933.6326338

INT2'
-AM1-

C	-2.822999	1.669179	0.750778
C	-1.636117	1.468692	0.018955
C	-1.514654	0.325211	-0.786435
C	-2.540668	-0.612674	-0.849184
C	-3.706687	-0.407763	-0.095979
C	-3.853180	0.739762	0.703036

C	-0.627482	2.491881	0.072955
O	0.680840	2.351278	0.016877
C	1.304726	1.174724	0.042962
C	2.751879	1.249247	-0.118990
O	3.342107	2.301801	-0.405031
N	-4.801481	-1.411229	-0.147089
O	-5.799551	-1.215562	0.493230
C	3.461411	-0.037780	0.050239
C	3.025876	-0.997457	0.971151
C	3.722940	-2.196493	1.110635
C	4.853888	-2.444370	0.331995
C	5.295530	-1.486772	-0.581200
C	4.606565	-0.283220	-0.719285
O	-4.659046	-2.392364	-0.826532
H	-0.894498	3.558375	0.178127
H	-0.615081	0.177822	-1.405888
H	-2.933033	2.571467	1.372664
H	-2.439475	-1.507718	-1.487789
H	-4.777481	0.896686	1.286076
H	0.757121	0.241139	0.184441
H	2.143150	-0.802461	1.598820
H	4.957087	0.487231	-1.424644
H	3.380647	-2.947008	1.838368
H	6.191422	-1.677680	-1.190427
H	5.399541	-3.393472	0.441723

Energy = 0.0702591
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -933.6717711

TS3
-AM1-

C	-1.250298	-0.771331	1.786130
C	-0.835419	0.585152	2.151201
C	-0.850854	1.590744	1.201400
C	-1.305540	1.316303	-0.167600
C	-1.698139	0.023910	-0.515279
C	-1.655147	-1.043052	0.491455
C	-0.388281	-1.714823	2.498808
C	0.559149	-0.943121	3.304997
C	0.282496	0.478105	3.089560
C	1.327531	1.384729	3.029279
C	0.255480	2.545407	1.135930
C	-0.439648	2.079092	-1.077515

C	-0.035613	1.535738	-2.283756
C	-0.450381	0.178909	-2.649382
C	-1.244787	-0.555015	-1.786677
C	-0.965232	-1.974454	-1.571588
C	-1.219126	-2.276226	-0.163184
C	-0.405644	-3.172061	0.510499
C	0.022079	-2.883518	1.879406
C	1.865053	-1.380903	3.447080
C	2.298797	-2.615818	2.791184
C	1.402797	-3.346383	2.029195
C	1.827721	-3.922570	0.752220
C	0.709564	-3.815292	-0.186598
C	0.949758	-3.529855	-1.519892
C	0.088576	-2.584151	-2.232077
C	0.927069	-1.806730	-3.144366
C	0.664734	-0.461887	-3.346382
C	0.509581	2.847135	-0.272578
C	4.022965	0.831230	-2.466069
C	3.613475	1.999279	-1.845390
C	4.041996	2.289657	-0.475999
C	4.857188	1.396308	0.198423
C	5.290370	0.161622	-0.457999
C	4.470332	-1.468634	-2.118475
C	3.352077	-1.362271	-3.057081
C	3.075086	0.059223	-3.271583
C	1.768918	0.496774	-3.412428
C	1.335411	1.730899	-2.755619
C	2.232468	2.461545	-1.994369
C	2.925794	2.931056	0.220810
C	2.685428	2.645051	1.553940
C	3.547759	1.701396	2.267344
C	4.603278	1.094100	1.608142
C	4.879643	-0.327288	1.822991
C	5.304343	-0.903595	0.546087
C	4.912152	-2.185826	0.200627
C	4.483560	-2.476216	-1.168704
C	2.307893	-2.269532	-2.995544
C	2.321802	-3.334748	-1.991412
C	3.379448	-3.435193	-1.103326
C	3.125558	-3.737328	0.306463
C	4.072844	-2.965189	1.112288
C	3.670843	-2.420015	2.320018
C	4.085484	-1.064337	2.685259

C	2.969674	-0.422315	3.382099
C	2.708335	0.922213	3.179168
C	1.807321	3.035933	-0.717951
C	1.313161	2.448074	2.024589
C	4.884952	-0.113034	-1.753238
C	-4.246979	0.424136	-1.010766
C	-3.575756	2.560466	-0.451232
O	-4.279445	1.456239	-0.174015
H	-3.067633	2.677874	-1.411514
C	-3.696987	3.614470	0.554438
O	-4.257943	3.429139	1.644641
C	-3.087067	4.909906	0.186411
C	-3.077348	5.367804	-1.136128
C	-2.531336	5.703456	1.199458
C	-2.503614	6.600491	-1.443095
H	-3.536130	4.766842	-1.935520
C	-1.952548	6.931805	0.886068
H	-2.565204	5.348153	2.241956
C	-1.936422	7.380353	-0.434712
H	-2.500895	6.958868	-2.483106
H	-1.512896	7.549029	1.683643
H	-1.480630	8.351040	-0.681135
H	-3.732707	0.500076	-1.977111
C	-5.047825	-0.718891	-0.644735
C	-5.719188	-0.791861	0.587240
C	-5.151590	-1.785281	-1.557099
C	-6.482639	-1.908640	0.909757
H	-5.639957	0.043151	1.303180
C	-5.909704	-2.906510	-1.246047
H	-4.628892	-1.733998	-2.524626
C	-6.575949	-2.965901	-0.009611
H	-7.009218	-1.963599	1.878665
H	-5.990103	-3.743337	-1.961520
N	-7.389051	-4.163194	0.326776
O	-7.461764	-5.059359	-0.471250
O	-7.953055	-4.204488	1.387222

Energy = 1.623354304882
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3219.85103362

TS4
-AM1-

C	1.102983	-1.131401	-1.824032

C	0.689791	0.134744	-2.433709
C	0.780698	1.311307	-1.711514
C	1.312621	1.306394	-0.341815
C	1.702485	0.099742	0.239882
C	1.578997	-1.146665	-0.525175
C	0.184770	-2.174404	-2.281411
C	-0.796119	-1.555055	-3.174147
C	-0.483584	-0.128104	-3.267673
C	-1.507849	0.801396	-3.335384
C	-0.304291	2.290115	-1.780355
C	0.514169	2.259828	0.440081
C	0.174473	1.983026	1.751946
C	0.588510	0.717764	2.362891
C	1.318437	-0.197203	1.625149
C	1.001543	-1.622538	1.719044
C	1.163918	-2.209783	0.389488
C	0.297102	-3.199849	-0.042402
C	-0.206971	-3.181858	-1.415594
C	-2.115303	-1.975232	-3.151727
C	-2.529405	-3.039371	-2.235550
C	-1.601582	-3.626064	-1.391617
C	-1.958595	-3.920186	-0.002587
C	-0.784581	-3.657374	0.831467
C	-0.939227	-3.101152	2.089867
C	-0.021045	-2.056236	2.546486
C	-0.790439	-1.087100	3.326733
C	-0.493876	0.262580	3.235950
C	-0.468663	2.876510	-0.450308
C	-3.877354	1.446339	2.298219
C	-3.486421	2.452744	1.431288
C	-3.991524	2.472459	0.057382
C	-4.860489	1.484942	-0.375209
C	-5.274044	0.421197	0.541491
C	-4.382879	-0.862662	2.450767
C	-3.208841	-0.600717	3.284895
C	-2.895835	0.826289	3.190186
C	-1.576469	1.245658	3.166453
C	-1.162670	2.308714	2.249199
C	-2.091445	2.895956	1.406533
C	-2.908482	2.927641	-0.816053
C	-2.753523	2.371848	-2.074539
C	-3.672680	1.328563	-2.532303
C	-4.696646	0.897144	-1.705915

C	-5.008986	-0.529900	-1.611583
C	-5.365902	-0.824027	-0.222647
C	-4.975022	-2.020646	0.354069
C	-4.469958	-2.040544	1.727955
C	-2.185283	-1.530845	3.351375
C	-2.277216	-2.775989	2.587015
C	-3.387793	-3.023844	1.797927
C	-3.224089	-3.611752	0.467214
C	-4.204993	-2.991676	-0.425133
C	-3.867268	-2.713464	-1.738905
C	-4.280475	-1.448319	-2.348624
C	-3.197945	-0.992212	-3.222041
C	-2.902671	0.357625	-3.311636
C	-1.734093	3.187985	0.018301
C	-1.415326	2.044720	-2.570147
C	-4.796075	0.402477	1.840984
C	4.332879	0.452163	0.325017
C	3.643687	2.413883	-0.746885
O	4.180583	1.180856	-0.770757
H	4.068275	0.840814	1.321291
C	5.031413	-0.805575	0.162668
C	5.464195	-1.266509	-1.090975
C	5.276573	-1.580590	1.310776
C	6.129256	-2.482654	-1.205891
H	5.275384	-0.659789	-1.991135
C	5.938257	-2.798498	1.209912
H	4.943983	-1.221241	2.297779
C	6.363909	-3.247328	-0.051884
H	6.468494	-2.843440	-2.192600
H	6.129616	-3.407167	2.111017
H	3.405555	2.731024	-1.771819
C	3.704022	3.312280	0.380607
O	4.074495	2.943029	1.514598
C	3.365287	4.725316	0.103532
C	2.448425	5.086777	-0.890125
C	3.983919	5.723324	0.870071
C	2.165050	6.431515	-1.123392
H	1.931307	4.311621	-1.476890
C	3.701698	7.066354	0.629245
H	4.687704	5.430782	1.665969
C	2.794234	7.421977	-0.368782
H	1.441338	6.710323	-1.903484
H	4.193096	7.845392	1.230747

H	2.571283	8.482598	-0.558168
N	7.073600	-4.549244	-0.165908
O	7.266734	-5.194457	0.829249
O	7.434752	-4.920434	-1.250303

Energy = 1.621211338894
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3219.85727947

TS3’
-AM1-

C	-4.254095	-2.589029	-0.814500
C	-4.593157	-1.318078	-1.317149
C	-5.867045	-0.793171	-1.054418
C	-6.790018	-1.513977	-0.298106
C	-6.433702	-2.775448	0.197620
C	-5.160002	-3.316328	-0.055768
C	-3.661206	-0.653990	-2.194722
O	-3.480448	0.628065	-2.447681
C	-3.555894	1.679221	-1.628781
C	-4.231526	1.852978	-0.359519
O	-4.635101	0.916713	0.352307
N	-7.412271	-3.553125	1.002502
O	-7.086172	-4.625015	1.437848
C	-4.373728	3.261374	0.080755
C	-4.585828	4.300790	-0.832460
C	-4.728573	5.610730	-0.378028
C	-4.660659	5.890847	0.987141
C	-4.460709	4.856653	1.901538
C	-4.323801	3.544425	1.452668
O	-8.505880	-3.092265	1.193067
H	-3.197052	-1.247264	-3.012714
H	-6.143825	0.200019	-1.439850
H	-3.250039	-3.000252	-1.009104
H	-7.787667	-1.090807	-0.088688
H	-4.886134	-4.306738	0.346937
H	-3.163749	2.557267	-2.177467
H	-4.657547	4.090067	-1.910129
H	-4.183220	2.718309	2.168278
H	-4.896917	6.424426	-1.098923
H	-4.414872	5.074001	2.979093
H	-4.769187	6.926706	1.342004
C	-0.476022	1.802644	-1.586350
C	0.242977	1.318086	-2.663250

C	0.137904	2.779011	-0.687792
C	-1.335861	0.910638	-0.790784
C	0.185005	-0.107823	-2.998074
C	1.608339	1.782753	-2.907059
C	-0.300376	2.476597	0.673979
C	1.429358	3.224480	-0.916956
C	-1.185137	1.313850	0.615987
C	-1.388183	-0.453944	-1.109373
C	1.513975	-0.520304	-3.447768
C	-0.587723	-0.962620	-2.233756
C	2.394777	0.647543	-3.392085
C	2.186417	2.712153	-2.058320
C	0.575416	2.636535	1.735002
C	2.356621	3.390594	0.203801
C	-1.137243	0.367391	1.622652
C	-1.298739	-1.450645	-0.033288
C	2.002879	-1.771853	-3.111276
C	-0.068937	-2.281695	-1.875371
C	3.714945	0.501460	-3.000885
C	3.581967	2.557867	-1.644109
C	0.622216	1.635128	2.799735
C	1.941378	3.104544	1.493076
C	3.687154	2.977555	-0.245520
C	-0.210807	0.530242	2.743297
C	-1.196368	-1.057988	1.288687
C	-0.508482	-2.583996	-0.514123
C	3.398383	-1.926503	-2.697185
C	1.187986	-2.677399	-2.302600
C	4.230702	-0.821244	-2.643238
C	4.325040	1.482984	-2.102097
C	2.017275	1.480658	3.215559
C	2.832833	2.389281	2.407814
C	4.530146	2.299842	0.619176
C	0.303781	-0.792093	3.102669
C	-0.305538	-1.772850	2.202636
C	0.333766	-3.265032	0.349448
C	3.445349	-2.930746	-1.632960
C	2.078797	-3.395815	-1.389625
C	5.157913	-0.657278	-1.522554
C	5.216263	0.766769	-1.188173
C	2.503970	0.229321	3.554003
C	4.091168	1.997610	1.982627
C	5.315934	1.163769	0.134701

C	1.623074	-0.938662	3.496496
C	0.438402	-2.848676	1.747387
C	1.663431	-3.681262	-0.100232
C	4.322260	-2.775465	-0.572590
C	5.202473	-1.607201	-0.515956
C	3.834094	-0.184675	3.104643
C	4.605700	0.674821	2.340816
C	5.362769	0.159497	1.198780
C	2.409604	-2.074925	3.013096
C	1.833485	-3.003560	2.162824
C	2.590821	-3.518627	1.020739
C	3.883206	-3.077641	0.790948
C	5.307586	-1.187434	0.882513
C	3.775741	-1.608777	2.770268
C	4.492228	-2.096195	1.690173

Energy = 1.639853769376
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3219.82867767

TS4’
-AM1-

C	4.027286	-2.846795	-1.337684
C	4.431766	-1.497494	-1.367550
C	5.538912	-1.102740	-0.598472
C	6.218170	-2.019924	0.196630
C	5.787941	-3.355219	0.228510
C	4.691687	-3.773372	-0.545542
C	3.752844	-0.604041	-2.270449
O	3.757411	0.721128	-2.251032
C	3.927868	1.422080	-1.125783
C	4.077453	2.866172	-1.335598
O	3.966039	3.382314	-2.456864
N	6.501455	-4.338182	1.084371
O	6.131979	-5.481682	1.087992
C	4.426495	3.652681	-0.134076
C	4.021748	3.273206	1.150402
C	4.384834	4.043796	2.253754
C	5.153150	5.195650	2.082479
C	5.550344	5.584220	0.802854
C	5.185077	4.820406	-0.303602
O	7.428966	-3.962739	1.750258
H	3.327611	-0.971241	-3.222238
H	5.907331	-0.065351	-0.644668

H	3.165648	-3.168994	-1.944300
H	7.089702	-1.700723	0.794840
H	4.363638	-4.827402	-0.521768
H	4.120083	0.927816	-0.169582
H	3.394538	2.378598	1.294660
H	5.480554	5.127498	-1.320027
H	4.061038	3.742724	3.261147
H	6.148705	6.497040	0.664391
H	5.441315	5.799563	2.956022
C	-3.563556	1.505618	-2.668151
C	-4.216214	0.195134	-2.655486
C	-4.064662	2.271399	-1.525399
C	-2.235961	1.614415	-3.046041
C	-3.506031	-0.935420	-3.022435
C	-5.119300	0.150609	-1.504318
C	-5.025617	1.433814	-0.805891
C	-3.210916	3.105082	-0.823046
C	-1.332712	2.494762	-2.303104
C	-1.484236	0.419250	-3.432879
C	-3.657937	-2.174941	-2.258527
C	-2.102532	-0.819922	-3.422376
C	-5.263248	-1.021952	-0.781901
C	-5.080968	1.474876	0.577134
C	-1.807457	3.220223	-1.223158
C	-3.269262	3.148373	0.639184
C	-0.023917	1.844910	-2.230798
C	-0.117579	0.560641	-2.929881
C	-4.512068	-2.217109	-1.169405
C	-2.348116	-2.824772	-2.186279
C	-1.387156	-1.985826	-2.904686
C	-5.321415	-0.978470	0.680187
C	-5.232783	0.235220	1.340768
C	-4.178226	2.355966	1.319839
C	-0.998867	3.332650	-0.009486
C	-1.901704	3.289765	1.142114
C	0.741942	1.950626	-1.084381
C	0.561661	-0.540855	-2.441685
C	-4.106002	-2.912351	0.053331
C	-1.964375	-3.482407	-1.030000
C	-0.094407	-1.847893	-2.426699
C	-4.606119	-2.146746	1.196424
C	-4.423729	0.350092	2.555413
C	-3.771996	1.660815	2.542511

C	0.237918	2.712970	0.056903
C	-1.517511	2.632330	2.298327
C	1.494917	0.795405	-0.575602
C	1.403996	-0.430190	-1.242140
C	-2.867599	-3.528088	0.121098
C	-0.597605	-3.337615	-0.526090
C	0.310453	-2.542286	-1.205210
C	-3.840720	-2.038109	2.345276
C	-3.747085	-0.754964	3.043742
C	-2.478657	1.795522	3.018606
C	0.644463	2.018968	1.278230
C	-0.208745	1.980082	2.368509
C	1.402503	0.828634	0.891040
C	1.215285	-1.662684	-0.465651
C	-2.058480	-3.413289	1.335772
C	-0.655450	-3.296882	0.934943
C	-2.531411	-2.688764	2.416825
C	-2.379871	-0.612534	3.546889
C	-1.763367	0.627232	3.535002
C	-0.360273	0.742744	3.133708
C	1.253509	-0.341224	1.614431
C	1.158800	-1.625094	0.915848
C	0.198837	-2.461986	1.635648
C	-1.628139	-1.807391	3.158841
C	0.350887	-0.386911	2.765310
C	-0.301017	-1.697484	2.779329

Energy = 1.630156437765
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = 1.630156437765

cis-**2a**
-AM1-

C	-1.479038	-0.854243	1.320747
C	-1.236865	0.550196	1.697669
C	-1.213031	1.520516	0.731091
C	-1.667812	1.327374	-0.713996
C	-1.925796	-0.176291	-1.118590
C	-1.675557	-1.179556	0.004787
C	-0.658825	-1.694332	2.189673
C	0.086404	-0.827653	3.101964
C	-0.272574	0.556187	2.794769
C	0.689953	1.549956	2.872153
C	-0.180248	2.540894	0.798468

C	-0.507462	1.987557	-1.463304
C	0.120509	1.463570	-2.561459
C	-0.120063	0.058935	-2.939090
C	-0.969244	-0.708907	-2.188063
C	-0.587483	-2.075558	-1.880429
C	-1.021686	-2.366621	-0.520997
C	-0.252150	-3.188210	0.289182
C	-0.063007	-2.841875	1.691552
C	1.385818	-1.146220	3.458671
C	2.017574	-2.353376	2.921487
C	1.312161	-3.179706	2.063345
C	1.971292	-3.743616	0.883682
C	1.001981	-3.753220	-0.213272
C	1.413786	-3.477131	-1.504685
C	0.593602	-2.620097	-2.362990
C	1.486657	-1.799719	-3.170436
C	1.137017	-0.486895	-3.444003
C	0.253634	2.832456	-0.560794
C	4.210654	1.118757	-2.139386
C	3.618524	2.260592	-1.627110
C	3.811962	2.617604	-0.220299
C	4.588838	1.813829	0.597670
C	5.216369	0.608106	0.054789
C	4.793901	-1.124336	-1.651037
C	3.823834	-1.138536	-2.746456
C	3.458726	0.247941	-3.045720
C	2.153533	0.562717	-3.384225
C	1.522682	1.764007	-2.838746
C	2.239245	2.592142	-1.989414
C	2.552801	3.169272	0.282562
C	2.140907	2.892035	1.573717
C	2.963739	2.047016	2.440819
C	4.153231	1.520863	1.964463
C	4.511718	0.134201	2.266025
C	5.169567	-0.429816	1.086124
C	4.943438	-1.748956	0.731402
C	4.751139	-2.106316	-0.675184
C	2.865193	-2.135481	-2.809290
C	2.819513	-3.173596	-1.777668
C	3.736548	-3.159261	-0.739676
C	3.300896	-3.452151	0.627171
C	4.046541	-2.580296	1.536092
C	3.422671	-2.046545	2.651546

C	3.661757	-0.651582	3.026612
C	2.404379	-0.096043	3.528286
C	2.065751	1.216247	3.245348
C	1.581477	3.144922	-0.812868
C	0.735908	2.576208	1.839219
C	5.032958	0.270555	-1.275918
C	-3.380667	-0.201031	-1.656608
C	-2.991109	2.054009	-1.046095
O	-3.948211	1.105576	-1.515984
H	-2.819670	2.771991	-1.899719
C	-3.617117	2.796520	0.133033
O	-4.247777	2.196579	1.006327
C	-3.441134	4.263096	0.150471
C	-3.598968	5.035074	-1.006410
C	-3.145603	4.891264	1.368494
C	-3.438233	6.418645	-0.947792
H	-3.872967	4.561985	-1.961895
C	-2.976739	6.273455	1.419251
H	-3.055446	4.284442	2.283342
C	-3.120126	7.037899	0.261137
H	-3.566339	7.022279	-1.858716
H	-2.736565	6.760668	2.376104
H	-2.988564	8.129705	0.302112
H	-3.360090	-0.401977	-2.769545
C	-4.278536	-1.205307	-0.996731
C	-5.043713	-0.870631	0.124698
C	-4.384364	-2.486671	-1.554818
C	-5.895163	-1.808971	0.704811
H	-4.980343	0.148995	0.547716
C	-5.226370	-3.437616	-0.987418
H	-3.799660	-2.750857	-2.449883
C	-5.980135	-3.093571	0.146939
H	-6.495975	-1.541985	1.591493
H	-5.304761	-4.448009	-1.424036
N	-6.883429	-4.103856	0.759051
O	-7.524032	-3.800598	1.729510
O	-6.949409	-5.198847	0.267151

Energy = 1.503060736098
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3219.91066992

trans-**2a**
-AM1-

C	-1.267383	-1.075396	1.737567
C	-0.879220	0.222088	2.320532
C	-0.961102	1.359335	1.562448
C	-1.674359	1.465822	0.214773
C	-2.091979	0.072812	-0.411012
C	-1.708823	-1.133367	0.442011
C	-0.359565	-2.088692	2.268966
C	0.584554	-1.435442	3.174844
C	0.261074	-0.009689	3.203378
C	1.280270	0.925766	3.286474
C	0.121289	2.325091	1.630820
C	-0.635333	2.233472	-0.596704
C	-0.237710	1.910542	-1.867348
C	-0.625853	0.613479	-2.451421
C	-1.378679	-0.264840	-1.718092
C	-1.027536	-1.674310	-1.744941
C	-1.231233	-2.212443	-0.406669
C	-0.382545	-3.194857	0.081201
C	0.069786	-3.132191	1.464572
C	1.904932	-1.849841	3.220839
C	2.359176	-2.945019	2.361142
C	1.465965	-3.570547	1.508083
C	1.873069	-3.911053	0.143334
C	0.727720	-3.683071	-0.739289
C	0.922196	-3.171177	-2.009608
C	0.016707	-2.143812	-2.528006
C	0.802046	-1.204280	-3.317384
C	0.488805	0.144859	-3.271035
C	0.325851	2.864034	0.292652
C	3.834844	1.388599	-2.277135
C	3.411460	2.423536	-1.460784
C	3.869837	2.495048	-0.072045
C	4.728521	1.528309	0.424673
C	5.177635	0.435827	-0.439680
C	4.359191	-0.920543	-2.331898
C	3.212946	-0.697004	-3.213580
C	2.884653	0.729798	-3.176191
C	1.561456	1.136617	-3.203640
C	1.109426	2.223979	-2.336628
C	2.012394	2.853647	-1.495047
C	2.753815	2.969840	0.747636
C	2.559692	2.458021	2.018001
C	3.469122	1.439638	2.545660

C	4.522704	0.986195	1.769090
C	4.844532	-0.441220	1.735276
C	5.250239	-0.781331	0.370431
C	4.886624	-2.000142	-0.176732
C	4.429538	-2.072181	-1.565641
C	2.200007	-1.638154	-3.284400
C	2.273983	-2.855605	-2.474257
C	3.358054	-3.066582	-1.638238
C	3.152148	-3.608716	-0.293795
C	4.096478	-2.949263	0.609346
C	3.711051	-2.627116	1.900094
C	4.095456	-1.338247	2.478653
C	2.981133	-0.859281	3.297277
C	2.677592	0.491091	3.331557
C	1.605605	3.183932	-0.135733
C	1.206520	2.132220	2.473141
C	4.743557	0.368281	-1.753219
C	-3.625260	0.216405	-0.631914
C	-3.014522	2.226964	0.380105
O	-4.063909	1.268043	0.244442
H	-3.803818	0.564842	-1.692577
C	-4.438660	-1.005510	-0.344088
C	-4.995739	-1.225359	0.920297
C	-4.681215	-1.917379	-1.379762
C	-5.773917	-2.354551	1.163681
H	-4.827449	-0.492234	1.726034
C	-5.452312	-3.053734	-1.154154
H	-4.262264	-1.738730	-2.382803
C	-5.995633	-3.269567	0.122769
H	-6.211966	-2.526828	2.161919
H	-5.638246	-3.774581	-1.968971
H	-3.132308	2.635893	1.422359
C	-3.230950	3.334286	-0.649089
O	-3.569989	3.055074	-1.803542
C	-3.110738	4.724389	-0.171925
C	-2.278048	5.073132	0.898250
C	-3.856395	5.720248	-0.820003
C	-2.201353	6.398237	1.321729
H	-1.662425	4.305801	1.395599
C	-3.782002	7.043113	-0.388307
H	-4.496640	5.444024	-1.673687
C	-2.956464	7.383098	0.683281
H	-1.542254	6.667000	2.160675

H	-4.373423	7.818884	-0.897265
H	-2.897126	8.428040	1.023444
N	-6.821485	-4.480833	0.373049
O	-7.281466	-4.654492	1.469696
O	-7.006694	-5.254589	-0.527748

Energy = 1.502544735010
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3219.91859725

2.6 Cartesian coordinates for the reaction of **1a** with C_{60} at the PM3 level

C_{60}
-PM3-

C	-3.51144	-0.21903	-0.44331
C	-3.34316	1.180163	-0.07155
C	-2.7277	2.05917	-0.94556
C	-2.24782	1.585685	-2.23775
C	-2.4076	0.257078	-2.59076
C	-3.05577	-0.66863	-1.67032
C	-3.30914	-1.02979	0.750848
C	-3.01585	-0.13167	1.860629
C	-3.03687	1.234152	1.352358
C	-2.13057	2.16443	1.830432
C	-1.77326	3.038868	-0.44209
C	-0.99679	2.272756	-2.5329
C	0.031355	1.596555	-3.16617
C	-0.13692	0.197364	-3.53792
C	-1.32484	-0.45504	-3.25765
C	-1.30381	-1.82087	-2.74939
C	-2.37357	-1.95287	-1.76836
C	-2.18148	-2.72272	-0.63443
C	-2.66138	-2.24924	0.657757
C	-2.08959	-0.49831	2.821332
C	-1.40741	-1.78255	2.723295
C	-1.6859	-2.63537	1.669481
C	-0.60315	-3.34749	1.002588
C	-0.90943	-3.40146	-0.42132
C	0.106377	-3.27612	-1.35286
C	-0.09592	-2.46538	-2.54702
C	1.155109	-1.77831	-2.84217
C	1.135142	-0.48139	-3.3248
C	-0.7035	3.170869	-1.42312
C	3.309146	1.029789	-0.75085

C	2.661378	2.249242	-0.65776
C	2.181486	2.722726	0.634436
C	2.373575	1.952867	1.768354
C	3.05575	0.668628	1.670311
C	3.343162	-1.18016	0.071548
C	3.036876	-1.23415	-1.35236
C	3.015848	0.131667	-1.86064
C	2.089586	0.49831	-2.82134
C	1.407401	1.782552	-2.72329
C	1.685897	2.635361	-1.66949
C	0.909432	3.401482	0.421324
C	-0.10637	3.276138	1.35287
C	0.09592	2.465381	2.547023
C	1.303809	1.820865	2.749387
C	1.324835	0.455046	3.257656
C	2.407592	-0.25708	2.590751
C	2.247814	-1.58568	2.237745
C	2.727707	-2.05917	0.945557
C	2.130583	-2.16443	-1.83044
C	1.482439	-3.09015	-0.90999
C	1.773261	-3.03887	0.442088
C	0.703495	-3.17089	1.423135
C	0.996782	-2.27276	2.532899
C	-0.03136	-1.59656	3.166168
C	0.136915	-0.19736	3.537924
C	-1.13514	0.481386	3.324805
C	-1.15511	1.778313	2.842173
C	0.603144	3.34748	-1.00259
C	-1.48242	3.090141	0.909996
C	3.511425	0.219033	0.443298

Energy = 1.292121073615
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -2286.17167898

Epoxide **1a**
-PM3-

C	5.844589	-1.16474	-1.02643
C	4.913122	-1.81823	-0.22518
C	3.794185	-1.13831	0.240445
C	3.606781	0.205612	-0.08991
C	4.547361	0.862108	-0.88615
C	5.660346	0.173675	-1.35651
C	2.42112	0.946375	0.418821

O	2.467406	2.114251	0.74885
C	1.120975	0.165649	0.457474
O	0.724011	-0.38616	1.721345
C	-0.07654	0.680081	1.19271
C	-1.44637	0.369387	0.709399
C	-2.10021	-0.81566	1.043676
C	-3.38943	-1.05584	0.583907
C	-4.03448	-0.10871	-0.21902
C	-3.37822	1.082676	-0.5524
C	-2.09215	1.318256	-0.08702
H	-0.01903	1.636102	1.753598
H	-1.59911	-1.56202	1.67287
H	-1.58183	2.254779	-0.34286
H	-3.8914	-1.99478	0.85831
H	-3.8714	1.838814	-1.17989
H	0.996923	-0.50973	-0.41214
H	3.062618	-1.65514	0.873218
H	4.41084	1.921523	-1.13399
H	5.061093	-2.87033	0.040538
H	6.394771	0.689719	-1.98402
H	6.723782	-1.70404	-1.39477
N	-5.42267	-0.36668	-0.71894
O	-5.97905	-1.40632	-0.42569
O	-5.97174	0.466714	-1.41215

Energy = 0.007086915507
-B3LYP/6-31G*//PM3-
E(RB+HF-LYP) = -933.7179858

TS1
-PM3-

C	-2.54834	-1.19901	0.966789
C	-1.68867	-0.70913	-0.02964
C	-2.16806	0.241103	-0.94054
C	-3.47897	0.690726	-0.8604
C	-4.33118	0.199138	0.134525
C	-3.85692	-0.7522	1.048133
C	-0.33576	-1.2115	-0.07199
O	0.472989	-0.86907	-1.10875
C	1.509132	-0.36787	-0.37078
C	2.848963	-0.9371	-0.56498
O	3.032514	-2.04284	-1.04846
N	-5.74483	0.686189	0.223364
O	-6.48089	0.227978	1.074634

C	3.971687	-0.07618	-0.09285
C	3.99585	1.282275	-0.41306
C	5.05116	2.078147	0.016504
C	6.08135	1.523871	0.770106
C	6.059914	0.170074	1.087965
C	5.010485	-0.63298	0.653908
O	-6.13331	1.534011	-0.55545
H	0.021392	-1.94054	0.669761
H	-1.51229	0.632951	-1.7278
H	-2.18409	-1.94573	1.683264
H	-3.83632	1.434968	-1.58688
H	-4.51514	-1.15048	1.833737
H	1.343039	0.526625	0.241577
H	3.185667	1.717519	-1.00966
H	5.001663	-1.70371	0.888859
H	5.071709	3.142382	-0.24046
H	6.873225	-0.26754	1.676415
H	6.9106	2.153351	1.109678

Energy = 0.072460586216
-B3LYP/6-31G*//PM3-
E(RB+HF-LYP) = -933.6589086

INT1
-PM3-

C	0.438727	-1.07913	-0.23309
C	-1.74543	-0.45623	-0.08964
O	-0.47127	-0.16785	-0.03429
H	-2.09868	-1.46983	-0.30625
C	-2.66674	0.667821	0.136684
O	-2.29225	1.808957	0.35128
C	-4.10875	0.294597	0.067204
C	-4.59325	-0.78279	0.810323
C	-4.97888	1.038938	-0.72981
C	-5.94164	-1.11479	0.751773
H	-3.91174	-1.36076	1.444889
C	-6.32564	0.696489	-0.79059
H	-4.60121	1.895928	-1.29945
C	-6.80741	-0.37833	-0.051
H	-6.32233	-1.95635	1.339882
H	-7.00779	1.279121	-1.4187
H	-7.8689	-0.64347	-0.09758
H	0.164584	-2.11742	-0.4568
C	1.821312	-0.65965	-0.14532

C	2.209541	0.656265	0.137908
C	2.807932	-1.63563	-0.35816
C	3.554955	0.989374	0.206952
H	1.459525	1.438505	0.308248
C	4.150651	-1.30447	-0.28961
H	2.515974	-2.66906	-0.58087
C	4.535367	0.01332	-0.00587
H	3.838418	2.028123	0.430519
H	4.907247	-2.08378	-0.4595
N	5.984764	0.372387	0.068604
O	6.823796	-0.48754	-0.11757
O	6.305598	1.518621	0.314186

Energy = 0.038838021550
-B3LYP/6-31G*//PM3-
E(RB+HF-LYP) = -933.6806024

TS2
-PM3-

C	0.332806	0.471012	-0.59121
C	-1.79449	-0.32406	-0.66367
O	-0.45723	-0.52589	-0.44482
H	-2.11877	-0.50177	-1.68537
C	-2.59748	0.006522	0.460493
O	-2.12036	0.325142	1.558345
C	-4.07267	-0.0124	0.220466
C	-4.66113	-1.07547	-0.46545
C	-4.86933	1.029928	0.695633
C	-6.0351	-1.0924	-0.67755
H	-4.03353	-1.89542	-0.83344
C	-6.24242	1.011704	0.475653
H	-4.4091	1.8542	1.252251
C	-6.82613	-0.04801	-0.21037
H	-6.49436	-1.92996	-1.21199
H	-6.86511	1.831221	0.848351
H	-7.90746	-0.06201	-0.37953
H	-0.04944	1.460558	-0.89622
C	1.766783	0.26832	-0.38207
C	2.281306	-0.89683	0.193838
C	2.6347	1.301805	-0.75719
C	3.653152	-1.03119	0.385819
H	1.612234	-1.70973	0.507673
C	4.003406	1.168088	-0.56858
H	2.235927	2.223673	-1.20077

C	4.516824	-0.00196	0.002783
H	4.043054	-1.95416	0.841449
H	4.672519	1.988533	-0.86857
N	6.005439	-0.14911	0.207242
O	6.730526	0.783541	-0.06748
O	6.438882	-1.19676	0.636945

Energy = 0.073622417161
-B3LYP/6-31G*//PM3-
E(RB+HF-LYP) = -933.6432352

INT2
-PM3-

C	-0.27091	0.2334	-0.05623
C	1.75497	-0.81019	0.184778
O	0.437737	-0.82926	0.195749
H	0.258913	1.191296	-0.28436
C	-1.71306	0.098264	-0.02176
C	-2.37248	-1.10331	0.265455
C	-2.46893	1.248571	-0.29447
C	-3.75911	-1.1552	0.280007
H	-1.80456	-2.01555	0.481967
C	-3.85378	1.198823	-0.28042
H	-1.95988	2.194217	-0.5206
C	-4.50953	-0.0056	0.007429
H	-4.25796	-2.10828	0.507773
H	-4.42787	2.111301	-0.49674
H	2.132297	-1.80471	0.431412
C	2.581284	0.349159	-0.08616
O	2.092474	1.45498	-0.33314
C	4.051943	0.128556	-0.0353
C	4.620084	-0.98535	-0.65612
C	4.868489	1.048939	0.623535
C	5.995842	-1.17791	-0.61251
H	3.981576	-1.70373	-1.18322
C	6.243705	0.846579	0.670286
H	4.424371	1.932785	1.096106
C	6.807821	-0.26492	0.053346
H	6.440427	-2.04947	-1.10415
H	6.882808	1.567627	1.190703
H	7.891182	-0.42046	0.088868
N	-6.00502	-0.06227	0.023355
O	-6.64359	0.944434	-0.21193
O	-6.55965	-1.1149	0.271522

Energy = 0.035503547498
-B3LYP/6-31G*//PM3-
E(RB+HF-LYP) = -933.6890175

TS1'
-PM3-

C	2.096734	1.217846	1.120937
C	1.306463	1.406184	-0.02384
C	1.607788	0.682739	-1.18626
C	2.676482	-0.20002	-1.20878
C	3.459153	-0.3856	-0.06241
C	3.160394	0.328689	1.104468
C	0.255753	2.401026	0.04569
O	-0.72272	2.559909	-0.87669
C	-1.34127	1.342537	-0.75245
C	-2.0929	0.964947	0.446046
O	-1.92116	1.475243	1.545769
N	4.609774	-1.34403	-0.08439
O	5.30148	-1.4683	0.906716
C	-3.09593	-0.11668	0.224322
C	-4.00325	-0.0287	-0.8326
C	-4.94383	-1.03398	-1.02431
C	-4.97854	-2.13002	-0.16776
C	-4.07618	-2.21747	0.887003
C	-3.13796	-1.21078	1.089101
O	4.834328	-1.98265	-1.09351
H	0.261304	3.170436	0.828112
H	0.994282	0.814065	-2.08644
H	1.86925	1.775462	2.038543
H	2.89864	-0.75124	-2.13396
H	3.762633	0.192955	2.014471
H	-1.44936	0.804816	-1.69826
H	-3.97672	0.835844	-1.506
H	-2.43761	-1.27066	1.930054
H	-5.65872	-0.96152	-1.85058
H	-4.10635	-3.0777	1.564001
H	-5.71857	-2.9222	-0.32263

Energy = 0.074870614581
-B3LYP/6-31G*//PM3-
E(RB+HF-LYP) = -933.648094602

INT1'
-PM3-

C	2.586446	1.744023	0.477422
C	1.385953	1.605152	-0.23373
C	1.102487	0.395035	-0.87466
C	2.000115	-0.66237	-0.80488
C	3.192671	-0.52375	-0.08686
C	3.478922	0.687299	0.558536
C	0.53261	2.767078	-0.36534
O	-0.75062	2.877221	-0.47552
C	-1.67916	1.970643	-0.30657
C	-1.67697	0.76516	0.514208
O	-0.84017	0.530104	1.374812
N	4.157438	-1.6644	-0.00387
O	5.17161	-1.54345	0.6551
C	-2.83775	-0.13964	0.268832
C	-3.20198	-0.46132	-1.03983
C	-4.26959	-1.31975	-1.27235
C	-4.9797	-1.85452	-0.20144
C	-4.61741	-1.53542	1.102774
C	-3.54446	-0.68275	1.341787
O	3.918581	-2.69444	-0.60339
H	0.965065	3.774125	-0.42974
H	0.164438	0.274596	-1.43199
H	2.81575	2.690993	0.980315
H	1.758881	-1.60538	-1.31594
H	4.407976	0.809166	1.13343
H	-2.60765	2.363536	-0.73444
H	-2.63966	-0.03494	-1.87911
H	-3.24758	-0.44236	2.369343
H	-4.55131	-1.57533	-2.29908
H	-5.17398	-1.95935	1.945233
H	-5.82237	-2.52894	-0.38647

Energy = 0.048532233817
-B3LYP/6-31G*//PM3-
E(RB+HF-LYP) = -933.667238755

TS2'
-PM3-

C	-2.92743	1.783507	0.371343
C	-1.64768	1.359126	-0.03314
C	-1.48542	0.039511	-0.46922
C	-2.56184	-0.83763	-0.49036
C	-3.82599	-0.41211	-0.07262
C	-4.00133	0.912076	0.356659

C	-0.60383	2.354698	-0.00323
O	0.687313	2.24876	-0.00535
C	1.37365	1.139164	0.013673
C	2.838407	1.295926	0.003027
O	3.398581	2.377178	-0.05861
N	-4.98388	-1.35818	-0.08633
O	-6.08354	-0.96198	0.24621
C	3.58437	0.005655	0.05724
C	3.290266	-0.93556	1.044835
C	3.999871	-2.12952	1.09778
C	4.998424	-2.38978	0.164186
C	5.293296	-1.45142	-0.81915
C	4.592482	-0.2511	-0.87232
O	-4.80812	-2.51111	-0.42902
H	-0.84307	3.426188	0.034915
H	-0.50725	-0.31936	-0.81925
H	-3.07709	2.817888	0.705213
H	-2.40505	-1.86811	-0.84078
H	-4.98927	1.266921	0.683707
H	0.900858	0.149986	0.04512
H	2.506189	-0.7289	1.782251
H	4.83514	0.496133	-1.63669
H	3.772703	-2.86509	1.876531
H	6.08243	-1.6541	-1.55093
H	5.554184	-3.33245	0.206145

Energy = 0.070687472860
-B3LYP/6-31G*//PM3-
E(RB+HF-LYP) = -933.620813145

INT2'
-PM3-

C	-2.92743	1.783507	0.371343
C	-1.64768	1.359126	-0.03314
C	-1.48542	0.039511	-0.46922
C	-2.56184	-0.83763	-0.49036
C	-3.82599	-0.41211	-0.07262
C	-4.00133	0.912076	0.356659
C	-0.60383	2.354698	-0.00323
O	0.687313	2.24876	-0.00535
C	1.37365	1.139164	0.013673
C	2.838407	1.295926	0.003027
O	3.398581	2.377178	-0.05861

N	-4.98388	-1.35818	-0.08633
O	-6.08354	-0.96198	0.24621
C	3.58437	0.005655	0.05724
C	3.290266	-0.93556	1.044835
C	3.999871	-2.12952	1.09778
C	4.998424	-2.38978	0.164186
C	5.293296	-1.45142	-0.81915
C	4.592482	-0.2511	-0.87232
O	-4.80812	-2.51111	-0.42902
H	-0.84307	3.426188	0.034915
H	-0.50725	-0.31936	-0.81925
H	-3.07709	2.817888	0.705213
H	-2.40505	-1.86811	-0.84078
H	-4.98927	1.266921	0.683707
H	0.900858	0.149986	0.04512
H	2.506189	-0.7289	1.782251
H	4.83514	0.496133	-1.63669
H	3.772703	-2.86509	1.876531
H	6.08243	-1.6541	-1.55093
H	5.554184	-3.33245	0.206145

Energy = 0.038631907656
-B3LYP/6-31G*//PM3-
E(RB+HF-LYP) = -933.670999667

TS3
-PM3-

C	-1.31769	-0.70574	1.769976
C	-0.85952	0.631592	2.132881
C	-0.83743	1.633712	1.182112
C	-1.31529	1.388276	-0.18299
C	-1.74736	0.099287	-0.53191
C	-1.72385	-0.96402	0.474779
C	-0.49645	-1.67204	2.485868
C	0.468628	-0.93546	3.292243
C	0.243657	0.487657	3.073053
C	1.31963	1.356743	3.018295
C	0.298535	2.541407	1.12113
C	-0.39863	2.099227	-1.08361
C	-0.00666	1.540929	-2.28472
C	-0.46501	0.203493	-2.64941
C	-1.28688	-0.49845	-1.78887
C	-1.05766	-1.91872	-1.57129
C	-1.32787	-2.20691	-0.1706

C	-0.55132	-3.13019	0.508494
C	-0.12383	-2.85596	1.872654
C	1.756861	-1.41798	3.442875
C	2.14938	-2.66344	2.795102
C	1.233194	-3.364	2.030336
C	1.64291	-3.9549	0.762406
C	0.539165	-3.81123	-0.17852
C	0.795912	-3.53748	-1.51033
C	-0.02401	-2.56738	-2.22546
C	0.840974	-1.82576	-3.13105
C	0.625923	-0.4734	-3.33571
C	0.569471	2.829168	-0.27975
C	4.013243	0.697176	-2.44464
C	3.642036	1.879614	-1.82891
C	4.071509	2.156689	-0.46387
C	4.851021	1.237319	0.216329
C	5.242437	-0.00763	-0.43255
C	4.376961	-1.60595	-2.09188
C	3.272866	-1.46351	-3.03239
C	3.047049	-0.03992	-3.24965
C	1.758215	0.441977	-3.39757
C	1.366117	1.68602	-2.74794
C	2.284484	2.386745	-1.98497
C	2.979286	2.834593	0.222795
C	2.722087	2.56004	1.554269
C	3.543862	1.593197	2.27123
C	4.580503	0.948439	1.619117
C	4.804959	-0.47498	1.837233
C	5.214221	-1.06588	0.569296
C	4.77973	-2.33374	0.224452
C	4.350403	-2.61083	-1.14057
C	2.198248	-2.33356	-2.97489
C	2.170242	-3.39195	-1.97306
C	3.218468	-3.52687	-1.07948
C	2.948039	-3.81571	0.323406
C	3.912913	-3.07829	1.129204
C	3.523767	-2.51705	2.332965
C	3.981365	-1.18166	2.696158
C	2.889771	-0.5027	3.38269
C	2.676777	0.848978	3.17612
C	1.874705	2.974257	-0.71801
C	1.347177	2.411593	2.015539
C	4.834562	-0.27063	-1.72868

C	-4.14944	0.560904	-1.00136
C	-3.38645	2.629629	-0.43838
O	-4.14632	1.583431	-0.18089
H	-2.97034	2.818978	-1.44194
C	-3.47413	3.720914	0.560064
O	-4.07619	3.588194	1.613493
C	-2.78605	4.990203	0.188813
C	-2.4721	5.276961	-1.14272
C	-2.46522	5.917989	1.182932
C	-1.85247	6.473867	-1.47618
H	-2.71084	4.541466	-1.92532
C	-1.8395	7.113707	0.845618
H	-2.71102	5.704584	2.230801
C	-1.53466	7.394255	-0.48149
H	-1.61264	6.691924	-2.52213
H	-1.58896	7.836101	1.629873
H	-1.04455	8.337562	-0.74487
H	-3.71568	0.632054	-2.00946
C	-4.98492	-0.56746	-0.62468
C	-5.60991	-0.67373	0.623748
C	-5.15376	-1.59229	-1.56774
C	-6.39265	-1.78099	0.921867
H	-5.48812	0.110795	1.381191
C	-5.93311	-2.69886	-1.27107
H	-4.66282	-1.52263	-2.54631
C	-6.56094	-2.7998	-0.02254
H	-6.87528	-1.84551	1.908012
H	-6.05193	-3.4915	-2.02375
N	-7.40632	-3.993	0.298574
O	-7.55354	-4.86205	-0.53819
O	-7.93427	-4.07456	1.389816

Energy = 1.342832117250
-B3LYP/6-31G*//PM3-
E(RB+HF-LYP) = -3219.8522496

TS4
-PM3-

C	1.121103	-1.065	-1.83446
C	0.71535	0.218245	-2.39894
C	0.80768	1.366685	-1.63632
C	1.355501	1.326093	-0.27465
C	1.734494	0.089135	0.269832

C	1.589193	-1.12504	-0.53581
C	0.20681	-2.08383	-2.33018
C	-0.76405	-1.43423	-3.20151
C	-0.44907	-0.01199	-3.2429
C	-1.47063	0.921133	-3.28423
C	-0.27125	2.342432	-1.67537
C	0.535439	2.234988	0.534682
C	0.186913	1.913396	1.832035
C	0.594199	0.63185	2.39935
C	1.32429	-0.25636	1.632916
C	1.003009	-1.67571	1.675606
C	1.168598	-2.21349	0.333563
C	0.303261	-3.18678	-0.13604
C	-0.19132	-3.12055	-1.50349
C	-2.08348	-1.85163	-3.20045
C	-2.5028	-2.94171	-2.32832
C	-1.58098	-3.55994	-1.50175
C	-1.94368	-3.90035	-0.13157
C	-0.77817	-3.67075	0.71288
C	-0.9371	-3.15879	1.988516
C	-0.02287	-2.13673	2.483123
C	-0.78931	-1.19865	3.290254
C	-0.48858	0.151933	3.246717
C	-0.43963	2.879696	-0.33266
C	-3.85587	1.369905	2.340931
C	-3.45922	2.404693	1.512104
C	-3.95587	2.473519	0.143504
C	-4.82464	1.504365	-0.32709
C	-5.24287	0.415012	0.546118
C	-4.36534	-0.93157	2.410065
C	-3.19968	-0.70312	3.25441
C	-2.88376	0.719209	3.210833
C	-1.56393	1.135102	3.207021
C	-1.14522	2.223196	2.332734
C	-2.06892	2.842579	1.508807
C	-2.87233	2.953514	-0.70486
C	-2.71295	2.442195	-1.98053
C	-3.62867	1.422822	-2.47686
C	-4.65678	0.965496	-1.67095
C	-4.9714	-0.45691	-1.62821
C	-5.33378	-0.79713	-0.25807
C	-4.94857	-2.01351	0.277854
C	-4.4521	-2.08259	1.646476

C	-2.17938	-1.63725	3.293081
C	-2.27063	-2.84931	2.488681
C	-3.37753	-3.06625	1.686653
C	-3.20988	-3.60524	0.342772
C	-4.18068	-2.95444	-0.52795
C	-3.83624	-2.63133	-1.82889
C	-4.2419	-1.35024	-2.39325
C	-3.15912	-0.86864	-3.24145
C	-2.86067	0.482044	-3.28273
C	-1.70602	3.179051	0.139911
C	-1.37888	2.129812	-2.47851
C	-4.77095	0.349591	1.845563
C	4.229371	0.413721	0.382377
C	3.535293	2.383669	-0.59659
O	4.12378	1.200621	-0.65896
H	3.989859	0.759195	1.401828
C	4.935405	-0.84312	0.175095
C	5.36533	-1.28761	-1.08079
C	5.178775	-1.6374	1.305087
C	6.028365	-2.5009	-1.20541
H	5.181701	-0.6884	-1.9805
C	5.838846	-2.85055	1.182876
H	4.84331	-1.29967	2.294172
C	6.270277	-3.28963	-0.07522
H	6.358066	-2.83213	-2.20092
H	6.018477	-3.45883	2.081226
H	3.378714	2.731523	-1.62426
C	3.595701	3.325098	0.528774
O	3.890129	2.991016	1.669077
C	3.338678	4.74785	0.164166
C	2.242029	5.096839	-0.62481
C	4.206636	5.739414	0.625361
C	2.021015	6.428365	-0.95654
H	1.544363	4.319004	-0.96762
C	3.984157	7.069033	0.284315
H	5.057402	5.469352	1.261749
C	2.89351	7.414418	-0.50677
H	1.156564	6.699836	-1.57157
H	4.667762	7.845177	0.644285
H	2.719027	8.462422	-0.77228
N	6.987244	-4.59872	-0.21012
O	7.175251	-5.27973	0.778087
O	7.370682	-4.95735	-1.3058

Energy = 1.343993710044
-B3LYP/6-31G*//PM3-
E(RB+HF-LYP) = -3219.8547931

TS3'
-PM3-

C	-1.317687	-0.705736	1.769976
C	-0.859523	0.631592	2.132881
C	-0.837430	1.633712	1.182112
C	-1.315292	1.388276	-0.182987
C	-1.747358	0.099287	-0.531907
C	-1.723849	-0.964022	0.474779
C	-0.496453	-1.672036	2.485868
C	0.468628	-0.935456	3.292243
C	0.243657	0.487657	3.073053
C	1.319630	1.356743	3.018295
C	0.298535	2.541407	1.121130
C	-0.398628	2.099227	-1.083611
C	-0.006664	1.540929	-2.284715
C	-0.465013	0.203493	-2.649414
C	-1.286881	-0.498449	-1.788868
C	-1.057664	-1.918721	-1.571291
C	-1.327867	-2.206914	-0.170597
C	-0.551318	-3.130193	0.508494
C	-0.123833	-2.855957	1.872654
C	1.756861	-1.417980	3.442875
C	2.149380	-2.663435	2.795102
C	1.233194	-3.363995	2.030336
C	1.642910	-3.954898	0.762406
C	0.539165	-3.811228	-0.178524
C	0.795912	-3.537479	-1.510328
C	-0.024008	-2.567380	-2.225459
C	0.840974	-1.825757	-3.131047
C	0.625923	-0.473399	-3.335705
C	0.569471	2.829168	-0.279745
C	4.013243	0.697176	-2.444639
C	3.642036	1.879614	-1.828906
C	4.071509	2.156689	-0.463866
C	4.851021	1.237319	0.216329
C	5.242437	-0.007632	-0.432545
C	4.376961	-1.605953	-2.091879
C	3.272866	-1.463511	-3.032387
C	3.047049	-0.039922	-3.249652

C	1.758215	0.441977	-3.397572
C	1.366117	1.686020	-2.747937
C	2.284484	2.386745	-1.984967
C	2.979286	2.834593	0.222795
C	2.722087	2.560040	1.554269
C	3.543862	1.593197	2.271230
C	4.580503	0.948439	1.619117
C	4.804959	-0.474978	1.837233
C	5.214221	-1.065876	0.569296
C	4.779730	-2.333738	0.224452
C	4.350403	-2.610833	-1.140569
C	2.198248	-2.333559	-2.974893
C	2.170242	-3.391954	-1.973062
C	3.218468	-3.526869	-1.079475
C	2.948039	-3.815712	0.323406
C	3.912913	-3.078292	1.129204
C	3.523767	-2.517054	2.332965
C	3.981365	-1.181661	2.696158
C	2.889771	-0.502700	3.382690
C	2.676777	0.848978	3.176120
C	1.874705	2.974257	-0.718006
C	1.347177	2.411593	2.015539
C	4.834562	-0.270634	-1.728684
C	-4.149438	0.560904	-1.001361
C	-3.386446	2.629629	-0.438378
O	-4.146324	1.583431	-0.180887
H	-2.970338	2.818978	-1.441942
C	-3.474133	3.720914	0.560064
O	-4.076190	3.588194	1.613493
C	-2.786045	4.990203	0.188813
C	-2.472099	5.276961	-1.142719
C	-2.465217	5.917989	1.182932
C	-1.852466	6.473867	-1.476177
H	-2.710836	4.541466	-1.925319
C	-1.839495	7.113707	0.845618
H	-2.711015	5.704584	2.230801
C	-1.534662	7.394255	-0.481490
H	-1.612637	6.691924	-2.522132
H	-1.588961	7.836101	1.629873
H	-1.044548	8.337562	-0.744873
H	-3.715683	0.632054	-2.009455
C	-4.984923	-0.567461	-0.624682
C	-5.609912	-0.673731	0.623748

C	-5.153756	-1.592294	-1.567735
C	-6.392647	-1.780994	0.921867
H	-5.488119	0.110795	1.381191
C	-5.933106	-2.698857	-1.271069
H	-4.662818	-1.522634	-2.546308
C	-6.560944	-2.799803	-0.022539
H	-6.875279	-1.845505	1.908012
H	-6.051933	-3.491501	-2.023747
N	-7.406323	-3.993001	0.298574
O	-7.553540	-4.862046	-0.538188
O	-7.934267	-4.074560	1.389816

Energy = 1.342832117250
-B3LYP/6-31G*//PM3-
E(RB+HF-LYP) = -3219.85224955

TS4’
-PM3-

C	1.121103	-1.065002	-1.834459
C	0.715350	0.218245	-2.398939
C	0.807680	1.366685	-1.636324
C	1.355501	1.326093	-0.274649
C	1.734494	0.089135	0.269832
C	1.589193	-1.125038	-0.535810
C	0.206810	-2.083831	-2.330182
C	-0.764050	-1.434233	-3.201509
C	-0.449072	-0.011989	-3.242898
C	-1.470625	0.921133	-3.284234
C	-0.271248	2.342432	-1.675372
C	0.535439	2.234988	0.534682
C	0.186913	1.913396	1.832035
C	0.594199	0.631850	2.399350
C	1.324290	-0.256361	1.632916
C	1.003009	-1.675706	1.675606
C	1.168598	-2.213494	0.333563
C	0.303261	-3.186778	-0.136042
C	-0.191322	-3.120552	-1.503490
C	-2.083480	-1.851627	-3.200448
C	-2.502796	-2.941709	-2.328324
C	-1.580975	-3.559937	-1.501748
C	-1.943680	-3.900354	-0.131565
C	-0.778174	-3.670746	0.712880
C	-0.937098	-3.158785	1.988516
C	-0.022873	-2.136729	2.483123

C	-0.789308	-1.198648	3.290254
C	-0.488582	0.151933	3.246717
C	-0.439633	2.879696	-0.332661
C	-3.855869	1.369905	2.340931
C	-3.459219	2.404693	1.512104
C	-3.955869	2.473519	0.143504
C	-4.824641	1.504365	-0.327089
C	-5.242868	0.415012	0.546118
C	-4.365340	-0.931566	2.410065
C	-3.199684	-0.703124	3.254410
C	-2.883764	0.719209	3.210833
C	-1.563925	1.135102	3.207021
C	-1.145220	2.223196	2.332734
C	-2.068916	2.842579	1.508807
C	-2.872330	2.953514	-0.704858
C	-2.712953	2.442195	-1.980533
C	-3.628665	1.422822	-2.476863
C	-4.656781	0.965496	-1.670947
C	-4.971400	-0.456913	-1.628214
C	-5.333776	-0.797128	-0.258065
C	-4.948573	-2.013514	0.277854
C	-4.452102	-2.082589	1.646476
C	-2.179379	-1.637245	3.293081
C	-2.270626	-2.849313	2.488681
C	-3.377530	-3.066254	1.686653
C	-3.209877	-3.605241	0.342772
C	-4.180676	-2.954438	-0.527947
C	-3.836243	-2.631326	-1.828886
C	-4.241902	-1.350239	-2.393249
C	-3.159116	-0.868636	-3.241453
C	-2.860667	0.482044	-3.282726
C	-1.706015	3.179051	0.139911
C	-1.378880	2.129812	-2.478507
C	-4.770949	0.349591	1.845563
C	4.229371	0.413721	0.382377
C	3.535293	2.383669	-0.596586
O	4.123780	1.200621	-0.658959
H	3.989859	0.759195	1.401828
C	4.935405	-0.843122	0.175095
C	5.365330	-1.287607	-1.080794
C	5.178775	-1.637398	1.305087
C	6.028365	-2.500903	-1.205413
H	5.181701	-0.688400	-1.980500

C	5.838846	-2.850547	1.182876
H	4.843310	-1.299665	2.294172
C	6.270277	-3.289625	-0.075222
H	6.358066	-2.832129	-2.200918
H	6.018477	-3.458829	2.081226
H	3.378714	2.731523	-1.624261
C	3.595701	3.325098	0.528774
O	3.890129	2.991016	1.669077
C	3.338678	4.747850	0.164166
C	2.242029	5.096839	-0.624810
C	4.206636	5.739414	0.625361
C	2.021015	6.428365	-0.956537
H	1.544363	4.319004	-0.967622
C	3.984157	7.069033	0.284315
H	5.057402	5.469352	1.261749
C	2.893510	7.414418	-0.506769
H	1.156564	6.699836	-1.571566
H	4.667762	7.845177	0.644285
H	2.719027	8.462422	-0.772277
N	6.987244	-4.598722	-0.210123
O	7.175251	-5.279734	0.778087
O	7.370682	-4.957348	-1.305802

Energy = 1.343993698638
-B3LYP/6-31G*//PM3-
E(RB+HF-LYP) = -3219.85479308

cis-**2a**
-PM3-

C	-1.49318	-0.78802	1.367403
C	-1.19517	0.604716	1.735871
C	-1.15173	1.574461	0.770494
C	-1.64254	1.395294	-0.66474
C	-1.96074	-0.10328	-1.06193
C	-1.72435	-1.11375	0.057871
C	-0.69341	-1.6498	2.221495
C	0.09312	-0.81213	3.115873
C	-0.21869	0.577119	2.81166
C	0.779596	1.535546	2.874029
C	-0.08606	2.550529	0.818203
C	-0.46768	2.010425	-1.42819
C	0.123923	1.454974	-2.5306
C	-0.17233	0.061964	-2.89971
C	-1.03822	-0.67629	-2.13904

C	-0.7017	-2.04748	-1.83348
C	-1.12362	-2.31795	-0.47175
C	-0.37023	-3.16256	0.329174
C	-0.14845	-2.82046	1.719873
C	1.383983	-1.17687	3.45479
C	1.960742	-2.4026	2.91489
C	1.213438	-3.20489	2.070785
C	1.831173	-3.79317	0.888716
C	0.849929	-3.77104	-0.18848
C	1.25122	-3.51342	-1.4861
C	0.452509	-2.63333	-2.33099
C	1.356908	-1.8506	-3.14945
C	1.050402	-0.52648	-3.41872
C	0.335366	2.822258	-0.54331
C	4.192082	0.962554	-2.17272
C	3.65068	2.126005	-1.65509
C	3.878617	2.477661	-0.25893
C	4.637871	1.648108	0.548693
C	5.20977	0.424399	0.002017
C	4.699214	-1.28938	-1.68974
C	3.71633	-1.27123	-2.76475
C	3.397777	0.12091	-3.06008
C	2.100353	0.481498	-3.3777
C	1.52461	1.700941	-2.82839
C	2.284652	2.505607	-1.99502
C	2.654118	3.073761	0.259496
C	2.25273	2.814794	1.556814
C	3.053619	1.945868	2.409604
C	4.214976	1.37556	1.916847
C	4.52571	-0.01647	2.215387
C	5.141649	-0.60431	1.032381
C	4.862531	-1.91448	0.685171
C	4.636613	-2.26648	-0.71111
C	2.722347	-2.2328	-2.81019
C	2.656206	-3.26203	-1.78001
C	3.588678	-3.27798	-0.75677
C	3.165715	-3.55046	0.611429
C	3.952552	-2.70744	1.502273
C	3.365567	-2.1488	2.62462
C	3.659581	-0.7685	2.990373
C	2.436513	-0.16878	3.506719
C	2.14197	1.153719	3.225835
C	1.669748	3.082632	-0.81635

C	0.847169	2.55236	1.843617
C	4.993203	0.090869	-1.32395
C	-3.42429	-0.06317	-1.59017
C	-2.95012	2.163064	-0.98721
O	-3.94822	1.251565	-1.427
H	-2.79358	2.847977	-1.86279
C	-3.50983	2.993441	0.186004
O	-4.18241	2.492017	1.063518
C	-3.20026	4.45207	0.170902
C	-3.05082	5.139392	-1.03618
C	-3.08624	5.147354	1.376986
C	-2.79089	6.503535	-1.0378
H	-3.1366	4.588538	-1.98508
C	-2.818	6.512118	1.371102
H	-3.21419	4.617398	2.328778
C	-2.672	7.191224	0.166456
H	-2.67971	7.036841	-1.98779
H	-2.7262	7.052373	2.31947
H	-2.46483	8.266688	0.164535
H	-3.4279	-0.22049	-2.69724
C	-4.34853	-1.07282	-0.95344
C	-5.01068	-0.82191	0.24723
C	-4.56075	-2.28592	-1.61526
C	-5.87134	-1.77174	0.786421
H	-4.86326	0.13247	0.771373
C	-5.41432	-3.24042	-1.08115
H	-4.05115	-2.49097	-2.56504
C	-6.07614	-2.98767	0.126618
H	-6.38466	-1.55192	1.733669
H	-5.56501	-4.18867	-1.61641
N	-7.0005	-4.01362	0.705198
O	-7.54147	-3.79827	1.771613
O	-7.19646	-5.04956	0.100136

Energy = 1.223173329463
-B3LYP/6-31G*//PM3-
E(RB+HF-LYP) = -3219.9161873

trans-**2a**
-PM3-

C	-1.22322	-1.02545	1.728664
C	-0.89312	0.311571	2.246413
C	-1.00499	1.405982	1.432249
C	-1.70675	1.413406	0.07437

C	-2.06283	-0.02808	-0.48429
C	-1.64356	-1.17334	0.433923
C	-0.29194	-1.96895	2.323434
C	0.608558	-1.23721	3.203074
C	0.23481	0.168999	3.151081
C	1.217495	1.144471	3.201169
C	0.036391	2.4072	1.463394
C	-0.677	2.172784	-0.75745
C	-0.24736	1.791969	-2.00052
C	-0.5783	0.455602	-2.51995
C	-1.31243	-0.41251	-1.75728
C	-0.91034	-1.79965	-1.70227
C	-1.11489	-2.27084	-0.34502
C	-0.23746	-3.19139	0.207352
C	0.18717	-3.03833	1.584447
C	1.940879	-1.5996	3.291429
C	2.44653	-2.71695	2.502537
C	1.591576	-3.41971	1.671955
C	2.031577	-3.81567	0.339793
C	0.898512	-3.67876	-0.56633
C	1.09478	-3.22832	-1.85851
C	0.164545	-2.2688	-2.44217
C	0.923776	-1.34771	-3.26426
C	0.560967	-0.0109	-3.29209
C	0.241805	2.880565	0.106383
C	3.834228	1.400987	-2.32414
C	3.361167	2.461019	-1.57101
C	3.792868	2.622512	-0.18817
C	4.677337	1.716084	0.371225
C	5.177163	0.601593	-0.42345
C	4.440497	-0.87681	-2.24882
C	3.306113	-0.74399	-3.15305
C	2.92676	0.663416	-3.19555
C	1.591108	1.017849	-3.26219
C	1.088253	2.12703	-2.46422
C	1.954132	2.835275	-1.64716
C	2.652636	3.096603	0.585595
C	2.456653	2.646346	1.877833
C	3.389199	1.695607	2.469327
C	4.470319	1.240799	1.733646
C	4.842191	-0.16735	1.780575
C	5.28027	-0.5624	0.447715
C	4.970297	-1.82045	-0.03834

C	4.540686	-1.98233	-1.42174
C	2.33026	-1.72439	-3.1883
C	2.435506	-2.88868	-2.31757
C	3.512275	-3.01407	-1.45635
C	3.305217	-3.48939	-0.0939
C	4.205702	-2.75126	0.782313
C	3.787566	-2.37563	2.047376
C	4.114013	-1.05023	2.559399
C	2.97483	-0.57192	3.331137
C	2.622602	0.76558	3.289192
C	1.51656	3.220711	-0.32043
C	1.11442	2.297141	2.328727
C	4.766885	0.448561	-1.73668
C	-3.59804	0.055137	-0.74385
C	-3.08439	2.124882	0.191148
O	-4.09803	1.142879	0.040334
H	-3.77015	0.317298	-1.8184
C	-4.37677	-1.18712	-0.39687
C	-4.80571	-1.45418	0.9035
C	-4.69426	-2.08156	-1.42236
C	-5.5417	-2.60017	1.179647
H	-4.56666	-0.7578	1.716883
C	-5.42413	-3.23139	-1.1534
H	-4.36807	-1.87782	-2.4502
C	-5.85342	-3.49689	0.152208
H	-5.87261	-2.79027	2.210754
H	-5.66075	-3.92348	-1.97423
H	-3.25668	2.508308	1.223696
C	-3.31292	3.271584	-0.81827
O	-3.45675	3.06691	-2.00511
C	-3.41356	4.634499	-0.22473
C	-2.43034	5.101915	0.64842
C	-4.49719	5.449856	-0.55419
C	-2.53432	6.376794	1.191385
H	-1.569	4.465435	0.896369
C	-4.60022	6.721558	-0.00026
H	-5.26252	5.088954	-1.25123
C	-3.62072	7.185532	0.871212
H	-1.75889	6.74401	1.871977
H	-5.45336	7.359025	-0.25577
H	-3.70217	8.188566	1.303349
N	-6.64487	-4.73413	0.446849
O	-7.00923	-4.95258	1.585256

O	-6.91055	-5.50191	-0.45671

Energy = 1.222637618734
-B3LYP/6-31G*//PM3-
E(RB+HF-LYP) = -3219.9206030

2.7 Cartesian coordinates for ring opening of **1a** at the B3LYP/6-31G* level
epoxide **1a**

C	5.407714	2.077835	-0.02182
C	4.105191	2.339446	-0.44932
C	3.151978	1.321437	-0.4507
C	3.492738	0.030343	-0.01509
C	4.805508	-0.21852	0.421535
C	5.756541	0.79544	0.413934
C	2.527307	-1.10801	0.029796
O	2.820594	-2.17941	0.53736
C	1.13454	-0.92887	-0.5393
O	0.484145	-2.13389	-0.94848
C	-0.01519	-1.50345	0.221981
C	-1.37338	-0.89428	0.164486
C	-2.04661	-0.75062	-1.05711
C	-3.3051	-0.16032	-1.10352
C	-3.88276	0.282809	0.085564
C	-3.24125	0.142912	1.315145
C	-1.98453	-0.45258	1.346828
H	0.24769	-2.01917	1.146493
H	-1.57993	-1.12287	-1.96323
H	-1.47352	-0.57586	2.29811
H	-3.84505	-0.04327	-2.03503
H	-3.72946	0.493516	2.215916
H	0.933766	-0.07967	-1.18796
H	2.143992	1.550671	-0.78031
H	5.051695	-1.21913	0.761037
H	3.830281	3.335858	-0.78336
H	6.769744	0.590903	0.748367
H	6.150002	2.871423	-0.02676
N	-5.21209	0.911198	0.042931
O	-5.69901	1.29129	1.107685
O	-5.75707	1.02172	-1.05509

E(RB+HF-LYP) = -933.729545556

TS1

C	0.000000	0.000000	0.000000
C	1.418020	0.000000	0.000000

C	2.106812	1.23945	0.000000
C	1.402872	2.43198	-0.02795
C	0.005537	2.3948	-0.03366
C	-0.70534	1.190327	-0.01796
C	2.120493	-1.23532	-0.03362
O	3.461299	-1.25721	-0.13638
C	3.799111	-2.1151	0.888924
C	4.602323	-3.26274	0.550797
O	4.8296	-3.53721	-0.63546
N	-0.73961	3.657772	-0.04719
O	-1.97011	3.594709	-0.05242
C	5.133653	-4.11563	1.664229
C	5.17201	-3.70536	3.006389
C	5.683411	-4.55212	3.989229
C	6.161101	-5.81771	3.643447
C	6.134562	-6.23101	2.308328
C	5.628623	-5.38443	1.326306
O	-0.09019	4.704523	-0.05295
H	1.614659	-2.19388	-0.01264
H	3.190961	1.242839	0.021864
H	-0.53495	-0.94556	0.006169
H	1.907818	3.389999	-0.03416
H	-1.78791	1.212281	-0.02005
H	3.434748	-1.84329	1.869494
H	4.829776	-2.71445	3.289797
H	5.605955	-5.68078	0.282708
H	5.714542	-4.22135	5.023815
H	6.510455	-7.2134	2.03538
H	6.557159	-6.47755	4.41077

E(RB+HF-LYP) = -933.668045586

INT1

C	-0.54903	1.351625	-0.13672
C	1.748921	0.748226	-0.06387
O	0.446212	0.519359	-0.04244
H	-0.32321	2.410125	-0.25102
C	-1.8789	0.840463	-0.08496
C	-2.14	-0.54656	0.057012
C	-2.9686	1.739081	-0.17838
C	-3.44287	-1.00951	0.105163
H	-1.3067	-1.23836	0.125504
C	-4.2732	1.275743	-0.13045
H	-2.77982	2.803557	-0.28824

C	-4.49854	-0.09544	0.011559
H	-3.66328	-2.06429	0.213333
H	-5.11858	1.948865	-0.19987
H	2.069164	1.775949	-0.19408
C	2.587632	-0.42503	0.019582
O	2.100313	-1.56148	0.056382
C	4.073844	-0.21731	0.026708
C	4.688332	1.011259	0.315737
C	4.880338	-1.33078	-0.25389
C	6.078261	1.124665	0.312197
H	4.091281	1.880956	0.574202
C	6.267304	-1.21564	-0.26418
H	4.390755	-2.27706	-0.45915
C	6.870406	0.013621	0.017023
H	6.542496	2.07905	0.545518
H	6.880936	-2.08383	-0.48909
H	7.953374	0.103954	0.011597
N	-5.87534	-0.58731	0.063422
O	-6.04631	-1.80146	0.189567
O	-6.78427	0.241803	-0.02199

E(RB+HF-LYP) = -933.693935272

TS2

C	0.000000	0.000000	0.000000
C	1.411314	0.000000	0.000000
C	2.115602	1.225436	0.000000
C	1.419995	2.423766	-0.00206
C	0.022642	2.390803	-0.00178
C	-0.70071	1.197261	-0.00295
C	2.100293	-1.25889	-0.05061
O	3.380454	-1.30379	-0.06611
C	3.966378	-2.62509	-0.0926
C	3.687507	-3.24548	-1.33665
O	2.967686	-2.67727	-2.19772
C	4.190427	-4.63994	-1.54633
C	5.255834	-5.16341	-0.80111
C	5.679966	-6.47603	-1.0063
C	5.052372	-7.2724	-1.96723
C	4.000946	-6.74943	-2.7251
C	3.57263	-5.44006	-2.51709
H	1.552396	-2.19797	0.002476
H	3.199832	1.216249	0.000804
H	-0.53917	-0.94294	-0.00561

H	1.929648	3.379091	-0.0018
H	-1.78289	1.227862	-0.00323
H	3.832479	-3.14212	0.851829
H	5.764873	-4.52758	-0.08186
H	2.761371	-5.01236	-3.09746
H	6.509713	-6.87303	-0.42714
H	3.516587	-7.36397	-3.47972
H	5.388096	-8.29303	-2.13204
N	-0.71619	3.665795	0.004445
O	-1.94513	3.60899	0.000175
O	-0.05609	4.703658	0.014262

E(RB+HF-LYP) = -933.657964911

INT2

C	6.877636	-0.27519	0.042738
C	6.051013	-1.35935	-0.25886
C	4.666555	-1.19716	-0.2886
C	4.091198	0.054596	-0.01785
C	4.93185	1.14065	0.269017
C	6.313793	0.976389	0.304465
C	2.613538	0.312151	-0.0369
O	2.176233	1.482141	-0.11285
C	1.736451	-0.80508	0.067172
O	0.401726	-0.68654	0.06129
C	-0.35189	0.372631	-0.06216
C	-1.77098	0.196847	-0.03497
C	-2.39179	-1.06643	0.124235
C	-3.77145	-1.17407	0.144694
C	-4.54763	-0.01856	0.006116
C	-3.96838	1.242019	-0.15291
C	-2.58648	1.345305	-0.17297
H	0.144085	1.327432	-0.1776
H	-1.77762	-1.95379	0.231375
H	-2.12011	2.318559	-0.29585
H	-4.26383	-2.13105	0.265583
H	-4.60519	2.11158	-0.25729
H	2.029673	-1.83225	0.217306
H	4.04236	-2.04561	-0.55273
H	4.474852	2.106133	0.459061
H	6.484553	-2.3314	-0.47774
H	6.953573	1.824228	0.534198
H	7.956411	-0.40396	0.067665
N	-6.00731	-0.13454	0.028596

O	-6.49026	-1.25983	0.169182
O	-6.66622	0.899654	-0.09431

E(RB+HF-LYP) = -933.702300109

TS1'

C	0.000000	0.000000	0.000000
C	1.411891	0.000000	0.000000
C	2.094741	1.241671	0.000000
C	1.390636	2.429785	0.004307
C	-0.0106	2.39509	0.022838
C	-0.71284	1.19212	0.021321
C	2.075009	-1.27479	-0.13299
O	3.399668	-1.46654	-0.04457
C	3.474349	-1.25423	1.3408
C	2.823298	-2.1943	2.215158
O	1.841271	-2.86971	1.857406
N	-0.75353	3.656486	0.03854
O	-1.98441	3.597333	0.045346
C	3.361529	-2.33623	3.607069
C	4.654612	-1.94216	3.988931
C	5.085879	-2.1151	5.303372
C	4.233814	-2.68548	6.25113
C	2.94902	-3.090000	5.8785
C	2.517703	-2.91955	4.566328
O	-0.10267	4.703379	0.043458
H	1.50867	-2.11972	-0.51514
H	3.179447	1.258329	-0.01622
H	-0.53198	-0.94675	-0.00198
H	1.895895	3.387538	-0.00888
H	-1.79562	1.205986	0.033971
H	4.242773	-0.55254	1.640536
H	5.340265	-1.52581	3.257576
H	1.525733	-3.23057	4.256377
H	6.090445	-1.812	5.58538
H	2.284542	-3.53727	6.612758
H	4.571251	-2.81791	7.275613

E(RB+HF-LYP) = -933.659551040

INT1'

C	0.000000	0.000000	0.000000
C	1.41998	0.000000	0.000000
C	2.095517	1.245797	0.000000
C	1.376351	2.433113	-0.01781

C	-0.01632	2.390161	0.01348
C	-0.71833	1.180562	0.023417
C	2.042276	-1.27841	-0.1215
O	3.300797	-1.62394	-0.14486
C	4.409403	-1.02245	0.33541
C	4.369619	-0.23756	1.526979
O	3.292115	0.014804	2.102453
N	-0.76899	3.648975	0.026989
O	-1.99923	3.578836	0.041698
C	5.680372	0.208907	2.103433
C	6.856593	0.302321	1.344309
C	8.043258	0.73732	1.933327
C	8.067663	1.08272	3.286181
C	6.897347	1.001971	4.045915
C	5.710614	0.572707	3.457425
O	-0.12782	4.700687	0.018898
H	1.421785	-2.12309	-0.40628
H	3.173781	1.283824	-0.03977
H	-0.53085	-0.94797	-0.00936
H	1.878087	3.392432	-0.03729
H	-1.80076	1.190294	0.041664
H	5.288311	-1.55954	0.007712
H	6.842886	0.06336	0.284422
H	4.788837	0.51359	4.026975
H	8.946893	0.813334	1.334531
H	6.911101	1.277267	5.097105
H	8.993314	1.420521	3.744544

E(RB+HF-LYP) = -933.686980862

INT2'

C	0.000000	0.000000	0.000000
C	1.422625	0.000000	0.000000
C	2.083681	1.256162	0.000000
C	1.359608	2.439906	-0.01747
C	-0.03347	2.393301	-0.0444
C	-0.72359	1.176765	-0.02877
C	2.045181	-1.28524	0.050241
O	3.299303	-1.61319	-0.10051
C	4.401089	-0.96449	-0.43352
C	5.614916	-1.75772	-0.43581
O	5.62732	-2.9242	-0.03283
N	-0.7903	3.645202	-0.07998
O	-2.02039	3.569021	-0.08315

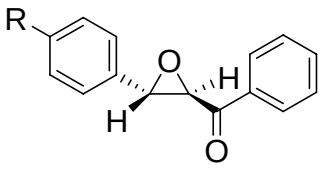
C	6.873433	-1.08352	-0.90139
C	6.890858	0.072496	-1.69777
C	8.101822	0.635835	-2.09963
C	9.308612	0.053833	-1.70763
C	9.300769	-1.10261	-0.92229
C	8.092519	-1.66958	-0.5279
O	-0.15281	4.699827	-0.10428
H	1.442397	-2.16507	0.241743
H	3.160696	1.319163	0.066275
H	-0.52711	-0.94975	0.012994
H	1.857183	3.401856	-0.00692
H	-1.80643	1.177919	-0.04049
H	4.335257	0.077303	-0.70108
H	5.963202	0.52419	-2.0377
H	8.062447	-2.57287	0.072553
H	8.10254	1.525585	-2.7234
H	10.23838	-1.56157	-0.62048
H	10.25155	0.496144	-2.01784

E(RB+HF-LYP) = -933.685236572

3. Computational details for the reaction of C_{60} with **1b**, **1c** and **3a-c** at the B3LYP/6-31G*// AM1 level

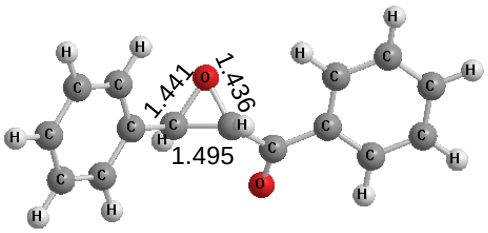
3.1 Optimized geometries

AM1-optimized geometries for the reaction of C_{60} with *trans*-2-benzoyl-3- aryloxiranes (**1b** and **1c**).

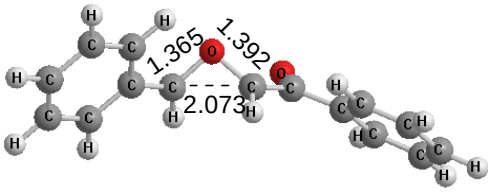


trans-**1**

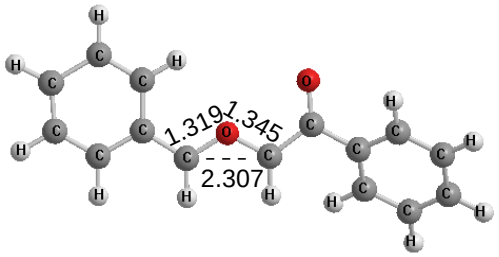
trans-**1b**, R = H
trans-**1c**, R = CH_3



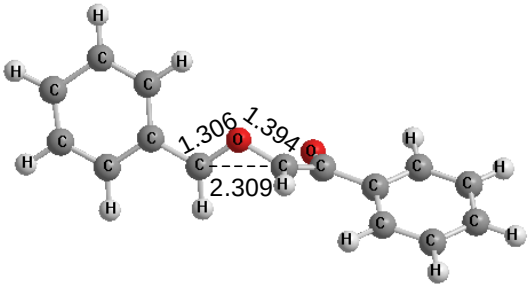
trans-epoxide (**1b**)



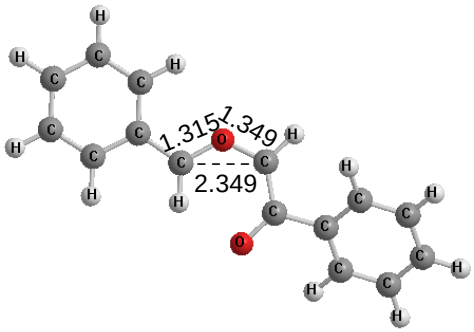
TS1 (303.59i cm^{-1})



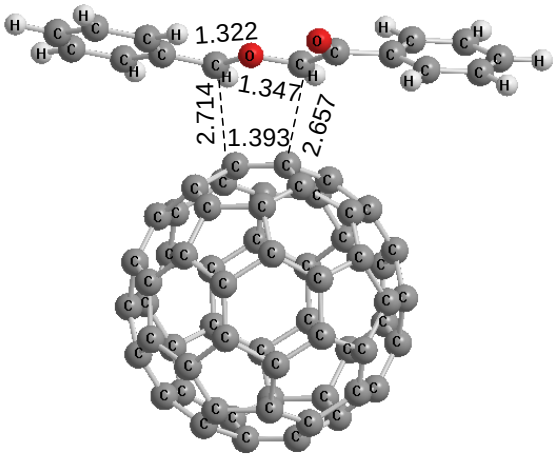
INT1



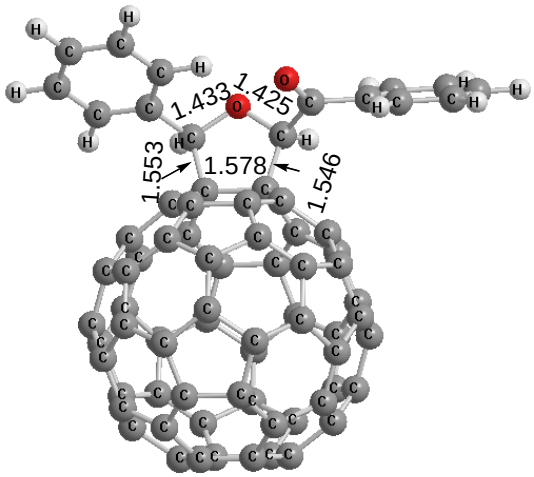
TS2 (363.39i cm^{-1})



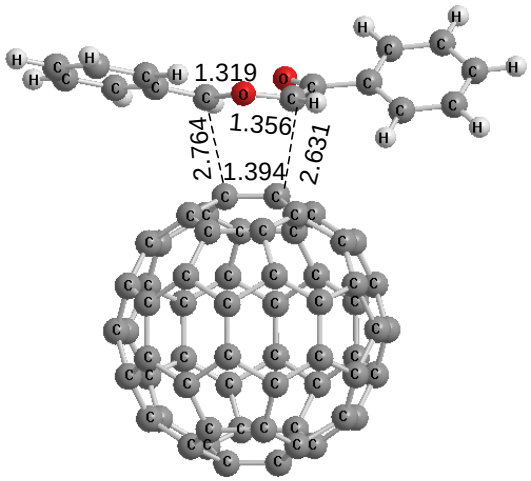
INT2



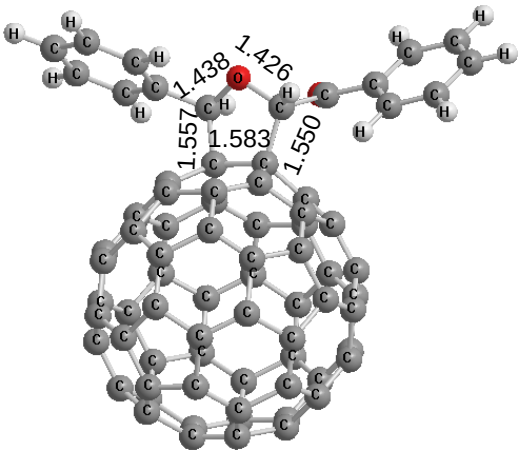
TS3 (71.15i cm^{-1})



cis-**2b**

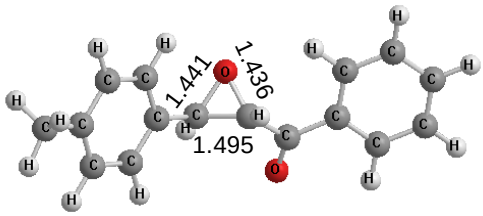


TS4 (110.38i cm^{-1})

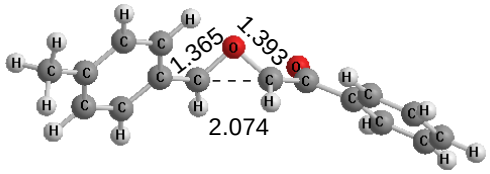


trans-**2b**

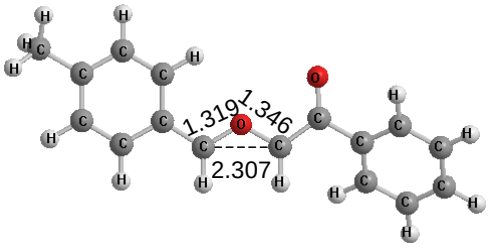
Figure S22. AM1-optimized geometries for the reaction of C_{60} with **1b** (R = H).



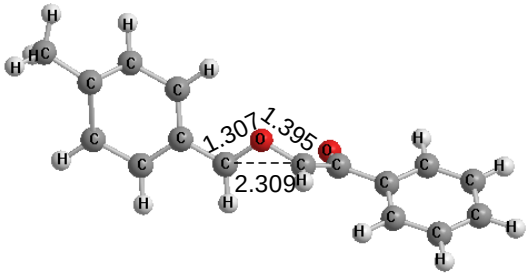
trans-epoxide (**1c**)



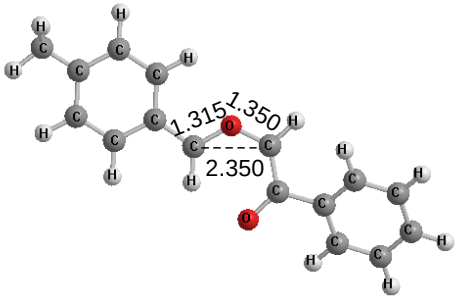
TS1 (297.82i cm^{-1})



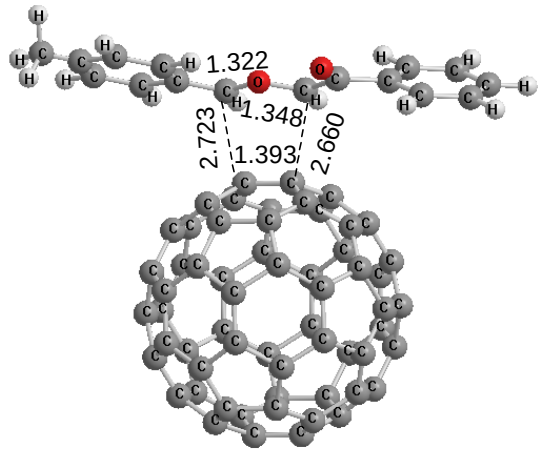
INT1



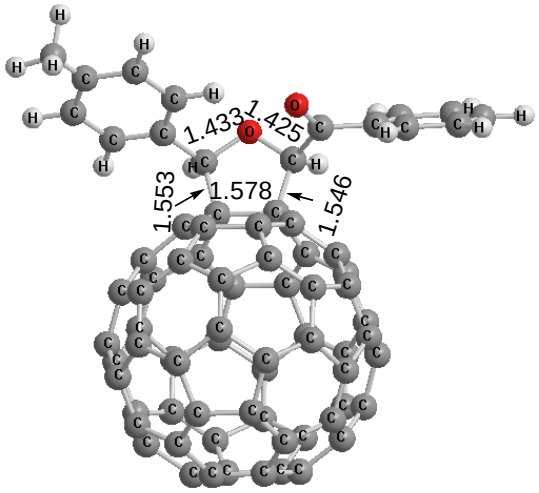
TS2 (340.70i cm^{-1})



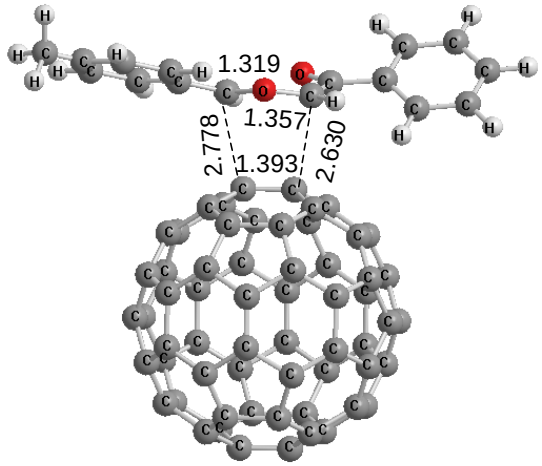
INT2



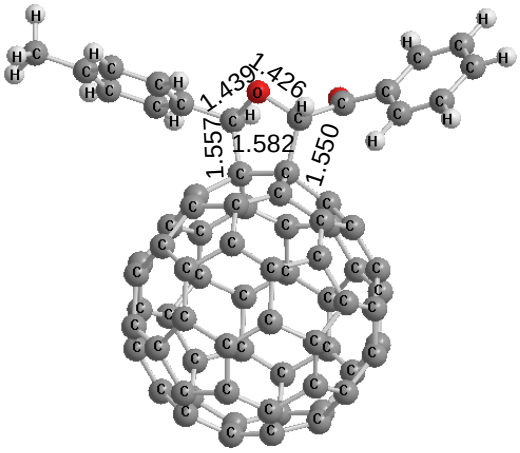
TS3 (70.32i cm^{-1})



cis-**2c**



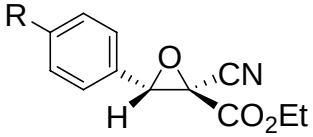
TS4 (108.92i cm^{-1})



trans-**2c**

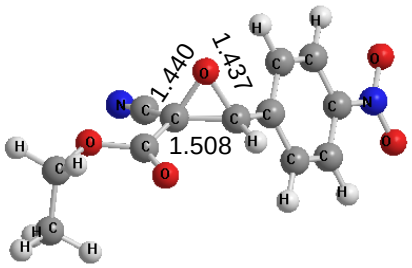
Figure S23. AM1-optimized geometries for the reaction of C_{60} with **1c** (R = CH_3)

AM1-optimized geometries for the reaction of C_{60} with *trans*-2-cyano-2-ethoxycarbonyl-3-aryloxiranes (**3a-c**, Figure S22-Figure S24).

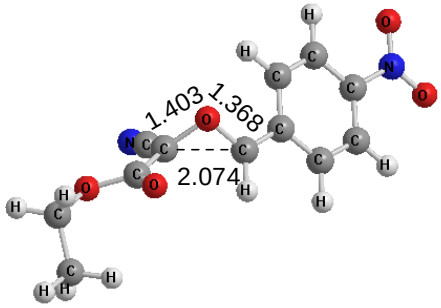


trans-**3**

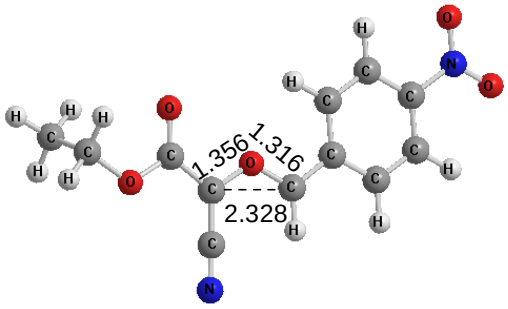
trans-**3a**, R = NO_2
trans-**3b**, R = H
trans-**3c**, R = OCH_3



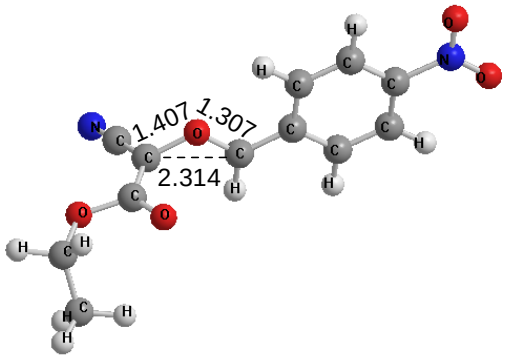
trans-epoxide (**3a**)



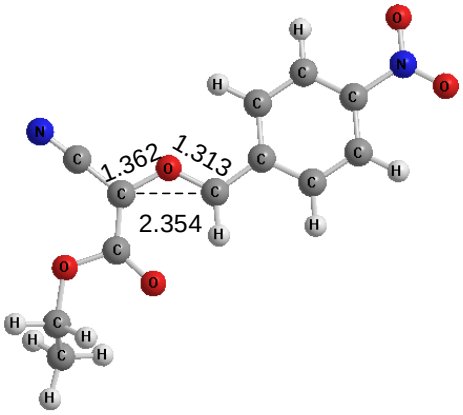
TS1 (254.67i cm^{-1})



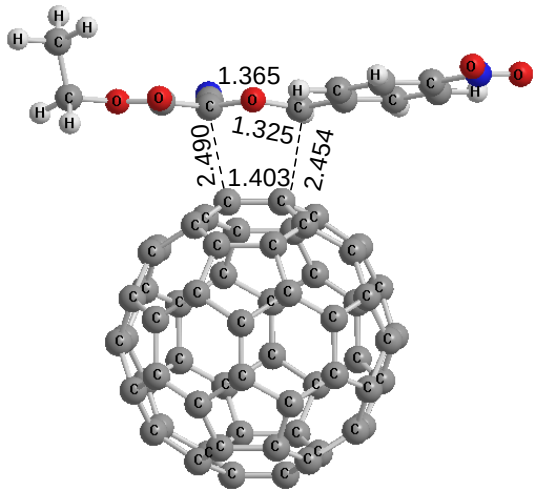
INT1



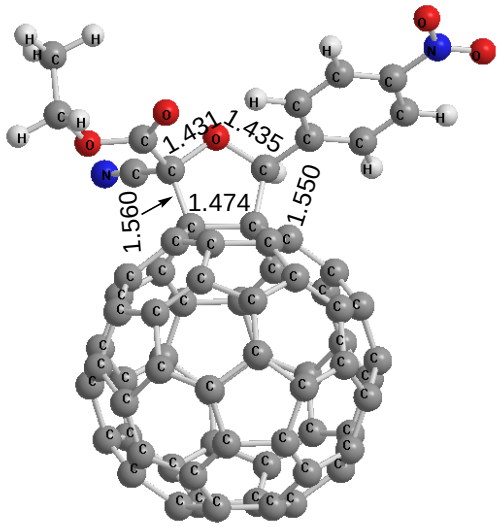
TS2 (199.53i cm^{-1})



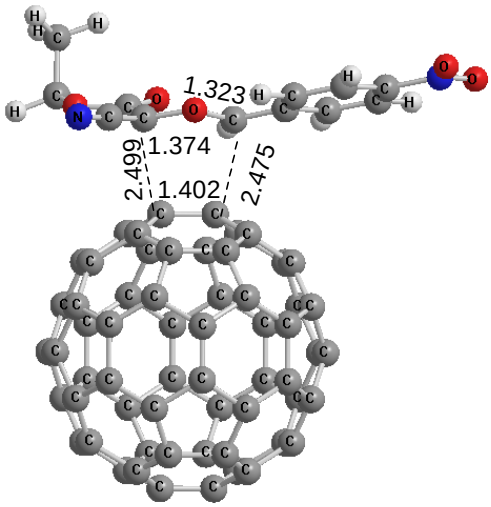
INT2



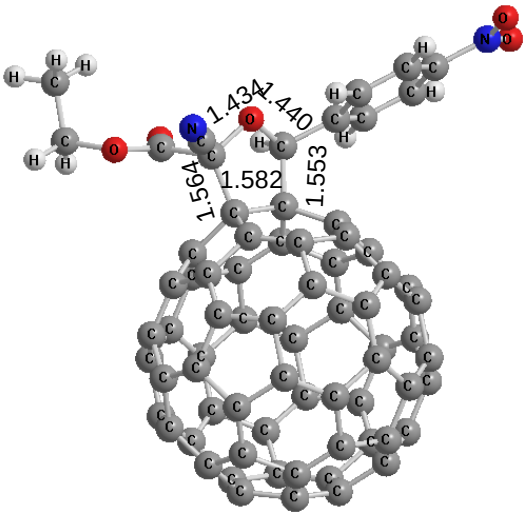
TS3 (171.21i cm^{-1})



cis-**4a**

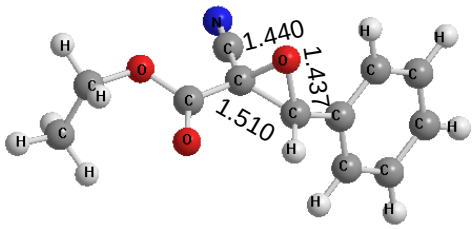


TS4 (154.23i cm^{-1})

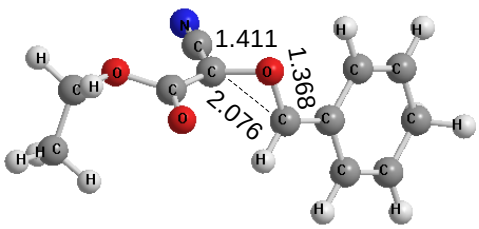


trans-**4a**

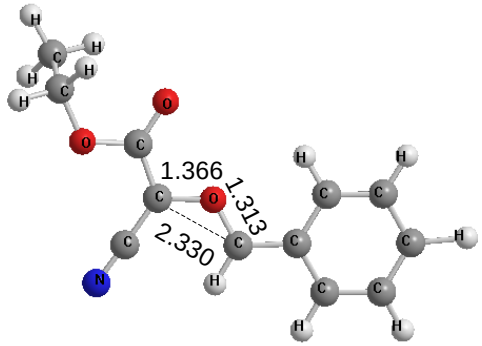
Figure S24. AM1-optimized geometries for the reaction of C_{60} with **3a** (R = NO_2).



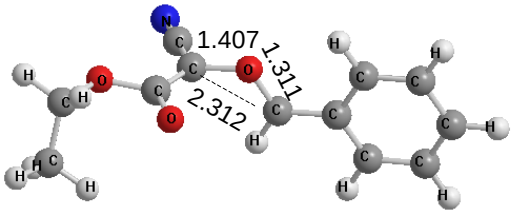
trans-epoxide (**3b**)



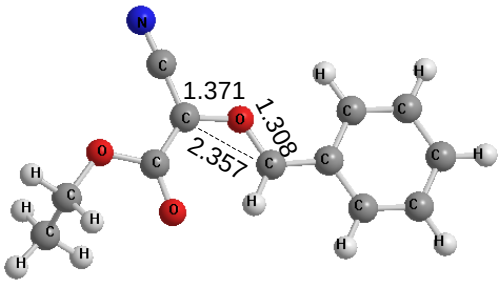
TS1 (256.00i cm^{-1})



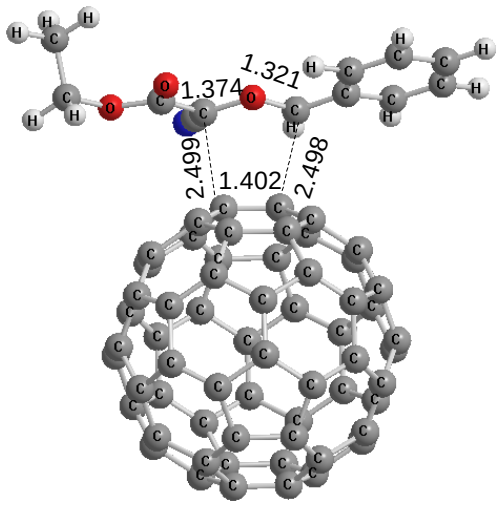
INT1



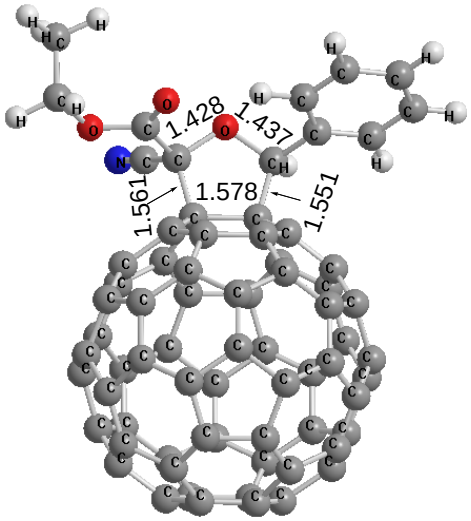
TS2 (117.49i cm^{-1})



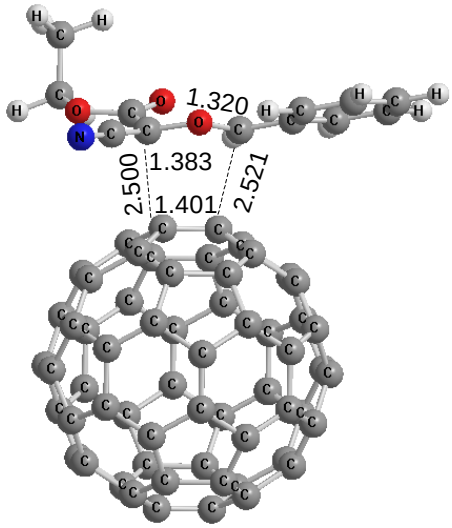
INT2



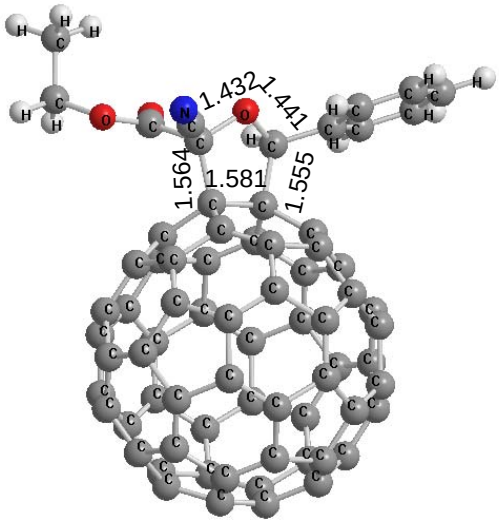
TS3 (147.19i cm^{-1})



cis-**4b**

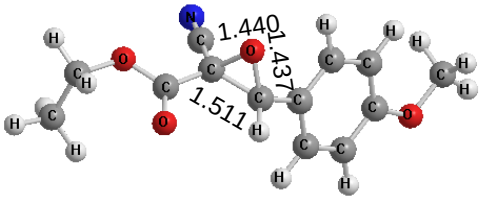


TS4 (138.33i cm^{-1})

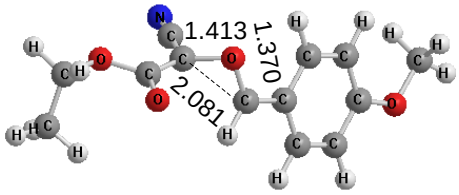


trans-**4b**

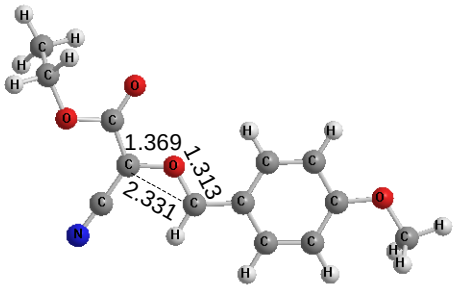
Figure S25. AM1-optimized geometries for the reaction of C_{60} with **3b** (R = H).



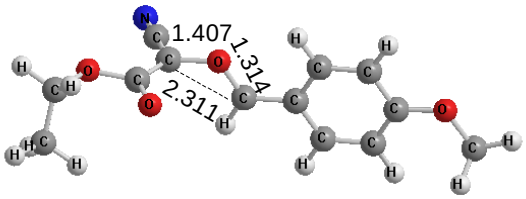
trans-epoxide (**3c**)



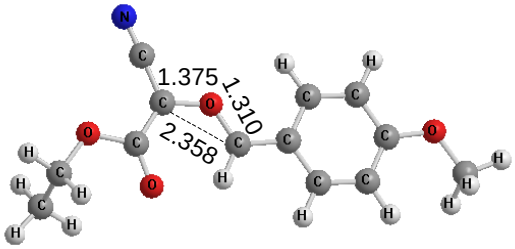
TS1 (243.50i cm^{-1})



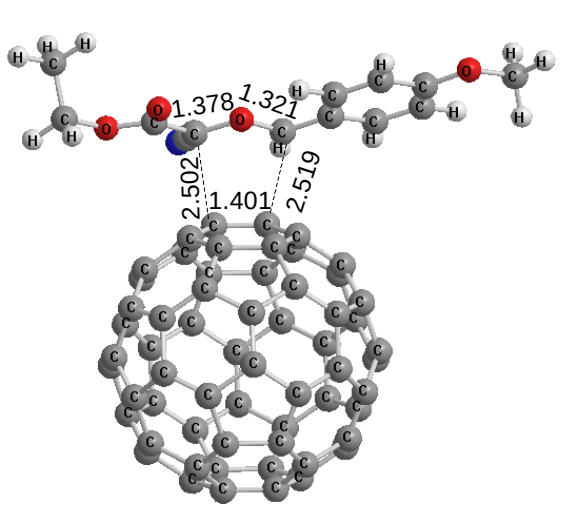
INT1



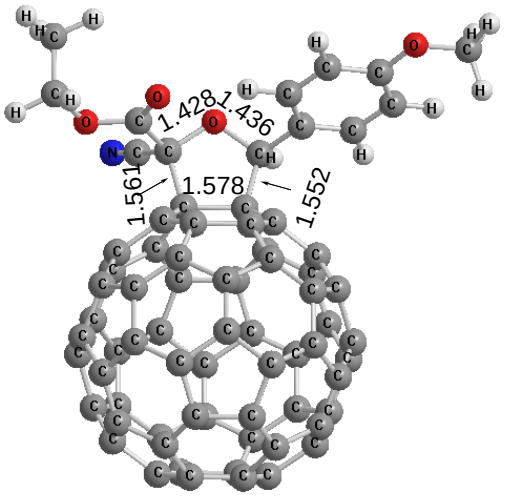
TS2 (117.49i cm^{-1})



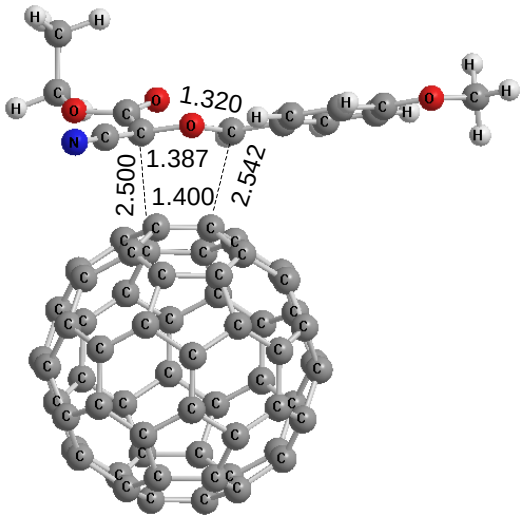
INT2



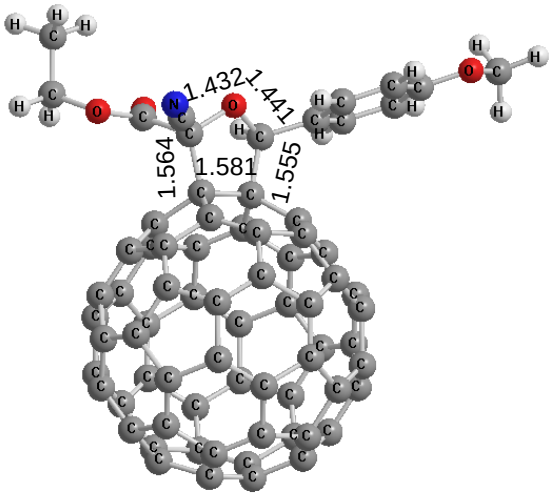
TS3 (142.14i cm^{-1})



cis -**4c**



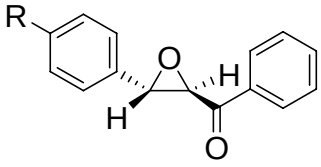
TS4 (133.60i cm^{-1})



trans-**4c**

Figure S26. AM1-optimized geometries for the reaction of C_{60} with **3c** (R = OCH_3).

3.2 IRCs for the ring opening of epoxides and 1,3-dipolar cycloaddition to C_{60}
IRCs for the reaction of C_{60} with epoxides **1b** and **1c**



trans-**1**

trans-**1a**, R = NO_2
trans-**1b**, R = H
trans-**1c**, R = CH_3

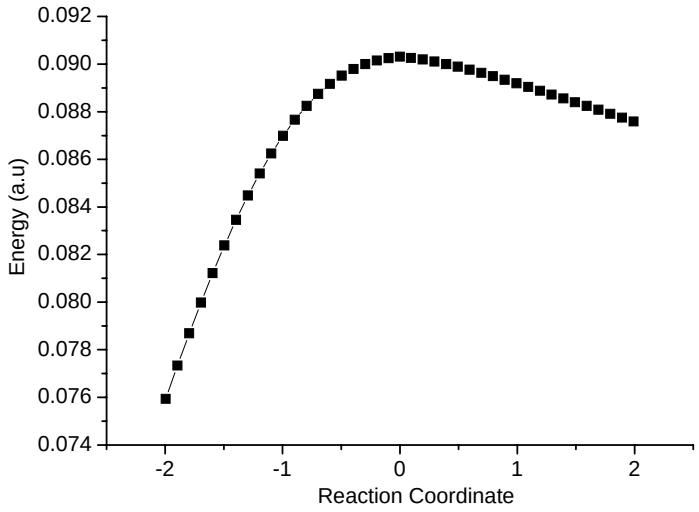


Figure S27. IRC for TS1 of the reaction of C_{60} with **1b** (R = H).

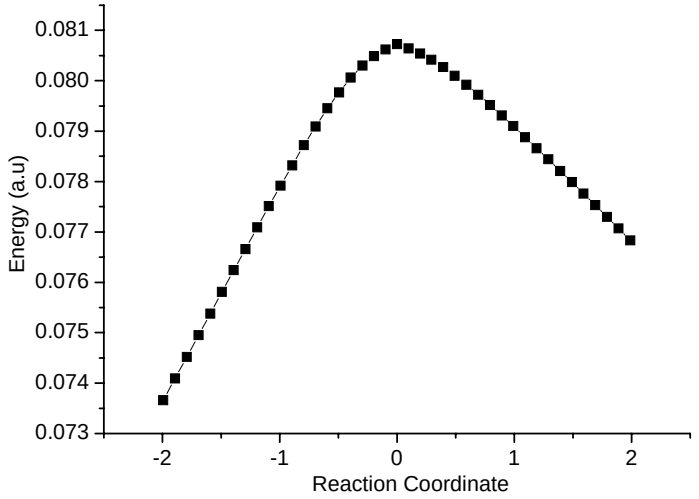


Figure S28. IRC for TS2 of the reaction of C_{60} with **1b** (R = H).

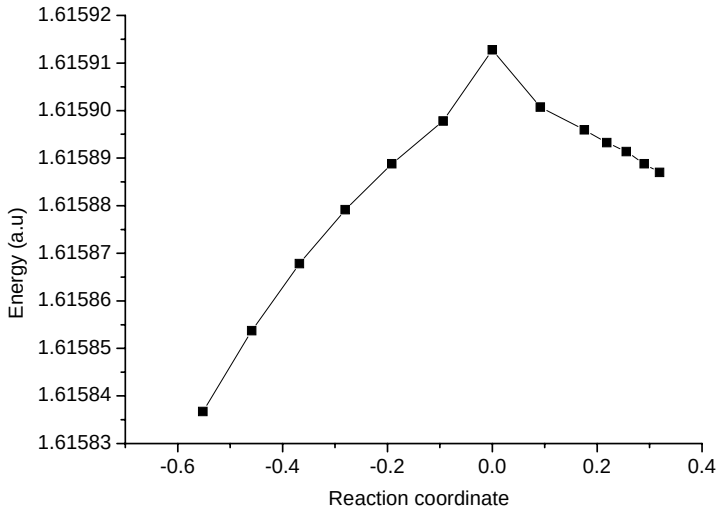


Figure S29. IRC for TS3 of the reaction of C_{60} with **1b** (R = H).

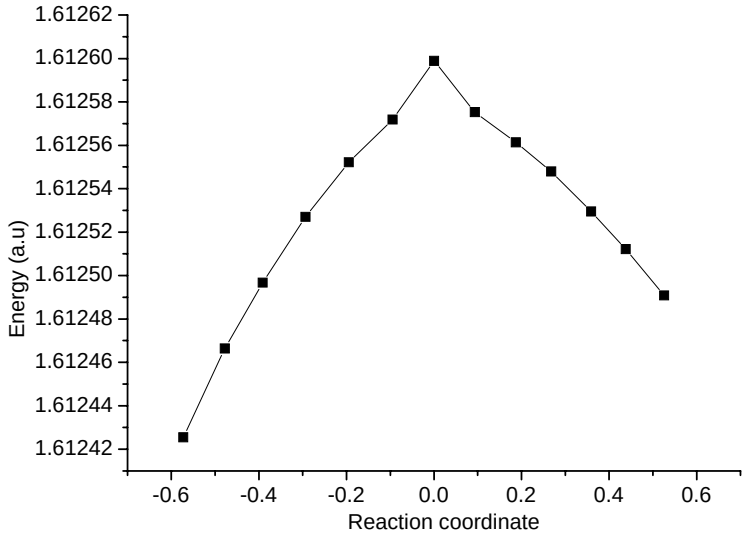


Figure S30. IRC for TS4 of the reaction of C_{60} with **1b** (R = H).

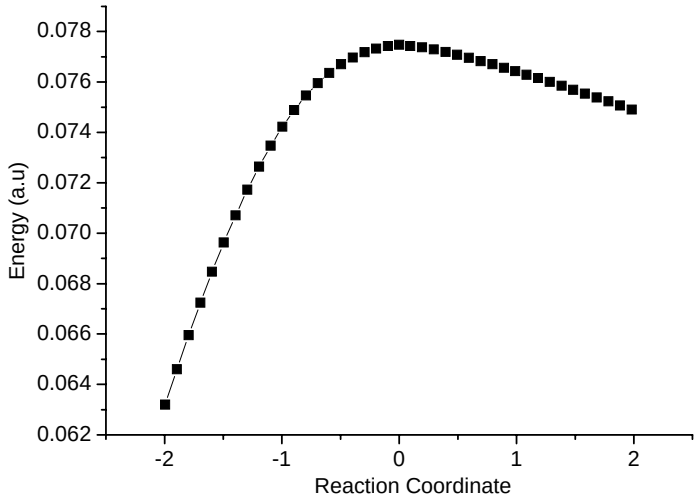


Figure S31. IRC for TS1 of reaction of C_{60} with **1c** (R = CH_3).

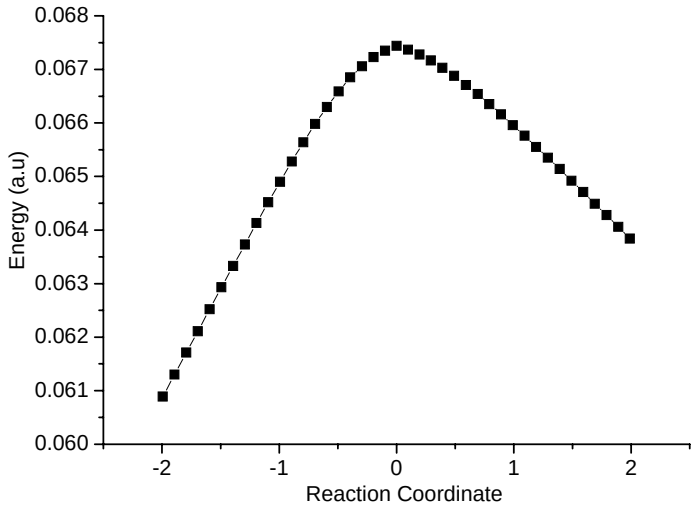


Figure S32. IRC for TS2 of reaction of C_{60} with **1c** (R = CH_3).

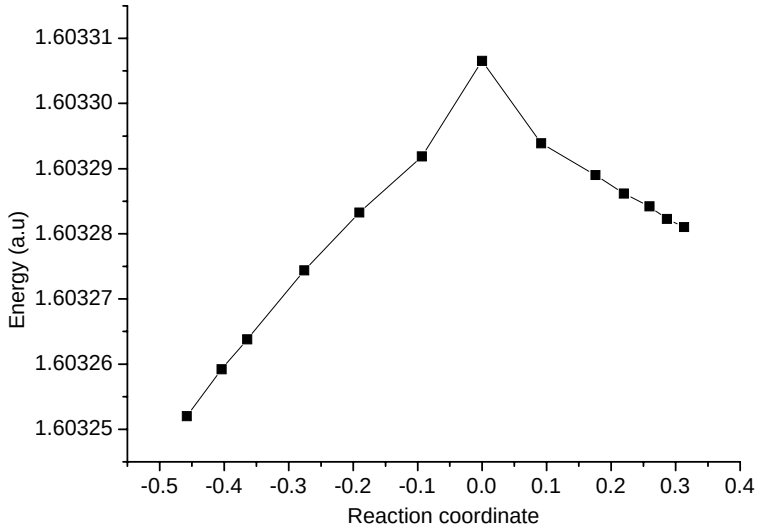


Figure S33. IRC for TS3 of reaction of C_{60} with **1c** (R = CH_3).

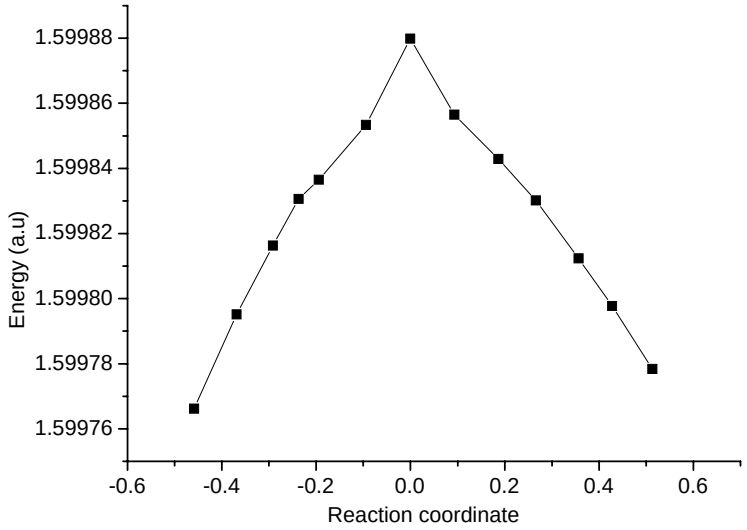
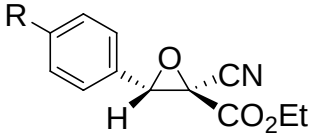


Figure S34. IRC for TS4 of reaction of C_{60} with **1c** (R = CH_3).

IRCs for the reaction of C_{60} with **3a-c**



trans-**3**

trans-**3a**, R = NO_2
trans-**3b**, R = H
trans-**3c**, R = OCH_3

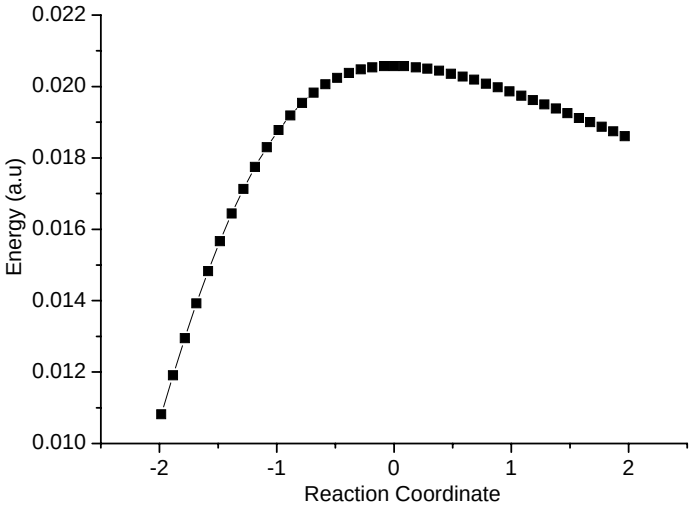


Figure S35. IRC for TS1 of reaction of C_{60} with **3a** (R = NO_2).

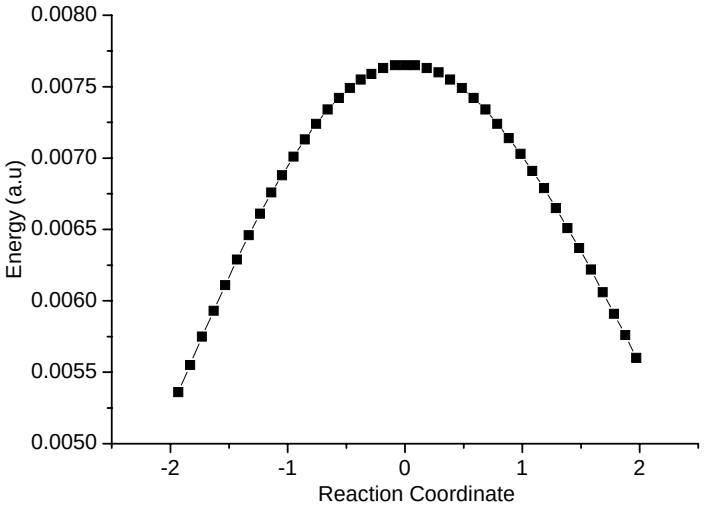


Figure S36. IRC for TS2 of reaction of C_{60} with **3a** (R = NO_2).

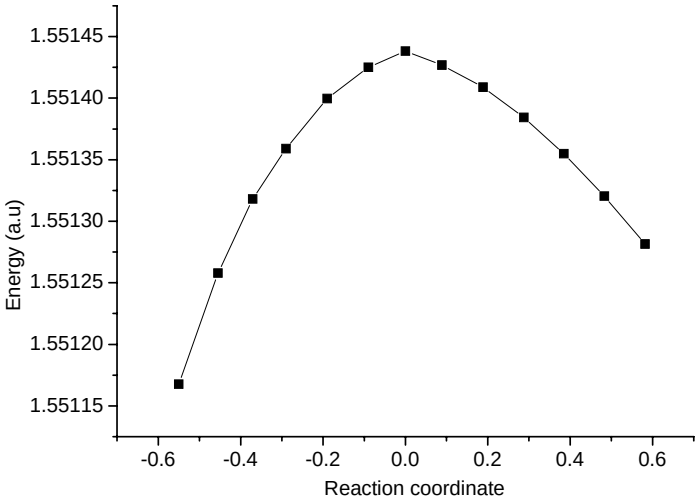


Figure S37. IRC for TS3 of reaction of C_{60} with **3a** (R = NO_2).

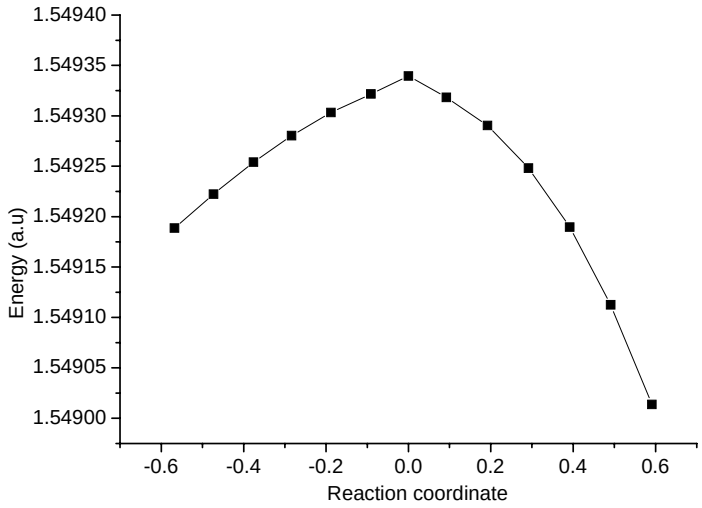


Figure S38. IRC for TS4 of reaction of C_{60} with **3a** (R = NO_2).

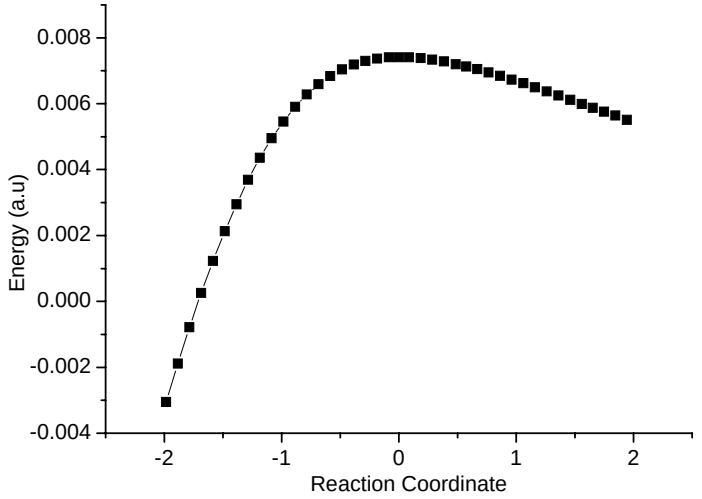


Figure S39. IRC for TS1 of reaction of C_{60} with **3b** (R = H).

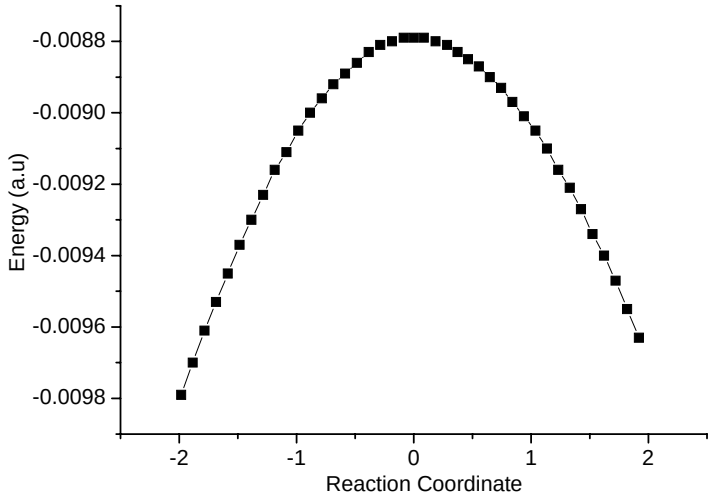


Figure S40. IRC for TS2 of reaction of C_{60} with **3b** (R = H).

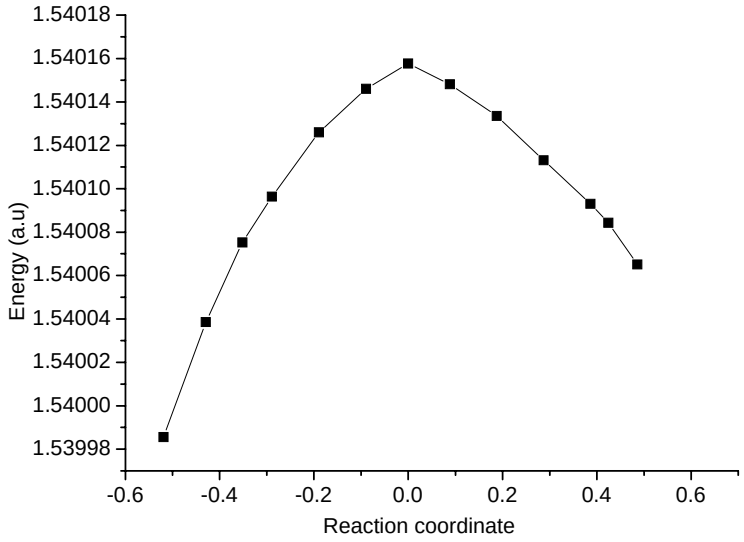


Figure S41. IRC for TS3 of reaction of C_{60} with **3b** (R = H).

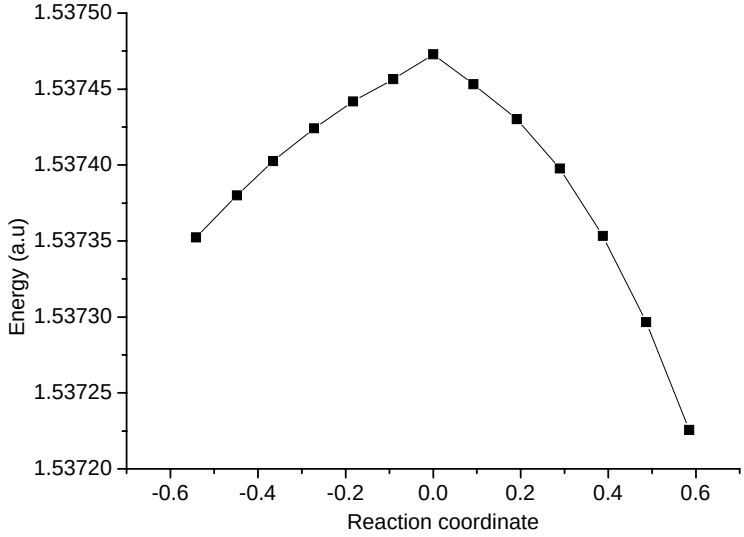


Figure S42. IRC for TS4 of reaction of C_{60} with **3b** (R = H).

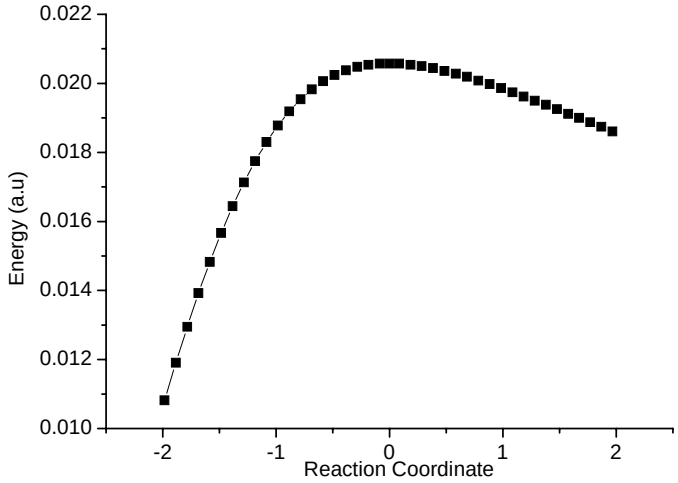


Figure S43. IRC for TS1 of reaction of C_{60} with **3c** (R = OCH_3).

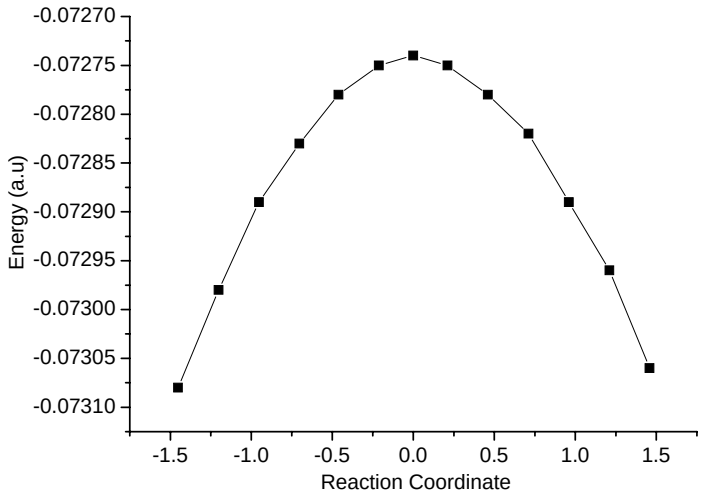


Figure S44. IRC for TS2 of reaction of C_{60} with **3c** (R = OCH_3).

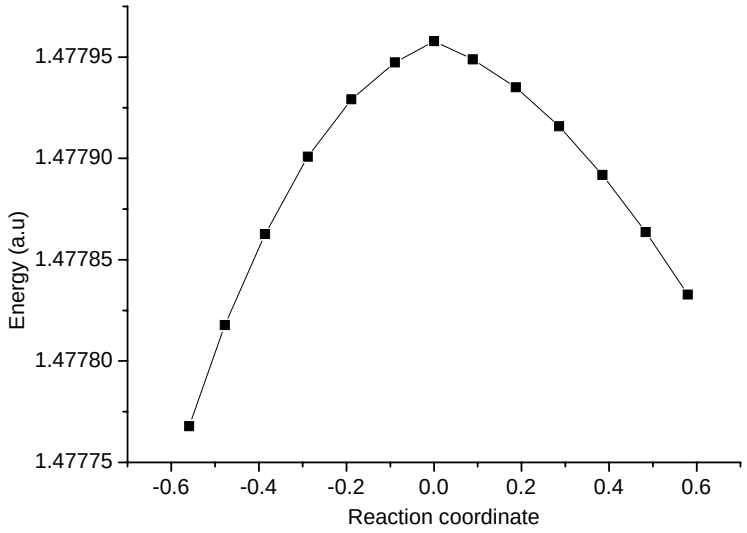


Figure S45. IRC for TS3 of reaction of C_{60} with **3c** (R = OCH_3).

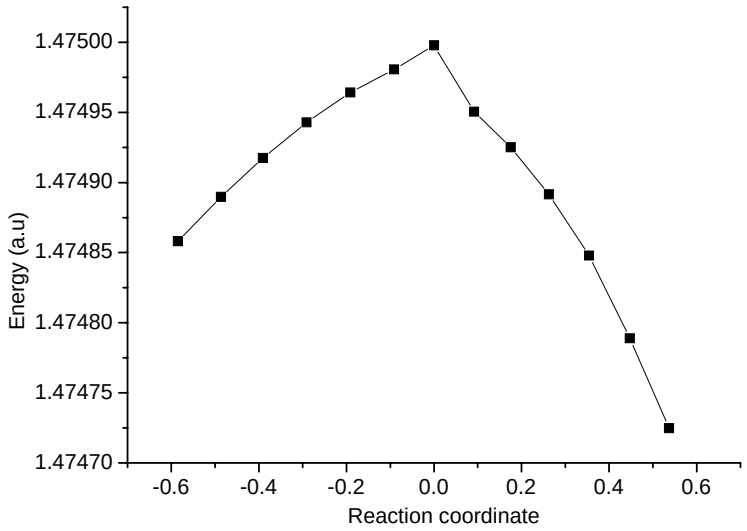
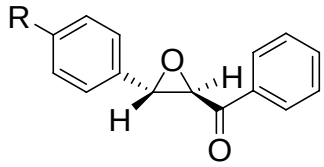


Figure S46. IRC for TS4 of the reaction of C_{60} with **3c** (R = OCH_3).

3.3 Cartesian coordinates

Reaction of C_{60} with *trans*-2-benzoyl-3-aryloxiranes (**1a-c**)



trans-**1**

trans-**1a**, R = NO_2
trans-**1b**, R = H
trans-**1c**, R = CH_3

Reaction of C_{60} with **1b** (R = H)

trans-epoxide (**1b**)

-AM1-

C	4.970806	-0.975115	-0.449688
C	3.849853	-1.726058	-0.093399
C	2.623317	-1.097739	0.113100
C	2.514850	0.291082	-0.033137
C	3.645767	1.043288	-0.379760
C	4.868134	0.408874	-0.592042
C	1.229249	0.978581	0.188002
O	1.147917	2.188818	0.422271
C	-0.001887	0.132207	0.059337
O	-0.399557	-0.598318	1.229532
C	-1.253610	0.479695	0.799210
C	-2.582291	0.124326	0.273572
C	-3.031782	-1.200729	0.262750
C	-4.299621	-1.503785	-0.231231
C	-5.122490	-0.488282	-0.717838
C	-4.677565	0.834175	-0.706880
C	-3.412757	1.143406	-0.210578
H	-1.240903	1.356796	1.482480
H	-2.377755	-1.996504	0.652586
H	-3.063921	2.187058	-0.197920
H	-4.649968	-2.546397	-0.235232
H	-5.326173	1.636144	-1.089028
H	-0.045261	-0.453910	-0.881187
H	1.740991	-1.689896	0.406577
H	3.555899	2.137355	-0.476871
H	3.933042	-2.816295	0.027056
H	5.752523	1.001980	-0.867873
H	5.937010	-1.474926	-0.615348
H	-6.122214	-0.728955	-1.108168

Energy = 0.027982330003

-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -729.221948502

TS1
-AM1-

C	5.141615	1.148318	0.620254
C	4.085056	1.867915	0.061816
C	2.909534	1.214504	-0.305421
C	2.786408	-0.166493	-0.115700
C	3.855461	-0.887865	0.431813
C	5.026380	-0.229813	0.803274
C	1.550906	-0.889697	-0.500634
O	1.577849	-2.085316	-0.845772
C	0.326503	-0.133121	-0.401452
O	-0.782513	-0.590193	-1.108079
C	-1.566908	-0.892489	-0.032273
C	-2.862844	-0.287816	0.092822
C	-3.342449	0.620603	-0.867394
C	-4.610505	1.178854	-0.728899
C	-5.410347	0.839804	0.362631
C	-4.941307	-0.062130	1.320949
C	-3.675570	-0.623264	1.192724
H	-1.189101	-1.624265	0.697862
H	-2.706402	0.878534	-1.729607
H	-3.306579	-1.334932	1.947147
H	-4.981521	1.887883	-1.484242
H	-5.575132	-0.328931	2.179935
H	0.225490	0.834277	0.091638
H	2.083824	1.784292	-0.758357
H	3.759839	-1.978596	0.554407
H	4.179293	2.952718	-0.092331
H	5.861517	-0.799810	1.236008
H	6.066827	1.666864	0.911713
H	-6.412335	1.282179	0.469578

Energy = 0.090311314353
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -729.166579309

INT1
-AM1-

C	1.706171	-0.906699	-0.230839
C	-0.544525	-0.417374	-0.103374
O	0.741202	-0.031509	-0.021960

H	1.471063	-1.949705	-0.480259
C	3.062214	-0.430879	-0.110945
C	3.356879	0.904888	0.206769
C	4.113312	-1.341472	-0.322226
C	4.682592	1.319694	0.311097
H	2.534348	1.619323	0.371621
C	5.433353	-0.916266	-0.215742
H	3.888970	-2.389075	-0.571872
C	5.721205	0.413101	0.100785
H	4.907737	2.367573	0.560332
H	6.253154	-1.630915	-0.381768
H	-0.794249	-1.450758	-0.344780
C	-1.507650	0.641863	0.103526
O	-1.187792	1.829035	0.287327
C	-2.925168	0.211763	0.055537
C	-3.327678	-1.035240	0.546175
C	-3.879524	1.087608	-0.478442
C	-4.670364	-1.406480	0.491439
H	-2.588057	-1.718944	0.989344
C	-5.219503	0.709172	-0.537594
H	-3.557883	2.076986	-0.840931
C	-5.615789	-0.538002	-0.054387
H	-4.983798	-2.385620	0.881988
H	-5.964792	1.397992	-0.961665
H	-6.673939	-0.834988	-0.099447
H	6.767015	0.743859	0.183833

Energy = 0.061077640509
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -729.185170431

TS2
-AM1-

C	-3.917284	1.069439	0.781785
C	-2.998775	0.318672	0.024553
C	-3.453349	-0.756932	-0.757421
C	-4.810259	-1.071353	-0.783612
C	-5.716644	-0.321637	-0.033500
C	-5.269475	0.747440	0.748376
C	-1.595571	0.658283	0.087958
O	-0.750606	0.009671	-0.668250
C	0.586759	0.401612	-0.621352
C	1.419965	-0.353689	0.229319
O	0.975476	-1.187161	1.058366

C	2.881247	-0.116617	0.100470
C	3.397855	1.131260	-0.262686
C	4.775926	1.313931	-0.374918
C	5.645970	0.252873	-0.126879
C	5.136308	-0.992256	0.242180
C	3.760293	-1.176705	0.360229
H	-1.245863	1.478060	0.747773
H	-2.726780	-1.349003	-1.339919
H	-3.563411	1.908417	1.401650
H	-5.164408	-1.915683	-1.394888
H	-5.988570	1.333447	1.340833
H	0.829648	1.221254	-1.286546
H	2.717663	1.974150	-0.453856
H	3.344884	-2.149978	0.666541
H	5.176190	2.297548	-0.659448
H	5.820712	-1.828928	0.443552
H	6.731820	0.398155	-0.219243
H	-6.788638	-0.573438	-0.054392

Energy = 0.080726409739
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -729.153568826

INT2
-AM1-

C	-5.626296	-0.306528	-0.039860
C	-4.776314	-1.300191	0.445805
C	-3.399151	-1.086461	0.485185
C	-2.865136	0.127274	0.038237
C	-3.723472	1.128597	-0.434950
C	-5.098774	0.908173	-0.478306
C	-1.406082	0.390625	0.068794
O	-0.968876	1.546215	0.275582
C	-0.571895	-0.741466	-0.172389
O	0.776861	-0.756592	-0.182498
C	1.520649	0.300452	0.061017
C	2.953279	0.104834	0.019300
C	3.535700	-1.139475	-0.268764
C	4.921826	-1.272005	-0.296590
C	5.737086	-0.169886	-0.038639
C	5.163672	1.070457	0.248262
C	3.779941	1.213044	0.278452
H	1.079521	1.284732	0.288516
H	2.890301	-2.007842	-0.472269

H	3.328579	2.191365	0.504661
H	5.372998	-2.249616	-0.522909
H	5.807326	1.939434	0.451512
H	-0.940258	-1.745052	-0.418685
H	-2.735202	-1.869500	0.881523
H	-3.296923	2.090233	-0.761818
H	-5.192175	-2.254373	0.800806
H	-5.768035	1.695468	-0.854919
H	-6.711999	-0.479340	-0.073014
H	6.831783	-0.277164	-0.061393

Energy = 0.054693405090
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -729.195581643

TS3
-AM1-

C	1.012874	1.485251	1.881998
C	1.186612	0.066230	2.200211
C	1.631593	-0.810628	1.226932
C	1.952846	-0.325031	-0.120535
C	1.783503	1.023902	-0.423360
C	1.292288	1.944498	0.606979
C	-0.173907	1.965558	2.590471
C	-0.734129	0.844799	3.347672
C	0.106868	-0.328714	3.105915
C	-0.471057	-1.581884	2.990982
C	1.017641	-2.132862	1.103772
C	1.498563	-1.344365	-1.075596
C	0.928246	-0.972389	-2.279968
C	0.754334	0.446719	-2.599200
C	1.160215	1.411491	-1.693992
C	0.317655	2.582961	-1.452912
C	0.399586	2.912652	-0.030148
C	-0.722386	3.370665	0.640287
C	-1.017794	2.883561	1.987801
C	-2.106809	0.702161	3.460345
C	-2.998503	1.672050	2.822138
C	-2.468997	2.732471	2.106309
C	-3.070577	3.127742	0.831528
C	-1.990820	3.522603	-0.074724
C	-2.068359	3.210747	-1.421488
C	-0.881700	2.728368	-2.130208
C	-1.309446	1.707475	-3.086696

C	-0.513295	0.597133	-3.313732
C	0.935407	-2.462650	-0.319249
C	-3.056857	-1.991562	-2.569250
C	-2.213944	-2.909172	-1.965255
C	-2.509381	-3.397980	-0.617297
C	-3.632033	-2.942879	0.053549
C	-4.523196	-1.972929	-0.585166
C	-4.417286	-0.092374	-2.178803
C	-3.337800	0.303134	-3.084930
C	-2.496605	-0.870523	-3.325918
C	-1.123793	-0.727576	-3.437226
C	-0.232519	-1.696953	-2.798223
C	-0.762667	-2.757847	-2.083123
C	-1.240759	-3.548459	0.097372
C	-1.163266	-3.236076	1.443944
C	-2.350189	-2.755616	2.153428
C	-3.550241	-2.612863	1.477394
C	-4.390927	-1.439050	1.718726
C	-4.992308	-1.043559	0.444022
C	-5.156556	0.297893	0.142590
C	-4.861077	0.786705	-1.205279
C	-2.760693	1.556443	-2.968819
C	-3.229784	2.485798	-1.939537
C	-4.250819	2.111597	-1.082269
C	-4.169020	2.441527	0.341655
C	-4.728839	1.320621	1.098609
C	-4.159681	0.946601	2.304278
C	-3.986063	-0.471651	2.622987
C	-2.717556	-0.622636	3.337710
C	-1.922288	-1.732954	3.109594
C	-0.161549	-3.151734	-0.808810
C	-0.002226	-2.509696	1.961408
C	-4.243676	-1.510561	-1.860135
C	4.368298	1.742849	-0.834803
C	4.591537	-0.508863	-0.375332
O	4.794291	0.779316	-0.036167
H	4.174259	-0.766079	-1.349685
C	5.112481	-1.464432	0.585433
O	5.559681	-1.130563	1.695360
C	5.056788	-2.881800	0.158774
C	5.238068	-3.252878	-1.178132
C	4.842909	-3.870048	1.129158
C	5.190368	-4.597879	-1.541934

H	5.434036	-2.487202	-1.943651
C	4.789239	-5.212643	0.759671
H	4.727314	-3.572052	2.183548
C	4.960838	-5.577584	-0.575768
H	5.336464	-4.885701	-2.593352
H	4.616204	-5.984395	1.524125
H	4.919752	-6.637733	-0.866512
H	3.909599	1.508953	-1.805232
C	4.635564	3.098977	-0.416317
C	5.209686	3.391215	0.831498
C	4.308185	4.149186	-1.292660
C	5.450449	4.714426	1.194230
H	5.467922	2.569085	1.518327
C	4.552061	5.466946	-0.919670
H	3.859392	3.926855	-2.272239
C	5.122630	5.752574	0.322523
H	5.900575	4.937921	2.173195
H	4.293986	6.286351	-1.607048
H	5.313007	6.796610	0.612419

Energy = 1.615912774921
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3015.35487897

TS4
-AM1-

C	-0.765158	1.808717	-1.838209
C	-0.878722	0.480539	-2.445023
C	-1.428482	-0.564653	-1.723983
C	-1.921012	-0.348087	-0.356783
C	-1.805078	0.914251	0.222017
C	-1.203465	2.011943	-0.541577
C	0.491550	2.406280	-2.289386
C	1.155672	1.449427	-3.176134
C	0.308485	0.259579	-3.271775
C	0.885867	-0.997567	-3.333467
C	-0.814297	-1.891060	-1.786286
C	-1.567910	-1.537241	0.429676
C	-1.153896	-1.412579	1.743642
C	-1.041332	-0.085279	2.352568
C	-1.348257	1.041187	1.609714
C	-0.498383	2.228692	1.706381
C	-0.409836	2.829697	0.375826
C	0.778448	3.398842	-0.050900

C	1.242607	3.181049	-1.421082
C	2.533780	1.318031	-3.145833
C	3.327234	2.136134	-2.227077
C	2.699363	3.041760	-1.388601
C	3.135521	3.175159	0.002567
C	1.948020	3.396444	0.829487
C	1.864896	2.826907	2.088770
C	0.607675	2.227631	2.540013
C	0.930407	1.035770	3.324555
C	0.128231	-0.089359	3.231746
C	-0.900917	-2.492201	-0.455126
C	2.780590	-2.508469	2.314003
C	2.030656	-3.282382	1.444548
C	2.495138	-3.501881	0.073701
C	3.684532	-2.935908	-0.353499
C	4.477394	-2.117929	0.565811
C	4.151162	-0.583032	2.469891
C	2.963948	-0.361214	3.296955
C	2.116429	-1.550922	3.200180
C	0.738486	-1.418672	3.168405
C	-0.054418	-2.235962	2.248601
C	0.573848	-3.142512	1.411390
C	1.325223	-3.497389	-0.806230
C	1.407934	-2.928198	-2.065543
C	2.665417	-2.330502	-2.517501
C	3.772025	-2.333950	-1.685025
C	4.619003	-1.143913	-1.588628
C	5.055013	-1.010454	-0.197557
C	5.162119	0.244840	0.376997
C	4.697792	0.464472	1.747807
C	2.387224	0.896191	3.357335
C	2.964961	2.003546	2.593704
C	4.088135	1.793769	1.811410
C	4.175764	2.395760	0.479867
C	4.839480	1.438460	-0.406647
C	4.426916	1.312276	-1.722458
C	4.313668	-0.014848	-2.329892
C	3.143873	-0.011239	-3.209804
C	2.342758	-1.136924	-3.301245
C	0.138199	-3.274089	0.020958
C	0.308309	-2.103229	-2.569185
C	4.037891	-1.910166	1.862418
C	-4.471047	1.642204	0.244855

C	-4.515823	-0.464739	-0.774631
O	-4.556310	0.888827	-0.834726
H	-4.390951	1.203025	1.253576
C	-4.628971	3.068211	0.054161
C	-4.789655	3.642344	-1.216935
C	-4.618255	3.894875	1.192191
C	-4.934194	5.021406	-1.346349
H	-4.801328	2.995995	-2.108343
C	-4.761530	5.271850	1.052185
H	-4.497875	3.449456	2.191892
C	-4.919316	5.837219	-0.214728
H	-5.059933	5.466572	-2.344705
H	-4.751489	5.916036	1.944267
H	-4.366581	-0.866279	-1.784208
C	-4.966677	-1.231874	0.349345
O	-5.223135	-0.720201	1.462751
C	-5.173304	-2.679168	0.110680
C	-4.406545	-3.393758	-0.816183
C	-6.167762	-3.343072	0.842702
C	-4.641847	-4.752859	-1.018848
H	-3.601442	-2.889771	-1.373633
C	-6.403091	-4.700300	0.633183
H	-6.751923	-2.778970	1.587427
C	-5.642465	-5.406036	-0.299268
H	-4.034522	-5.310222	-1.746952
H	-7.187323	-5.215081	1.207409
H	-5.828438	-6.477564	-0.464097
H	-5.032612	6.926714	-0.319918

Energy = 1.612598915459
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3015.36142676

cis-**2b**
-AM1-

C	1.186568	1.532549	1.580869
C	1.501095	0.114088	1.829790
C	1.899456	-0.687815	0.793017
C	2.298607	-0.189909	-0.594514
C	1.960861	1.327792	-0.862693
C	1.291092	2.037185	0.311661
C	0.067918	1.896944	2.446234
C	-0.312203	0.722614	3.230742
C	0.574142	-0.375304	2.847043

C	0.078020	-1.667156	2.775681
C	1.349511	-2.030206	0.704390
C	1.522289	-1.170665	-1.477339
C	0.782868	-0.824992	-2.576823
C	0.466381	0.592927	-2.827304
C	0.914366	1.550466	-1.957008
C	0.013776	2.623998	-1.576250
C	0.244384	2.923820	-0.169725
C	-0.817837	3.297510	0.640157
C	-0.911117	2.766965	1.993648
C	-1.645190	0.474568	3.511649
C	-2.678957	1.388900	3.021857
C	-2.321761	2.505257	2.284865
C	-3.102240	2.883661	1.105118
C	-2.172021	3.378149	0.088686
C	-2.390493	3.094184	-1.247485
C	-1.266013	2.712986	-2.104186
C	-1.731530	1.695342	-3.036961
C	-0.882980	0.655463	-3.382430
C	1.119581	-2.330230	-0.702094
C	-3.126429	-2.138656	-2.440149
C	-2.153642	-3.006053	-1.973039
C	-2.246742	-3.548499	-0.616175
C	-3.309075	-3.195252	0.199539
C	-4.338222	-2.279991	-0.295784
C	-4.563937	-0.358619	-1.827829
C	-3.635046	0.140081	-2.842492
C	-2.742418	-0.958620	-3.218032
C	-1.406265	-0.706636	-3.479717
C	-0.375859	-1.616814	-2.981244
C	-0.741961	-2.738453	-2.254197
C	-0.893123	-3.615415	-0.063107
C	-0.675102	-3.330282	1.272843
C	-1.797803	-2.961930	2.137041
C	-3.078491	-2.894082	1.613646
C	-3.965235	-1.792843	1.992007
C	-4.744508	-1.413744	0.812186
C	-5.041639	-0.081975	0.577115
C	-4.949749	0.460357	-0.779554
C	-3.144044	1.431768	-2.756451
C	-3.551427	2.297715	-1.648172
C	-4.429473	1.825202	-0.686716
C	-4.198776	2.126280	0.727436

C	-4.576846	0.947532	1.508285
C	-3.838064	0.589417	2.623789
C	-3.523821	-0.818860	2.872322
C	-2.170310	-0.889846	3.423836
C	-1.331745	-1.932512	3.068108
C	0.032964	-3.106902	-1.076891
C	0.480618	-2.522193	1.667164
C	-4.249675	-1.766808	-1.579222
C	3.309211	1.971188	-1.285474
C	3.813343	-0.307910	-0.880887
O	4.339493	0.978775	-1.195533
H	3.969817	-0.944707	-1.799528
C	4.632816	-0.871352	0.278523
O	4.915043	-0.186222	1.263407
C	5.081933	-2.272410	0.134979
C	5.622840	-2.746759	-1.065572
C	4.992791	-3.127746	1.241720
C	6.048472	-4.070801	-1.162564
H	5.736083	-2.075115	-1.930525
C	5.410725	-4.452872	1.136164
H	4.596806	-2.742017	2.194330
C	5.936406	-4.926126	-0.066255
H	6.476070	-4.439109	-2.106959
H	5.330744	-5.122822	2.005168
H	6.267917	-5.972127	-0.148428
H	3.254164	2.247772	-2.380532
C	3.708410	3.176124	-0.491349
C	4.461816	3.059204	0.681153
C	3.358923	4.447139	-0.966606
C	4.841524	4.203076	1.383386
H	4.762761	2.059290	1.039447
C	3.737296	5.585976	-0.259172
H	2.785391	4.548826	-1.900132
C	4.477519	5.465583	0.917687
H	5.432453	4.103626	2.305932
H	3.454844	6.581018	-0.632857
H	4.776155	6.366289	1.473857

Energy = 1.496828684663
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3015.41267569

trans-**2b**
-AM1-

C	-0.763829	1.799122	-1.865435
C	-1.031595	0.442784	-2.377664
C	-1.652612	-0.476626	-1.575153
C	-2.346186	-0.158359	-0.250646
C	-2.059535	1.297515	0.299498
C	-1.139219	2.128860	-0.589738
C	0.522482	2.230228	-2.406128
C	1.053445	1.159218	-3.248679
C	0.091849	0.057792	-3.227999
C	0.545163	-1.251902	-3.234684
C	-1.158003	-1.841946	-1.563501
C	-1.805907	-1.281408	0.629360
C	-1.316761	-1.116796	1.898573
C	-1.048911	0.238888	2.412744
C	-1.285376	1.327009	1.615089
C	-0.307279	2.401186	1.594863
C	-0.215953	2.897832	0.228473
C	1.002978	3.332987	-0.270044
C	1.386985	2.988073	-1.632258
C	2.412643	0.895311	-3.265127
C	3.322766	1.689538	-2.437258
C	2.824029	2.709012	-1.644214
C	3.328565	2.889789	-0.281468
C	2.202414	3.280402	0.568245
C	2.116056	2.807654	1.865479
C	0.825511	2.362125	2.394556
C	1.061313	1.207350	3.250892
C	0.145276	0.167396	3.250775
C	-1.249289	-2.339614	-0.197051
C	2.510009	-2.565444	2.431584
C	1.655055	-3.318988	1.645425
C	2.040160	-3.674782	0.278344
C	3.260645	-3.259150	-0.227994
C	4.164971	-2.464580	0.604529
C	4.067641	-0.781351	2.406599
C	2.942922	-0.386652	3.255324
C	1.976759	-1.487151	3.267056
C	0.618913	-1.216165	3.264172
C	-0.285581	-2.004998	2.428665
C	0.219336	-3.032313	1.647746
C	0.841897	-3.608027	-0.559800

C	0.928627	-3.135523	-1.856978
C	2.218613	-2.700179	-2.394562
C	3.352312	-2.758525	-1.600782
C	4.313152	-1.654580	-1.616348
C	4.816229	-1.473405	-0.253601
C	5.069026	-0.199977	0.227688
C	4.685329	0.155717	1.594944
C	2.497750	0.924347	3.249441
C	3.150358	1.915127	2.391216
C	4.214054	1.541312	1.586539
C	4.305596	2.041971	0.213721
C	4.833559	0.965711	-0.625971
C	4.355970	0.794776	-1.914807
C	4.088549	-0.551773	-2.423698
C	2.889842	-0.489404	-3.260592
C	1.981637	-1.534331	-3.248092
C	-0.280114	-3.203973	0.290115
C	-0.102074	-2.232890	-2.373900
C	3.800187	-2.127833	1.897569
C	-3.479656	1.912359	0.472708
C	-3.885321	-0.199877	-0.432594
O	-4.355296	1.145562	-0.372462
H	-3.810238	1.743923	1.540189
C	-3.610407	3.354425	0.105906
C	-3.927851	3.748528	-1.198260
C	-3.455258	4.324834	1.104308
C	-4.067962	5.101646	-1.504976
H	-4.078739	2.984054	-1.976030
C	-3.591138	5.675866	0.791528
H	-3.227596	4.020923	2.137290
C	-3.895834	6.066200	-0.512922
H	-4.317298	5.405570	-2.532262
H	-3.462069	6.434479	1.577492
H	-4.168779	-0.558580	-1.461451
C	-4.613025	-1.021505	0.628655
O	-4.786118	-0.568815	1.764558
C	-5.171516	-2.318837	0.201194
C	-4.586548	-3.078351	-0.818956
C	-6.321742	-2.797116	0.845720
C	-5.151206	-4.294828	-1.196827
H	-3.664892	-2.728277	-1.312170
C	-6.887353	-4.010680	0.459382
H	-6.768184	-2.204207	1.660576

C	-6.304086	-4.759596	-0.562552
H	-4.684572	-4.889413	-1.996226
H	-7.792705	-4.378093	0.965118
H	-6.750274	-5.718394	-0.866716
H	-4.004013	7.133309	-0.756762

Energy = 1.495759344633
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3015.42076201

Reaction of C_{60} with **1c** (R = CH_3)

trans-epoxide (**1c**)
-AM1-

C	5.347046	-1.103903	-0.521565
C	4.220293	-1.799595	-0.081382
C	3.021421	-1.123615	0.136884
C	2.946867	0.257856	-0.081874
C	4.084008	0.955031	-0.512892
C	5.278284	0.272822	-0.736446
C	1.691194	0.995504	0.150043
O	1.654285	2.218610	0.319910
C	0.432321	0.181623	0.115658
O	0.060964	-0.471538	1.339029
C	-0.778890	0.606769	0.882065
C	-2.136476	0.263905	0.428243
C	-2.624046	-1.045115	0.504397
C	-3.916914	-1.336934	0.077146
C	-4.740628	-0.326912	-0.433291
C	-4.249225	0.982447	-0.507714
C	-2.958912	1.278496	-0.077841
C	-6.120204	-0.634338	-0.874552
H	-0.713955	1.519186	1.514211
H	-1.977808	-1.839577	0.909974
H	-2.582415	2.311100	-0.135725
H	-4.293710	-2.368654	0.141692
H	-4.889126	1.782916	-0.908250
H	-6.833061	-0.488002	-0.023723
H	-6.432115	0.038586	-1.710947
H	-6.203933	-1.693410	-1.222146
H	0.335098	-0.453334	-0.788422
H	2.134982	-1.671573	0.496424
H	4.021548	2.044444	-0.667023
H	4.277033	-2.883723	0.096049

H	6.167469	0.822614	-1.078590
H	6.291167	-1.641382	-0.696304

Energy = 0.015659408667
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -768.538384537

TS1
-AM1-

C	5.521409	1.335339	0.597331
C	4.447314	1.972738	-0.023921
C	3.307331	1.248081	-0.368958
C	3.237587	-0.122181	-0.093779
C	4.324473	-0.761469	0.516914
C	5.459597	-0.032194	0.865778
C	2.040583	-0.920122	-0.453055
O	2.125364	-2.132675	-0.722653
C	0.784791	-0.212897	-0.420125
O	-0.292995	-0.762270	-1.110817
C	-1.076886	-1.038410	-0.027631
C	-2.399472	-0.488995	0.049671
C	-2.912215	0.335854	-0.967277
C	-4.204147	0.841822	-0.874878
C	-5.010141	0.536835	0.229084
C	-4.499582	-0.284906	1.244875
C	-3.209726	-0.792018	1.160909
C	-6.390799	1.062489	0.318909
H	-0.674286	-1.707430	0.748294
H	-2.279786	0.571201	-1.838845
H	-2.817317	-1.437289	1.962084
H	-4.597230	1.486472	-1.675870
H	-5.128572	-0.527049	2.115076
H	-7.106880	0.321068	-0.119147
H	-6.682267	1.242527	1.383145
H	-6.493443	2.022439	-0.244668
H	0.633917	0.779780	0.004849
H	2.467793	1.752489	-0.871298
H	4.271548	-1.845400	0.706982
H	4.499642	3.048695	-0.245219
H	6.308812	-0.537779	1.348247
H	6.418404	1.910039	0.871030

Energy = 0.077484645806
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -768.484239416

INT1
-AM1-

C	-1.214159	0.996936	-0.243210
C	1.022989	0.450409	-0.106550
O	-0.273189	0.095587	-0.037152
H	1.299178	1.479582	-0.336155
C	1.957646	-0.633824	0.095849
O	1.608193	-1.814672	0.267486
C	3.385915	-0.238820	0.059478
C	3.816929	0.992670	0.564660
C	4.320912	-1.133010	-0.478336
C	5.168812	1.330599	0.520616
H	3.092265	1.690240	1.010903
C	5.670258	-0.787860	-0.526733
H	3.976467	-2.110451	-0.852031
C	6.095112	0.444101	-0.028954
H	5.504528	2.297676	0.922495
H	6.400343	-1.490978	-0.953744
H	7.160571	0.714877	-0.065737
H	-0.950878	2.036260	-0.480121
C	-2.582152	0.555374	-0.137324
C	-2.915381	-0.775410	0.162221
C	-3.609763	1.493136	-0.344393
C	-4.250006	-1.157876	0.253324
H	-2.113241	-1.513770	0.323438
C	-4.939666	1.102247	-0.251514
H	-3.358390	2.537836	-0.580961
C	-5.274076	-0.225575	0.049057
H	-4.502092	-2.203508	0.487273
H	-5.739179	1.840388	-0.416040
C	-6.693022	-0.631699	0.161933
H	-6.823859	-1.710117	-0.101905
H	-7.047882	-0.483415	1.213583
H	-7.339944	-0.020328	-0.514401

Energy = 0.048526952301
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -768.50237103

TS2
-AM1-

C	-3.426957	1.188097	0.779329
C	-2.522688	0.414408	0.027475
C	-3.003646	-0.656620	-0.745629

C	-4.364375	-0.943394	-0.768669
C	-5.265455	-0.173117	-0.022088
C	-4.783579	0.895262	0.750758
C	-1.114609	0.724411	0.086624
O	-0.283010	0.050537	-0.663615
C	1.061813	0.417343	-0.620058
C	1.882512	-0.348914	0.232314
O	1.426366	-1.171769	1.065754
C	-6.710763	-0.491175	-0.032794
C	3.347679	-0.137098	0.100228
C	3.884793	1.101391	-0.265272
C	5.265548	1.260436	-0.380565
C	6.117891	0.184963	-0.133230
C	5.587806	-1.050905	0.238200
C	4.209096	-1.211706	0.359288
H	-0.746599	1.543186	0.737592
H	-2.291122	-1.268079	-1.325775
H	-3.056082	2.024901	1.392492
H	-4.735664	-1.784065	-1.375309
H	-5.488957	1.502104	1.339255
H	-6.945517	-1.200316	0.802206
H	-7.326119	0.431503	0.108811
H	-7.009413	-0.974199	-0.995865
H	1.319939	1.226977	-1.291748
H	3.218532	1.955460	-0.455909
H	3.777732	-2.177369	0.667576
H	5.681930	2.236784	-0.666943
H	6.258262	-1.898900	0.439045
H	7.205847	0.311590	-0.227987

Energy = 0.067444551504
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -768.472144604

INT2
-AM1-

C	6.094953	-0.339929	0.049142
C	5.237906	-1.325493	-0.440565
C	3.862705	-1.099982	-0.483377
C	3.337768	0.117465	-0.035885
C	4.203282	1.110611	0.441393
C	5.576535	0.878439	0.488241
C	1.880917	0.393168	-0.069959
O	1.454734	1.553243	-0.276401

C	1.037172	-0.731612	0.167296
O	-0.312620	-0.735117	0.174322
C	-1.045929	0.329070	-0.069554
C	-2.479647	0.147713	-0.031319
C	-3.077089	-1.090116	0.253065
C	-4.462762	-1.210173	0.277672
C	-5.277526	-0.100830	0.020624
C	-4.680279	1.134874	-0.264464
C	-3.296850	1.262794	-0.290937
C	-6.751898	-0.225649	0.062396
H	-0.594729	1.309484	-0.294724
H	-2.441623	-1.966073	0.456374
H	-2.836569	2.237511	-0.515619
H	-4.922538	-2.185011	0.500325
H	-5.314226	2.010899	-0.469774
H	-7.125212	0.029085	1.086958
H	-7.233049	0.471114	-0.667633
H	-7.074231	-1.268720	-0.177734
H	1.395652	-1.738796	0.412783
H	3.193095	-1.876609	-0.882785
H	3.783923	2.075253	0.768683
H	5.646584	-2.282631	-0.795916
H	6.251419	1.659388	0.867981
H	7.179033	-0.522005	0.085092

Energy = 0.042073169516
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -768.512857150

TS3
-AM1-

C	-1.147774	-1.236842	1.833112
C	-1.094876	0.184776	2.181321
C	-1.383818	1.141676	1.224738
C	-1.765147	0.741864	-0.135173
C	-1.811007	-0.610104	-0.466462
C	-1.484456	-1.618785	0.546460
C	-0.060449	-1.915985	2.538484
C	0.664705	-0.915590	3.323775
C	0.025201	0.382453	3.102467
C	0.797705	1.528705	3.018890
C	-0.564577	2.350473	1.134683
C	-1.144050	1.694656	-1.064628
C	-0.628818	1.260904	-2.273173

C	-0.681550	-0.160784	-2.622456
C	-1.245810	-1.066416	-1.741294
C	-0.604471	-2.362742	-1.520639
C	-0.752328	-2.704364	-0.106023
C	0.274965	-3.350303	0.561443
C	0.631260	-2.944893	1.921237
C	2.041308	-0.997520	3.448462
C	2.772228	-2.084558	2.794857
C	2.086659	-3.031182	2.052437
C	2.629709	-3.491441	0.773194
C	1.509663	-3.689033	-0.148507
C	1.649576	-3.365873	-1.487553
C	0.562719	-2.684722	-2.193178
C	1.158112	-1.726151	-3.124162
C	0.552601	-0.497945	-3.331858
C	-0.416388	2.692152	-0.280196
C	3.470838	1.632901	-2.514089
C	2.780006	2.661220	-1.895513
C	3.136601	3.068275	-0.535235
C	4.165041	2.425088	0.132691
C	4.895436	1.338085	-0.521429
C	4.505177	-0.467707	-2.156726
C	3.385294	-0.665965	-3.078321
C	2.745624	0.632234	-3.298866
C	1.368826	0.713850	-3.422187
C	0.638221	1.800302	-2.767799
C	1.324488	2.747309	-2.026094
C	1.901492	3.405648	0.174327
C	1.761539	3.081969	1.513166
C	2.848956	2.402624	2.219570
C	4.017251	2.083101	1.548362
C	4.656396	0.784820	1.769244
C	5.199207	0.324374	0.490071
C	5.149212	-1.019524	0.160255
C	4.792577	-1.426575	-1.199933
C	2.613548	-1.812503	-2.993566
C	2.917304	-2.826197	-1.981968
C	3.976571	-2.638573	-1.110075
C	3.828788	-2.980475	0.305679
C	4.553561	-1.979880	1.090736
C	4.039791	-1.544365	2.300629
C	4.092685	-0.123537	2.649348
C	2.857769	0.214301	3.358979

C	2.253130	1.442356	3.150198
C	0.781680	3.206161	-0.747344
C	0.493959	2.540863	2.006984
C	4.558068	0.953058	-1.808052
C	-4.482369	-0.896591	-0.907890
C	-4.340625	1.352464	-0.403961
O	-4.753770	0.107447	-0.092285
H	-3.877082	1.555913	-1.369897
C	-4.709721	2.361109	0.571504
O	-5.218012	2.084449	1.671071
C	-4.419057	3.758529	0.174670
C	-4.522886	4.179782	-1.155583
C	-4.057514	4.679899	1.166811
C	-4.252634	5.505696	-1.491177
H	-4.832614	3.471036	-1.938160
C	-3.781741	6.002575	0.825590
H	-4.003571	4.346844	2.215642
C	-3.877025	6.416146	-0.503286
H	-4.338397	5.833552	-2.537498
H	-3.493572	6.720971	1.607104
H	-3.660546	7.460736	-0.771727
H	-3.979941	-0.721595	-1.869173
C	-4.969137	-2.198858	-0.520215
C	-5.597461	-2.420679	0.715857
C	-4.805424	-3.272944	-1.413143
C	-6.051820	-3.692488	1.050057
H	-5.728200	-1.581486	1.418293
C	-5.261528	-4.539830	-1.070651
H	-4.314595	-3.108933	-2.384238
C	-5.889491	-4.763090	0.162687
H	-6.542043	-3.857822	2.021678
H	-5.128550	-5.376831	-1.772811
C	-6.386597	-6.112190	0.514682
H	-6.383212	-6.264767	1.622125
H	-7.437097	-6.237130	0.147522
H	-5.755692	-6.906823	0.045357

Energy = 1.603306547734
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3054.67176766

TS4
-AM1-

C	0.925329	-1.592226	-1.805597

C	0.848918	-0.269320	-2.429486
C	1.237955	0.853447	-1.720516
C	1.749265	0.727676	-0.348804
C	1.813176	-0.530697	0.246218
C	1.381333	-1.713474	-0.504787
C	-0.229347	-2.370897	-2.253152
C	-1.020078	-1.531407	-3.154802
C	-0.353318	-0.232837	-3.263236
C	-1.106045	0.926699	-3.343614
C	0.438739	2.076150	-1.802509
C	1.223731	1.863090	0.420610
C	0.824981	1.696366	1.734647
C	0.902223	0.374565	2.360769
C	1.372648	-0.704950	1.633868
C	0.702983	-2.001662	1.743384
C	0.709427	-2.625894	0.420601
C	-0.381770	-3.366246	-0.002718
C	-0.865164	-3.235150	-1.377285
C	-2.402848	-1.600352	-3.131075
C	-3.074608	-2.512960	-2.204342
C	-2.326899	-3.307591	-1.351742
C	-2.746673	-3.485118	0.039538
C	-1.544123	-3.521895	0.873466
C	-1.550994	-2.930487	2.125376
C	-0.396071	-2.150045	2.573058
C	-0.891940	-1.007580	3.340585
C	-0.260369	0.220491	3.235671
C	0.430388	2.700262	-0.479118
C	-3.229659	2.218755	2.276652
C	-2.594823	3.081963	1.399639
C	-3.078784	3.214669	0.024389
C	-4.171549	2.477284	-0.399427
C	-4.842748	1.564889	0.527866
C	-4.308265	0.117452	2.453254
C	-3.105923	0.080135	3.287336
C	-2.438814	1.378594	3.177763
C	-1.056075	1.446648	3.152557
C	-0.384725	2.358355	2.224777
C	-1.132944	3.153870	1.373433
C	-1.915797	3.368348	-0.851304
C	-1.908572	2.777348	-2.103242
C	-3.063979	1.998404	-2.551624
C	-4.163928	1.852260	-1.723150

C	-4.830455	0.553543	-1.613951
C	-5.250064	0.375978	-0.222768
C	-5.177640	-0.874264	0.367999
C	-4.693818	-1.007121	1.743212
C	-2.353778	-1.079763	3.366386
C	-2.761238	-2.268578	2.615484
C	-3.898723	-2.233345	1.826561
C	-3.891230	-2.858422	0.502820
C	-4.681606	-2.018450	-0.398620
C	-4.284545	-1.850525	-1.714536
C	-4.361102	-0.528744	-2.339110
C	-3.198361	-0.374216	-3.214795
C	-2.567929	0.854258	-3.318340
C	-0.713421	3.329538	-0.017088
C	-0.698528	2.113828	-2.592055
C	-4.384799	1.439247	1.828642
C	4.570712	-0.864790	0.279937
C	4.300383	1.215380	-0.760126
O	4.541975	-0.118714	-0.807465
H	4.425297	-0.431427	1.284026
C	4.936346	-2.253010	0.104771
C	5.178993	-2.813797	-1.159194
C	5.047958	-3.061721	1.250305
C	5.523690	-4.156333	-1.274939
H	5.094940	-2.183680	-2.058559
C	5.390960	-4.402576	1.126216
H	4.863613	-2.628971	2.246026
C	5.632846	-4.963377	-0.135610
H	5.711061	-4.588294	-2.269809
H	5.474264	-5.031022	2.026067
C	6.013327	-6.388547	-0.258656
H	7.123877	-6.493943	-0.160166
H	5.531946	-7.001695	0.542770
H	5.709604	-6.801603	-1.252012
H	4.091527	1.579554	-1.773089
C	4.636845	2.050886	0.354100
O	4.968955	1.593879	1.471616
C	4.627301	3.510657	0.101507
C	3.759543	4.095813	-0.826998
C	5.516904	4.320551	0.821362
C	3.791766	5.472669	-1.043479
H	3.034492	3.473411	-1.374693
C	5.549393	5.695488	0.598129

H	6.180991	3.855617	1.567594
C	4.689017	6.272716	-0.336030
H	3.105766	5.927619	-1.772880
H	6.252201	6.325457	1.162858
H	4.714884	7.358231	-0.511714

Energy = 1.599879825414
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3054.67889463

cis-**2c**
-AM1-

C	-5.130309	-4.719271	0.540152
C	-5.316851	-3.434878	1.062583
C	-4.764535	-2.324500	0.427311
C	-4.010404	-2.485606	-0.739203
C	-3.835641	-3.768368	-1.274742
C	-4.385262	-4.875474	-0.635600
C	-3.427550	-1.311569	-1.461659
C	-2.011829	-0.888087	-0.984482
C	-2.138259	0.646567	-0.640854
C	-3.614289	0.992736	-0.943936
O	-4.309256	-0.188461	-1.334945
C	-1.475789	-1.744013	0.160498
C	-1.330254	-1.324413	1.456355
C	-1.447242	0.109875	1.775794
C	-1.704770	1.011773	0.777334
C	-0.484048	0.410477	2.831945
C	0.229649	-0.820202	3.170062
C	-0.294214	-1.887350	2.318139
C	0.562486	-2.863486	1.834891
C	0.426317	-3.306047	0.453696
C	-0.553812	-2.744717	-0.351373
C	0.190738	1.620745	2.837408
C	-0.061843	2.579394	1.770095
C	-0.969172	2.265214	0.769085
C	-0.667097	2.600465	-0.615634
C	-1.211428	1.550630	-1.457851
C	-0.503143	1.159668	-2.562658
C	-0.384094	-0.274275	-2.883647
C	-0.982409	-1.201349	-2.072746
C	-0.251132	-2.409814	-1.735989
C	1.988901	-2.819777	2.161430
C	2.482976	-1.804289	2.962482

C	1.577510	-0.778491	3.484419
C	2.291598	0.500225	3.477808
C	1.616756	1.668078	3.165405
C	1.204965	3.234178	1.437464
C	2.244457	2.666818	2.298012
C	1.491511	3.552905	0.122206
C	0.526424	3.233135	-0.931518
C	1.268429	2.818705	-2.114726
C	0.764668	1.798728	-2.906297
C	1.667736	0.778097	-3.436790
C	0.955757	-0.499178	-3.420580
C	1.641458	-1.664990	-3.118189
C	1.016222	-2.652431	-2.248470
C	2.056063	-3.231823	-1.395990
C	1.769328	-3.549270	-0.080413
C	2.735991	-3.243426	0.975513
C	3.633841	0.265873	2.944275
C	3.752009	-1.158312	2.625691
C	4.458260	-1.560645	1.504203
C	3.935748	-2.632640	0.655728
C	4.239270	-2.297707	-0.736888
C	3.325698	-2.592185	-1.735538
C	3.071563	-1.622976	-2.803320
C	3.744837	-0.413204	-2.813335
C	3.027834	0.820614	-3.142793
C	4.949728	-1.018187	-0.750271
C	4.708338	-0.101952	-1.760568
C	3.558685	1.891380	-2.296208
C	4.596667	1.317643	-1.439144
C	4.727844	1.746121	-0.128567
C	3.829166	2.773673	0.399356
C	2.847740	3.317917	-0.412634
C	2.709603	2.864940	-1.798175
C	3.514447	2.444519	1.791631
C	4.218556	1.208007	2.134353
C	4.968954	0.773005	0.955103
C	5.090160	-0.561484	0.633500
C	-4.372428	1.607263	0.231128
C	-4.617579	3.063108	0.154783
C	-5.060454	3.668215	-1.026963
C	-5.294181	5.042249	-1.060639
C	-5.087215	5.817509	0.080440
C	-4.659198	5.215545	1.263921

C	-4.433429	3.841155	1.305995
C	-5.727595	-5.897796	1.208536
O	-4.769916	0.920490	1.174176
H	-3.658271	1.691196	-1.829442
H	-5.247765	3.063179	-1.927480
H	-4.116069	3.356437	2.242677
H	-5.645282	5.513725	-1.990585
H	-4.504975	5.823462	2.167821
H	-5.266994	6.902595	0.048413
H	-3.386799	-1.537249	-2.568924
H	-4.928600	-1.311879	0.835658
H	-3.262118	-3.904821	-2.204010
H	-5.905772	-3.297649	1.981991
H	-4.236797	-5.880399	-1.057949
H	-6.734471	-6.114189	0.769426
H	-5.085470	-6.802696	1.072580
H	-5.855854	-5.715758	2.303926

Energy = 1.484492601129
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3054.72705468

trans-**2c**
-AM1-

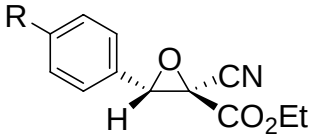
C	-0.965066	1.590595	-1.801543
C	-1.025860	0.222477	-2.347685
C	-1.489512	-0.801627	-1.565860
C	-2.210181	-0.627565	-0.229065
C	-2.145632	0.840760	0.357509
C	-1.373599	1.826205	-0.515211
C	0.233840	2.228448	-2.338703
C	0.914814	1.273708	-3.212564
C	0.134690	0.036926	-3.214940
C	0.784300	-1.186548	-3.259090
C	-0.790317	-2.074127	-1.593400
C	-1.494293	-1.675579	0.617533
C	-1.023300	-1.469420	1.887548
C	-0.962275	-0.102009	2.435676
C	-1.371746	0.956257	1.668481
C	-0.571120	2.168690	1.670527
C	-0.571489	2.707670	0.317195
C	0.560625	3.338116	-0.177303
C	0.979163	3.090932	-1.550547

C	2.298205	1.223188	-3.244542
C	3.083540	2.127273	-2.401726
C	2.441837	3.037311	-1.578900
C	2.926491	3.259461	-0.215051
C	1.762395	3.450156	0.651742
C	1.763272	2.937292	1.936558
C	0.562312	2.284817	2.461791
C	0.982038	1.159098	3.285818
C	0.237233	-0.009413	3.263981
C	-0.789769	-2.614113	-0.240029
C	2.986274	-2.323172	2.358019
C	2.249598	-3.179611	1.557616
C	2.670842	-3.437246	0.179218
C	3.807435	-2.825680	-0.323627
C	4.587043	-1.922264	0.523894
C	4.250052	-0.320043	2.370381
C	3.086742	-0.125082	3.236295
C	2.301870	-1.361422	3.225026
C	0.918526	-1.303210	3.237833
C	0.137836	-2.200909	2.387481
C	0.786958	-3.118058	1.576541
C	1.468040	-3.535142	-0.649312
C	1.467576	-3.022459	-1.934074
C	2.669479	-2.379912	-2.468068
C	3.806737	-2.282563	-1.683259
C	4.585785	-1.043538	-1.675695
C	5.068932	-0.821217	-0.311829
C	5.127422	0.463465	0.201336
C	4.707586	0.721214	1.579898
C	2.444828	1.101250	3.267843
C	2.928109	2.202120	2.432004
C	4.028372	2.017263	1.611067
C	4.027541	2.560392	0.251407
C	4.706379	1.599942	-0.619728
C	4.247595	1.389811	-1.909601
C	4.185638	0.031344	-2.452196
C	2.983088	-0.070981	-3.279594
C	2.246919	-1.243513	-3.288992
C	0.305978	-3.330550	0.218015
C	0.304839	-2.276981	-2.420476
C	4.188050	-1.678444	1.827647
C	-3.641790	1.224849	0.555865

C	-3.726358	-0.901356	-0.402413
O	-4.397340	0.353425	-0.303834
H	-3.931183	0.980392	1.620563
C	-3.996682	2.637691	0.228241
C	-4.381814	3.013458	-1.062744
C	-3.985292	3.596117	1.249647
C	-4.730802	4.334543	-1.333813
H	-4.419215	2.256060	-1.861100
C	-4.329467	4.916379	0.974574
H	-3.704461	3.306228	2.273692
C	-4.704508	5.298354	-0.319579
H	-5.030750	4.621351	-2.352842
H	-4.310513	5.665223	1.780509
C	-5.086379	6.700239	-0.604665
H	-6.179939	6.843020	-0.411652
H	-4.520882	7.409532	0.048633
H	-4.882636	6.962640	-1.671948
H	-3.961592	-1.273561	-1.438614
C	-4.307773	-1.852036	0.641105
O	-4.536760	-1.460756	1.789847
C	-4.664399	-3.208663	0.182548
C	-3.979523	-3.843008	-0.860647
C	-5.721156	-3.874441	0.820649
C	-4.354089	-5.121958	-1.267423
H	-3.127440	-3.342865	-1.349608
C	-6.097207	-5.150421	0.405494
H	-6.245520	-3.378116	1.653438
C	-5.415640	-5.774535	-0.639200
H	-3.809341	-5.617188	-2.084924
H	-6.930392	-5.665492	0.906408
H	-5.712050	-6.782574	-0.966116

Energy = 1.483404314037
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3054.73784276

Geometries (XYZ) of reactants, products and transition states for reaction of C_{60} with *trans*-2-cyano-2-ethoxycarbonyl-3-aryloxiranes (**3a-c**)



trans-**3**

trans-**3a**, R = NO_2
trans-**3b**, R = H
trans-**3c**, R = OCH_3

Reaction of C_{60} with **3a** (R = NO_2)

trans-epoxide (**3a**)
-AM1-

C	-0.569800	0.065600	-1.120910
H	-0.852070	0.847107	-1.865050
C	-1.666300	-0.470820	-0.235700
O	-1.175720	-1.213220	-1.367930
C	0.844877	0.085401	-0.711290
C	1.629422	-1.072110	-0.763430
C	1.411167	1.298657	-0.298720
C	2.974223	-1.028120	-0.403610
H	1.177964	-2.023080	-1.092690
C	2.752306	1.359292	0.068236
H	0.795998	2.211611	-0.262600
C	3.530537	0.191447	0.012650
H	3.593921	-1.940940	-0.444200
H	3.199906	2.313082	0.397839
C	-1.398030	-1.031560	1.057167
N	-1.195670	-1.474450	2.111366
C	-3.045970	0.092416	-0.424800
O	-3.355020	0.991100	-1.207030
O	-3.983020	-0.488350	0.367009
C	-5.337340	-0.008420	0.259585
H	-5.925920	-0.861900	0.693363
H	-5.598870	0.140472	-0.820300
C	-5.522370	1.260972	1.051456
H	-4.917510	2.087229	0.604695
H	-6.599760	1.552849	1.036719
H	-5.201280	1.115753	2.110753
N	4.966796	0.249464	0.399253
O	5.624119	-0.754360	0.341435
O	5.428810	1.299351	0.756934
C	-0.569800	0.065600	-1.120910
H	-0.852070	0.847107	-1.865050
C	-1.666300	-0.470820	-0.235700
O	-1.175720	-1.213220	-1.367930
C	0.844877	0.085401	-0.711290
C	1.629422	-1.072110	-0.763430
C	1.411167	1.298657	-0.298720
C	2.974223	-1.028120	-0.403610
H	1.177964	-2.023080	-1.092690
C	2.752306	1.359292	0.068236

H	0.795998	2.211611	-0.262600
C	3.530537	0.191447	0.012650
H	3.593921	-1.940940	-0.444200
H	3.199906	2.313082	0.397839
C	-1.398030	-1.031560	1.057167
N	-1.195670	-1.474450	2.111366
C	-3.045970	0.092416	-0.424800
O	-3.355020	0.991100	-1.207030
O	-3.983020	-0.488350	0.367009
C	-5.337340	-0.008420	0.259585
H	-5.925920	-0.861900	0.693363
H	-5.598870	0.140472	-0.820300
C	-5.522370	1.260972	1.051456
H	-4.917510	2.087229	0.604695
H	-6.599760	1.552849	1.036719
H	-5.201280	1.115753	2.110753
N	4.966796	0.249464	0.399253
O	5.624119	-0.754360	0.341435
O	5.428810	1.299351	0.756934

Energy = -0.033164839785
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -948.756187837

TS1
-AM1-

C	0.344992	-0.753860	-0.423240
H	0.853106	-1.620180	0.033349
C	2.025983	0.448995	-0.253440
O	1.079709	0.079575	-1.221470
C	-1.064960	-0.522480	-0.270340
C	-1.697790	0.565843	-0.896060
C	-1.822960	-1.414830	0.512369
C	-3.068500	0.762479	-0.751680
H	-1.100730	1.265767	-1.506060
C	-3.191710	-1.229590	0.662889
H	-1.330780	-2.267280	1.008066
C	-3.809760	-0.138400	0.027785
H	-3.565330	1.617967	-1.243440
H	-3.788420	-1.928450	1.275784
C	1.663088	1.415624	0.693747
N	1.387980	2.220857	1.490310
C	3.367886	-0.057100	-0.464850
O	3.688842	-1.041220	-1.142130

O	4.336582	0.648185	0.194758
C	5.692480	0.197114	0.046125
H	6.282298	1.112730	0.323093
H	5.885643	-0.083740	-1.021980
C	5.983916	-0.955390	0.974741
H	5.381082	-1.848440	0.679766
H	7.067840	-1.214870	0.917079
H	5.731265	-0.686120	2.028088
N	-5.279110	0.063799	0.186997
O	-5.796180	0.996359	-0.364130
O	-5.898220	-0.714200	0.860067

Energy = 0.020573048795
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -948.708698741

INT1
-AM1-

C	-0.051440	1.214457	0.011287
H	-0.263950	2.290933	0.097400
C	-2.321580	0.711907	-0.111700
O	-1.020520	0.330507	-0.099270
C	1.297080	0.695188	0.013726
C	2.360303	1.608884	0.130329
C	1.564725	-0.678710	-0.096050
C	3.674591	1.157794	0.137461
H	2.154664	2.687595	0.217225
C	2.877250	-1.142010	-0.090370
H	0.730616	-1.395390	-0.187690
C	3.929016	-0.220060	0.026636
H	4.511139	1.873021	0.228665
H	3.087784	-2.222900	-0.176710
C	-2.708980	2.052654	-0.009160
N	-3.065620	3.159452	0.073810
C	-3.226370	-0.418350	-0.241690
O	-2.922050	-1.612440	-0.334030
O	-4.543080	-0.048490	-0.267980
N	5.336145	-0.707060	0.033532
O	5.540982	-1.886570	-0.061630
O	6.225022	0.094697	0.134160
C	-5.513730	-1.103190	-0.379460
H	-5.173790	-1.853980	-1.139460
H	-6.421230	-0.553360	-0.749850
C	-5.761910	-1.753400	0.958557

H	-6.590230	-2.495320	0.863745
H	-4.840320	-2.280590	1.306480
H	-6.044990	-0.989270	1.721399

Energy = -0.010028525671
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -948.734956487

TS2
-AM1-

C	0.344992	-0.753860	-0.423240
H	0.853106	-1.620180	0.033349
C	2.025983	0.448995	-0.253440
O	1.079709	0.079575	-1.221470
C	-1.064960	-0.522480	-0.270340
C	-1.697790	0.565843	-0.896060
C	-1.822960	-1.414830	0.512369
C	-3.068500	0.762479	-0.751680
H	-1.100730	1.265767	-1.506060
C	-3.191710	-1.229590	0.662889
H	-1.330780	-2.267280	1.008066
C	-3.809760	-0.138400	0.027785
H	-3.565330	1.617967	-1.243440
H	-3.788420	-1.928450	1.275784
C	1.663088	1.415624	0.693747
N	1.387980	2.220857	1.490310
C	3.367886	-0.057100	-0.464850
O	3.688842	-1.041220	-1.142130
O	4.336582	0.648185	0.194758
C	5.692480	0.197114	0.046125
H	6.282298	1.112730	0.323093
H	5.885643	-0.083740	-1.021980
C	5.983916	-0.955390	0.974741
H	5.381082	-1.848440	0.679766
H	7.067840	-1.214870	0.917079
H	5.731265	-0.686120	2.028088
N	-5.279110	0.063799	0.186997
O	-5.796180	0.996359	-0.364130
O	-5.898220	-0.714200	0.860067

Energy = 0.007654219692
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -948.700385807

INT2
-AM1-

C	0.293902	-0.315380	-0.133750
H	0.807994	-1.287740	-0.239460
C	2.303403	0.910308	-0.094070
O	0.944634	0.822190	-0.054360
C	-1.150850	-0.224230	-0.074050
C	-1.887500	-1.419840	-0.154380
C	-1.821260	1.001503	0.058956
C	-3.276290	-1.392680	-0.102510
H	-1.364560	-2.384360	-0.258850
C	-3.211620	1.041751	0.111990
H	-1.244410	1.939172	0.121925
C	-3.934750	-0.158440	0.030869
H	-3.856890	-2.330150	-0.165390
H	-3.739160	2.006494	0.216691
C	2.753398	2.239240	0.005002
N	3.154226	3.329272	0.084047
C	3.175437	-0.226930	-0.221440
O	2.852988	-1.425010	-0.311500
O	4.502956	0.098302	-0.251950
C	5.442538	-0.983930	-0.363400
H	6.362359	-0.461080	-0.742840
H	5.077882	-1.729840	-1.116440
C	5.681953	-1.631770	0.977427
H	4.750177	-2.134950	1.333120
H	6.492350	-2.393290	0.883291
H	5.986468	-0.869620	1.734060
N	-5.422900	-0.124680	0.086810
O	-5.973310	0.936511	0.200809
O	-6.027480	-1.160050	0.016239

Energy = -0.011884230695
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -948.737229710

TS3
-AM1-

C	-0.393250	0.106863	2.723643
C	0.039330	1.487250	2.486661
C	-0.380180	2.155864	1.352099
C	-1.294150	1.513404	0.391792
C	-1.706800	0.191135	0.617526
C	-1.218100	-0.521460	1.809254

C	0.723213	-0.617970	3.329460
C	1.845748	0.311396	3.468633
C	1.421868	1.611865	2.947884
C	2.317405	2.401540	2.246295
C	0.568266	2.983427	0.609014
C	-0.843290	1.905895	-0.954170
C	-0.861660	1.001785	-1.999360
C	-1.294130	-0.378630	-1.764180
C	-1.678160	-0.770480	-0.495400
C	-1.250510	-2.068990	0.021605
C	-0.965260	-1.914860	1.446786
C	0.088986	-2.606570	2.020917
C	0.958158	-1.939880	2.989266
C	3.140942	-0.130400	3.257959
C	3.388520	-1.527380	2.896237
C	2.327424	-2.407300	2.766058
C	2.302929	-3.365780	1.659804
C	0.918763	-3.489920	1.199662
C	0.648079	-3.636020	-0.150150
C	-0.467870	-2.907150	-0.755610
C	-0.062230	-2.490440	-2.097120
C	-0.463610	-1.258300	-2.586130
C	0.282208	2.828855	-0.816570
C	2.899198	0.062661	-3.406580
C	2.666187	1.383977	-3.064380
C	3.536719	2.053957	-2.096650
C	4.593668	1.366523	-1.524030
C	4.840119	-0.030230	-1.886230
C	3.584728	-2.042800	-2.565510
C	2.200655	-2.168400	-3.025100
C	1.776351	-0.866770	-3.544070
C	0.481648	-0.424650	-3.330890
C	0.234855	0.971553	-2.967650
C	1.297038	1.850778	-2.839380
C	2.705183	2.934217	-1.274070
C	2.975989	3.080409	0.075642
C	4.094018	2.354719	0.680951
C	4.880010	1.521053	-0.096730
C	5.303406	0.219784	0.423201
C	5.278915	-0.738960	-0.682810
C	4.870594	-2.043100	-0.459740
C	4.000119	-2.713230	-1.427290
C	1.306678	-2.958000	-2.321920

C	1.745689	-3.666500	-1.118370
C	3.054935	-3.547530	-0.683430
C	3.341246	-3.393030	0.744002
C	4.463344	-2.463190	0.882164
C	4.486270	-1.556280	1.928377
C	4.918006	-0.177470	1.692525
C	4.087075	0.703713	2.514505
C	3.686915	1.934810	2.023027
C	1.320683	2.806614	-1.732730
C	1.877647	3.107408	1.043329
C	4.016446	-0.663990	-2.801350
C	-4.088290	0.508455	1.115406
H	-3.678080	0.567156	2.136986
C	-3.459850	2.705607	0.685772
O	-4.139150	1.575807	0.331729
C	-4.846810	-0.642790	0.664732
C	-4.995290	-1.729620	1.544127
C	-5.428080	-0.691100	-0.612070
C	-5.713660	-2.854090	1.153920
H	-4.540850	-1.696200	2.547257
C	-6.151240	-1.810940	-1.013310
H	-5.311020	0.162388	-1.301920
C	-6.290940	-2.889820	-0.126610
H	-5.830240	-3.709860	1.842275
H	-6.608250	-1.849410	-2.018180
C	-3.201680	3.007551	2.034742
N	-2.976780	3.293205	3.141934
C	-3.512510	3.717615	-0.369270
O	-3.942380	3.575677	-1.517710
O	-2.998370	4.922313	0.021090
N	-7.063330	-4.092030	-0.547900
O	-7.551630	-4.110650	-1.644790
O	-7.175270	-5.006300	0.222933
C	-2.986830	5.975728	-0.958180
H	-2.661670	5.568737	-1.950810
H	-2.209090	6.674841	-0.546570
C	-4.338560	6.637606	-1.054370
H	-4.274630	7.514886	-1.741370
H	-5.092260	5.916906	-1.455340
H	-4.678350	6.987437	-0.050300

Energy = 1.551438210126
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3234.89846215

TS4
-AM1-

C	0.636924	0.947210	-2.268620
C	0.149747	2.182198	-1.647680
C	0.436960	2.447750	-0.321930
C	1.263532	1.521228	0.470182
C	1.727149	0.338456	-0.123130
C	1.380630	0.050838	-1.523670
C	-0.395590	0.465325	-3.185430
C	-1.520770	1.400470	-3.133840
C	-1.182650	2.461038	-2.183690
C	-2.162570	2.991907	-1.361660
C	-0.600640	3.002159	0.545922
C	0.673000	1.467141	1.818223
C	0.608612	0.274875	2.514794
C	1.095541	-0.960930	1.895686
C	1.613755	-0.928620	0.614272
C	1.271995	-1.988920	-0.332160
C	1.127059	-1.383040	-1.654420
C	0.152374	-1.843950	-2.524470
C	-0.631470	-0.893630	-3.312130
C	-2.819530	0.926494	-3.209480
C	-3.068280	-0.510260	-3.341380
C	-2.004520	-1.395170	-3.391630
C	-2.067710	-2.658120	-2.654010
C	-0.733900	-2.936210	-2.118590
C	-0.596140	-3.510180	-0.866290
C	0.435775	-3.024560	0.051575
C	-0.112020	-3.056410	1.406921
C	0.208479	-2.050100	2.303051
C	-0.454980	2.395969	1.868665
C	-3.250330	-1.031060	3.153963
C	-3.016180	0.327944	3.278438
C	-3.801510	1.281073	2.492244
C	-4.778990	0.823532	1.624626
C	-5.026650	-0.613260	1.493428
C	-3.797280	-2.748900	1.617628
C	-2.463460	-3.028140	2.152129
C	-2.124810	-1.965900	3.101047
C	-0.826330	-1.490730	3.174497
C	-0.578260	-0.054210	3.304697
C	-1.643050	0.829654	3.356326
C	-2.913380	2.371075	2.084612

C	-3.051350	2.945091	0.832468
C	-4.085250	2.462256	-0.084500
C	-4.924790	1.430470	0.300487
C	-5.262460	0.368799	-0.649120
C	-5.325620	-0.894320	0.088205
C	-4.865680	-2.061650	-0.497510
C	-4.080420	-3.014840	0.288473
C	-1.484830	-3.558630	1.328711
C	-1.784030	-3.839450	-0.076600
C	-3.045700	-3.575110	-0.582310
C	-3.191440	-2.968100	-1.906590
C	-4.316250	-2.032760	-1.854090
C	-4.256310	-0.837970	-2.551540
C	-4.742640	0.396178	-1.932300
C	-3.855060	1.486689	-2.339180
C	-3.535920	2.491175	-1.441160
C	-1.578980	2.090454	2.617837
C	-1.862610	3.270819	0.042334
C	-4.283620	-1.514730	2.236886
C	4.156853	0.791506	-0.244600
H	3.831679	1.202122	-1.218930
C	3.425913	2.697630	0.899355
O	4.100308	1.501315	0.870023
C	4.914916	-0.445310	-0.163060
C	5.181555	-1.136750	-1.357710
C	5.378975	-0.955820	1.058946
C	5.900245	-2.327110	-1.333570
H	4.822113	-0.737120	-2.320080
C	6.100867	-2.145520	1.096196
H	5.170726	-0.412490	1.995845
C	6.358100	-2.827370	-0.103330
H	6.109821	-2.872810	-2.270730
H	6.465609	-2.548030	2.057946
C	3.217698	3.158298	2.216835
N	3.017726	3.556739	3.291895
C	3.459612	3.590121	-0.243680
O	3.841178	3.314054	-1.393420
O	3.010254	4.850616	0.021485
C	3.009267	5.792195	-1.066380
H	2.271348	6.562433	-0.712080
H	2.639308	5.295200	-2.000390
C	4.381732	6.384030	-1.267410
H	5.094612	5.595167	-1.610180

H	4.330275	7.187212	-2.040670
H	4.765209	6.821814	-0.314810
N	7.130005	-4.101950	-0.072490
O	7.516734	-4.517620	0.985521
O	7.342174	-4.673730	-1.106940

Energy = 1.549339511882
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3234.89953227

cis-**4a**
-AM1-

C	0.111620	0.262927	-2.900796
C	-0.214758	1.646062	-2.509102
C	0.378335	2.198951	-1.405160
C	1.570080	1.598809	-0.655775
C	1.919833	0.117779	-1.074597
C	1.002627	-0.460536	-2.154588
C	-1.107987	-0.352183	-3.418082
C	-2.185946	0.633876	-3.352420
C	-1.630901	1.864881	-2.790918
C	-2.399635	2.639682	-1.937219
C	-0.438257	2.984480	-0.496531
C	1.098316	1.749921	0.790263
C	1.175350	0.771376	1.745758
C	1.503809	-0.611748	1.356070
C	1.724645	-0.910393	0.037898
C	1.146768	-2.129110	-0.503685
C	0.702440	-1.850651	-1.862325
C	-0.441694	-2.460048	-2.356234
C	-1.379049	-1.686405	-3.159727
C	-3.471283	0.237673	-3.023918
C	-3.753533	-1.171384	-2.740661
C	-2.736490	-2.108292	-2.808956
C	-2.632898	-3.152465	-1.787758
C	-1.212630	-3.373729	-1.510741
C	-0.790771	-3.638281	-0.220151
C	0.424723	-3.003954	0.294359
C	0.208907	-2.684568	1.699373
C	0.732353	-1.508784	2.212550
C	0.005639	2.705068	0.861805
C	-2.427306	-0.111523	3.551562
C	-2.167233	1.221708	3.283879
C	-3.109842	2.005542	2.483405

C	-4.263315	1.413754	1.995635
C	-4.538907	0.004876	2.281100
C	-3.322447	-2.110446	2.649824
C	-1.902633	-2.335126	2.923697
C	-1.347061	-1.097883	3.476527
C	-0.067605	-0.698027	3.129918
C	0.208489	0.708067	2.838676
C	-0.812307	1.641379	2.920763
C	-2.335546	2.907706	1.629243
C	-2.757316	3.172922	0.338814
C	-3.978882	2.551907	-0.176016
C	-4.709657	1.694363	0.629714
C	-5.261051	0.458837	0.071310
C	-5.156405	-0.585240	1.092140
C	-4.849744	-1.884588	0.725095
C	-3.908018	-2.668940	1.525764
C	-1.145045	-3.108556	2.060733
C	-1.763681	-3.698579	0.871980
C	-3.107230	-3.484781	0.611720
C	-3.553652	-3.204218	-0.754264
C	-4.630061	-2.214924	-0.684089
C	-4.727515	-1.227044	-1.649990
C	-5.051755	0.146942	-1.261823
C	-4.278206	1.052151	-2.112399
C	-3.758208	2.222055	-1.585433
C	-0.915256	2.674218	1.898475
C	-1.781332	3.218706	-0.751942
C	-3.646723	-0.736440	3.037950
C	3.376172	0.181037	-1.602027
H	3.371318	0.047652	-2.724856
C	2.876149	2.404348	-0.938226
O	3.896145	1.498571	-1.369420
C	4.316547	-0.811750	-0.986211
C	4.498180	-2.050466	-1.615557
C	5.044659	-0.501903	0.166982
C	5.379292	-2.988131	-1.086131
H	3.943797	-2.291560	-2.536177
C	5.934435	-1.427559	0.708714
H	4.923625	0.488097	0.645464
C	6.094648	-2.671941	0.080625
H	5.518074	-3.966200	-1.578182
H	6.506740	-1.181763	1.620137
C	2.672273	3.396449	-1.994442

N	2.537675	4.193863	-2.827142
C	3.435188	3.077641	0.321326
O	4.158523	2.552428	1.165502
O	3.074310	4.381399	0.438386
C	3.581379	5.115891	1.570000
H	3.508785	4.483187	2.492419
H	2.867714	5.982007	1.628938
C	4.997402	5.570560	1.323829
H	5.330647	6.218079	2.169835
H	5.679821	4.688794	1.251681
H	5.065317	6.152471	0.373495
N	7.038755	-3.669047	0.652938
O	7.645900	-3.388937	1.651255
O	7.168402	-4.729231	0.101674

Energy = 1.440281741253
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3234.94777764

trans-**4a**
-AM1-

C	0.565792	1.027113	-2.349118
C	0.104274	2.238629	-1.646981
C	0.485419	2.465086	-0.350495
C	1.569035	1.683712	0.389254
C	2.065296	0.383487	-0.362521
C	1.368575	0.128852	-1.698268
C	-0.520637	0.574033	-3.213873
C	-1.648764	1.491326	-3.057448
C	-1.259257	2.516650	-2.090301
C	-2.195491	3.010681	-1.196201
C	-0.509219	2.951024	0.590789
C	0.866632	1.411883	1.719577
C	0.850569	0.204412	2.365415
C	1.312659	-1.007866	1.665058
C	1.755018	-0.918390	0.371858
C	1.339390	-1.938358	-0.576509
C	1.101672	-1.289689	-1.858788
C	0.085336	-1.743134	-2.686766
C	-0.754693	-0.780751	-3.387508
C	-2.945886	1.007423	-3.073120
C	-3.190649	-0.426286	-3.245555
C	-2.124967	-1.296375	-3.400807
C	-2.126449	-2.586790	-2.708898

C	-0.757841	-2.865651	-2.270779
C	-0.531554	-3.482304	-1.053353
C	0.549946	-3.009848	-0.186401
C	0.097041	-3.104007	1.195047
C	0.466328	-2.117799	2.095647
C	-0.272121	2.300574	1.872058
C	-2.938327	-1.186148	3.222226
C	-2.713820	0.170340	3.384279
C	-3.560465	1.141123	2.687966
C	-4.587263	0.702321	1.868411
C	-4.825543	-0.731915	1.699424
C	-3.566641	-2.854139	1.662308
C	-2.197727	-3.135018	2.096530
C	-1.806478	-2.101048	3.057188
C	-0.512575	-1.608176	3.055260
C	-0.272591	-0.175010	3.218549
C	-1.344114	0.687731	3.385258
C	-2.712571	2.255750	2.261718
C	-2.938417	2.872923	1.044503
C	-4.026370	2.413014	0.179758
C	-4.826549	1.355605	0.580130
C	-5.212767	0.324951	-0.384736
C	-5.213101	-0.965209	0.307146
C	-4.780277	-2.104022	-0.350766
C	-3.934919	-3.075388	0.345586
C	-1.271244	-3.624905	1.191873
C	-1.660162	-3.858470	-0.200322
C	-2.955393	-3.591090	-0.611961
C	-3.194878	-2.937860	-1.900311
C	-4.322238	-2.018520	-1.738606
C	-4.320426	-0.797817	-2.393006
C	-4.778057	0.406393	-1.697268
C	-3.931092	1.522466	-2.119471
C	-3.567286	2.498886	-1.207864
C	-1.342031	1.967704	2.689344
C	-1.806134	3.235556	0.189552
C	-4.024335	-1.649890	2.358004
C	3.583958	0.628728	-0.578180
H	3.737679	1.060637	-1.612684
C	2.873149	2.517926	0.608304
O	3.983525	1.644790	0.360437
C	4.469424	-0.559953	-0.375012
C	4.775916	-1.368537	-1.477433

C	5.027085	-0.846451	0.875435
C	5.611802	-2.471763	-1.332269
H	4.356590	-1.135039	-2.469003
C	5.870064	-1.943638	1.038280
H	4.809259	-0.192712	1.735898
C	6.155327	-2.757027	-0.069147
H	5.848442	-3.112340	-2.199486
C	3.001949	2.999397	1.979351
N	3.119742	3.398473	3.062719
C	2.980706	3.674703	-0.391537
O	3.350027	3.578112	-1.561212
O	2.647823	4.881909	0.130872
C	2.760134	6.035179	-0.726000
H	2.099959	6.781604	-0.206526
H	2.353457	5.790219	-1.741406
C	4.189399	6.507965	-0.804610
H	4.823896	5.738628	-1.308520
H	4.234120	7.455920	-1.392349
H	4.599692	6.695141	0.216650
H	6.308903	-2.169002	2.025812
N	7.050200	-3.934387	0.094672
O	7.509155	-4.168486	1.180094
O	7.288840	-4.619760	-0.863126

Energy = 1.441079
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3234.9530296

Reaction of C_{60} with **3b** (R = H)

trans-epoxide (**3b**)
-AM1-

C	-0.546506	-0.511851	-0.853850
H	-0.284886	-1.522276	-1.246018
C	0.595747	0.344188	-0.361972
O	-0.019071	0.565183	-1.645223
C	-1.917313	-0.381119	-0.336946
C	-2.746124	0.675442	-0.731051
C	-2.403337	-1.357933	0.542208
C	-4.050314	0.755579	-0.245090
H	-2.360718	1.438120	-1.426387
C	-3.706176	-1.269436	1.027756
H	-1.755784	-2.193266	0.848504
C	-4.530356	-0.213930	0.635098

H	-4.699078	1.587588	-0.556885
H	-4.084356	-2.034704	1.721659
C	0.410718	1.376139	0.617178
N	0.274203	2.203306	1.420653
C	1.978927	-0.232351	-0.441204
O	2.276301	-1.345107	-0.876077
O	2.944998	0.600861	0.027456
C	4.304334	0.127897	-0.000401
H	4.890860	1.084475	0.060815
H	4.502681	-0.392090	-0.973607
C	4.583767	-0.776757	1.173097
H	3.979305	-1.712772	1.091467
H	5.667088	-1.045358	1.184719
H	4.326324	-0.268324	2.133010
H	-5.558879	-0.147236	1.019963

Energy = -0.041491602927
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -744.261234131

TS1
-AM1-

C	-0.760720	-0.719060	-0.364920
H	-0.224720	-1.567040	0.098255
C	0.923762	0.493736	-0.312410
O	-0.063260	0.077617	-1.230630
C	-2.152610	-0.478980	-0.138010
C	-2.827750	0.577789	-0.779300
C	-2.862370	-1.323500	0.741289
C	-4.185570	0.778744	-0.548160
H	-2.268670	1.240091	-1.461730
C	-4.217590	-1.113930	0.963305
H	-2.338080	-2.148660	1.248675
C	-4.880300	-0.063420	0.320948
H	-4.709460	1.606821	-1.050010
H	-4.770770	-1.773850	1.648959
C	0.624414	1.589062	0.505040
N	0.395154	2.498024	1.198110
C	2.226297	-0.100850	-0.489370
O	2.485621	-1.168720	-1.061990
O	3.249855	0.607289	0.084784
C	4.570006	0.056818	-0.026490
H	5.223376	0.955357	0.142318
H	4.728678	-0.351780	-1.058490

C	4.804687	-1.004540	1.020145
H	4.140435	-1.882460	0.830683
H	5.868470	-1.339170	0.980638
H	4.587244	-0.606280	2.039880
H	-5.953950	0.100064	0.504266

Energy = 0.007414504490
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -744.217827968

INT1
-AM1-

C	1.175939	0.894934	0.023078
H	1.096695	1.990789	0.108650
C	-1.141360	0.689283	-0.111490
O	0.108833	0.139216	-0.093140
C	2.453856	0.223299	0.032471
C	3.617189	1.005403	0.155523
C	2.561319	-1.172990	-0.077000
C	4.865423	0.392308	0.168117
H	3.537554	2.100015	0.241060
C	3.817122	-1.775630	-0.062990
H	1.649301	-1.785150	-0.173550
C	4.967846	-0.996760	0.059120
H	5.774882	1.004511	0.264392
H	3.897944	-2.869980	-0.149100
C	-1.345510	2.067172	-0.009550
N	-1.549560	3.212541	0.073371
C	-2.176250	-0.312590	-0.245410
O	-2.034590	-1.538240	-0.337620
O	-3.439690	0.219713	-0.277230
C	-4.531450	-0.704980	-0.394990
H	-4.283170	-1.495130	-1.150650
H	-5.362440	-0.049680	-0.773040
C	-4.869640	-1.317190	0.941811
H	-5.781740	-1.952140	0.841532
H	-4.021800	-1.951880	1.297665
H	-5.062380	-0.522130	1.701118
H	5.958675	-1.476130	0.069998

Energy = -0.020707614071
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -744.241188084

TS2
-AM1-

C	-4.988638	-0.627319	-0.179043
C	-4.489777	-0.554172	1.125520
C	-3.152719	-0.245739	1.344510
C	-2.299990	-0.004841	0.248405
C	-2.807544	-0.081247	-1.061947
C	-4.149091	-0.391684	-1.268599
C	-0.915823	0.301936	0.498919
O	-0.135663	0.573383	-0.519085
C	1.202916	0.886187	-0.217995
C	2.093518	-0.216981	-0.338913
O	3.426769	0.114296	-0.300318
C	4.364578	-0.963232	-0.411140
C	4.567239	-1.646272	0.919625
C	1.472715	2.212021	0.095582
N	1.716650	3.321791	0.361393
O	1.782191	-1.417302	-0.457578
H	-0.516635	0.328811	1.534576
H	2.757762	-0.189821	2.371697
H	-2.133827	0.102138	-1.916939
H	-5.157590	-0.742541	1.980413
H	-4.545066	-0.452500	-2.294391
H	5.299235	-0.440586	-0.751804
H	4.022349	-1.694069	-1.189399
H	3.622787	-2.152530	1.235120
H	5.376628	-2.408971	0.830320
H	4.852445	-0.904015	1.702756
H	-6.049783	-0.873426	-0.345782

Energy = -0.008790771611
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -744.212356018

INT2
-AM1-

C	-0.830040	-0.338410	-0.104920
H	-0.296380	-1.300070	-0.224410
C	1.163993	0.918640	-0.086760
O	-0.202500	0.809116	-0.027390
C	-2.273570	-0.285440	-0.024540
C	-2.983160	-1.497960	-0.105520
C	-2.974300	0.921702	0.129373
C	-4.372280	-1.493720	-0.032980

H	-2.437310	-2.446820	-0.226360
C	-4.365210	0.914184	0.201184
H	-2.418710	1.871179	0.192984
C	-5.064720	-0.290240	0.120276
H	-4.926390	-2.442570	-0.096240
H	-4.911280	1.862197	0.321733
C	1.586983	2.254003	0.011410
N	1.963898	3.353046	0.089690
C	2.043729	-0.201810	-0.230300
O	1.741722	-1.407210	-0.321580
O	3.370490	0.137752	-0.277720
C	4.317182	-0.933810	-0.406530
H	5.227277	-0.403510	-0.798670
H	3.949185	-1.682580	-1.155170
C	4.584332	-1.583710	0.928528
H	3.661848	-2.094580	1.297257
H	5.399048	-2.338420	0.819819
H	4.894192	-0.820810	1.682122
H	-6.164090	-0.293120	0.177275

Energy = -0.023058536440
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -744.243753371

TS3
-AM1-

C	0.736470	0.585704	2.623987
C	0.753097	-0.876900	2.530780
C	1.328510	-1.491880	1.434722
C	1.963813	-0.695450	0.370703
C	1.942809	0.703467	0.457825
C	1.294237	1.344591	1.611498
C	-0.533210	0.984953	3.229936
C	-1.302290	-0.228170	3.513229
C	-0.506390	-1.377890	3.081100
C	-1.128280	-2.471890	2.503072
C	0.666698	-2.642140	0.821524
C	1.622019	-1.340520	-0.908290
C	1.324560	-0.583270	-2.025730
C	1.308080	0.879237	-1.935200
C	1.585370	1.494231	-0.728300
C	0.786849	2.641391	-0.299690
C	0.606087	2.548503	1.147782
C	-0.594820	2.932301	1.722130

C	-1.181700	2.128249	2.793026
C	-2.676320	-0.233100	3.342310
C	-3.360880	0.974981	2.878249
C	-2.634280	2.123082	2.611512
C	-2.944670	2.927138	1.428171
C	-1.683770	3.428360	0.878718
C	-1.512170	3.516594	-0.492260
C	-0.241800	3.113978	-1.098190
C	-0.534820	2.460891	-2.373150
C	0.219191	1.371808	-2.778150
C	0.847925	-2.548570	-0.626650
C	-2.580510	-1.001690	-3.284240
C	-1.933970	-2.144670	-2.845030
C	-2.521170	-2.952190	-1.774380
C	-3.723570	-2.573390	-1.201290
C	-4.407040	-1.365180	-1.665920
C	-3.868300	0.859709	-2.586510
C	-2.607930	1.362185	-3.135680
C	-1.811340	0.211724	-3.566020
C	-0.437640	0.216468	-3.392310
C	0.246096	-0.991000	-2.926790
C	-0.481560	-2.139070	-2.662000
C	-1.431430	-3.444990	-0.930270
C	-1.603060	-3.533330	0.440552
C	-2.874380	-3.133890	1.046463
C	-3.905060	-2.666740	0.248260
C	-4.700700	-1.516200	0.679580
C	-5.011120	-0.711840	-0.503490
C	-5.027160	0.670005	-0.416550
C	-4.440080	1.477628	-1.487040
C	-1.987200	2.455695	-2.555870
C	-2.591480	3.108756	-1.393270
C	-3.783760	2.633367	-0.873670
C	-3.965250	2.540058	0.576023
C	-4.733680	1.326620	0.858473
C	-4.439750	0.565822	1.977577
C	-4.422850	-0.895130	1.885659
C	-3.333440	-1.388930	2.729379
C	-2.580930	-2.477440	2.321691
C	-0.171180	-2.940530	-1.478670
C	-0.524130	-3.122330	1.340818
C	-3.851410	-0.601260	-2.678480
C	4.360478	1.201415	0.843830

H	3.988009	1.118064	1.879319
C	4.411521	-1.117240	0.645019
O	4.708953	0.130772	0.152758
C	4.713622	2.480683	0.267669
C	4.547170	3.636934	1.051899
C	5.214425	2.591481	-1.040220
C	4.877565	4.882312	0.527855
H	4.155260	3.555164	2.077546
C	5.543009	3.843855	-1.553670
H	5.344437	1.684643	-1.654000
C	5.374852	4.988015	-0.773340
H	4.745700	5.786479	1.141395
H	5.934722	3.927561	-2.578950
C	4.319971	-1.338450	2.028746
N	4.237703	-1.557690	3.170731
C	4.733068	-2.160320	-0.320270
O	5.048779	-2.017090	-1.506280
O	4.635197	-3.422740	0.201598
C	4.907729	-4.518480	-0.686620
H	4.433514	-4.328310	-1.684490
H	4.401440	-5.378470	-0.169900
C	6.392648	-4.746600	-0.823300
H	6.574063	-5.663290	-1.433320
H	6.870026	-3.872620	-1.329760
H	6.864472	-4.878820	0.179579
H	5.633743	5.976584	-1.182890

Energy = 1.540157650284
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3030.40465695

TS4
-AM1-

C	-1.152490	-0.416380	-2.264650
C	-1.069120	-1.737140	-1.635120
C	-1.422810	-1.893150	-0.307910
C	-1.921410	-0.751320	0.477593
C	-1.994020	0.511957	-0.123170
C	-1.581670	0.670392	-1.524990
C	-0.022660	-0.281850	-3.183300
C	0.759574	-1.518000	-3.124730
C	0.111999	-2.416570	-2.168110
C	0.881453	-3.218530	-1.341960
C	-0.605250	-2.734750	0.564343

C	-1.342330	-0.873720	1.826312
C	-0.912210	0.245299	2.514771
C	-0.995290	1.567196	1.888005
C	-1.499030	1.687348	0.605709
C	-0.848500	2.585439	-0.347220
C	-0.898990	1.955949	-1.665490
C	0.169074	2.088147	-2.537890
C	0.620678	0.937347	-3.318710
C	2.141129	-1.468140	-3.202540
C	2.820572	-0.179030	-3.343480
C	2.081301	0.990386	-3.400120
C	2.531860	2.176950	-2.670550
C	1.349483	2.856266	-2.138110
C	1.396950	3.452709	-0.889560
C	0.266695	3.315213	0.030632
C	0.799319	3.184999	1.386160
C	0.185140	2.332084	2.288398
C	-0.555180	-2.104630	1.883256
C	3.162470	0.301549	3.148462
C	2.520706	-0.918180	3.281370
C	2.972904	-2.072010	2.501937
C	4.042876	-1.943760	1.632249
C	4.721335	-0.654230	1.492035
C	4.210517	1.757165	1.601565
C	3.028513	2.437469	2.133273
C	2.380050	1.537514	3.088667
C	0.998381	1.486320	3.164036
C	0.319542	0.197204	3.303295
C	1.059907	-0.971580	3.361470
C	1.791415	-2.837600	2.100747
C	1.744100	-3.434130	0.852436
C	2.875364	-3.299370	-0.066760
C	3.992758	-2.574450	0.312205
C	4.640151	-1.674710	-0.643930
C	5.090660	-0.487980	0.085289
C	5.012361	0.760567	-0.508270
C	4.560271	1.914387	0.270951
C	2.259921	3.238528	1.305708
C	2.629468	3.404435	-0.101140
C	3.747593	2.760806	-0.604160
C	3.697426	2.130082	-1.924370
C	4.479114	0.893892	-1.865040
C	4.052723	-0.228590	-2.554820

C	4.135586	-1.548600	-1.927320
C	2.954490	-2.314800	-2.327880
C	2.342160	-3.166100	-1.423630
C	0.609204	-2.155930	2.631193
C	0.511800	-3.382540	0.063565
C	4.293393	0.437143	2.229123
C	-4.491330	0.831063	-0.246810
H	-4.271380	0.332945	-1.210850
C	-4.342490	-1.202150	0.906249
O	-4.645100	0.147277	0.871459
C	-4.848960	2.233299	-0.190150
C	-4.901210	2.954479	-1.397380
C	-5.140820	2.881629	1.021407
C	-5.238090	4.304208	-1.383710
H	-4.677060	2.449119	-2.350090
C	-5.477770	4.232762	1.023186
H	-5.101170	2.315928	1.966371
C	-5.525760	4.944535	-0.176150
H	-5.277720	4.867723	-2.328380
H	-5.705150	4.738244	1.974148
C	-4.260420	-1.687770	2.226550
N	-4.169000	-2.113210	3.306364
C	-4.676130	-2.042020	-0.221960
O	-4.975010	-1.668260	-1.370140
O	-4.628530	-3.381870	0.041932
C	-4.928820	-4.276420	-1.042180
H	-4.454310	-5.235630	-0.698840
H	-4.440860	-3.913670	-1.983810
C	-6.419170	-4.424830	-1.221720
H	-6.864070	-3.455420	-1.553880
H	-6.625440	-5.202960	-1.994590
H	-6.902590	-4.728760	-0.262580
H	-5.790880	6.013179	-0.171310

Energy = 1.537472820604
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3030.40657084

cis-**4b**
-AM1-

C	0.566741	0.432857	2.807603
C	0.634109	-1.025860	2.606270
C	1.317307	-1.534250	1.533327
C	2.257676	-0.731690	0.631311

C	2.186221	0.829898	0.846035
C	1.183880	1.268523	1.915917
C	-0.756720	0.747580	3.339142
C	-1.509830	-0.499080	3.470753
C	-0.648440	-1.590510	3.017381
C	-1.196400	-2.655730	2.320854
C	0.724098	-2.630200	0.787209
C	1.792679	-1.200430	-0.747340
C	1.549590	-0.376050	-1.814110
C	1.484673	1.083020	-1.615670
C	1.661595	1.604050	-0.361490
C	0.781196	2.675167	0.074993
C	0.487876	2.468276	1.486411
C	-0.762380	2.795798	1.990453
C	-1.407610	1.906596	2.947322
C	-2.866630	-0.524060	3.195877
C	-3.550470	0.699578	2.771388
C	-2.841510	1.882866	2.652543
C	-3.080390	2.768155	1.510979
C	-1.794440	3.336933	1.103980
C	-1.516190	3.533252	-0.236830
C	-0.191110	3.199855	-0.763530
C	-0.361270	2.648031	-2.101060
C	0.455971	1.606606	-2.510440
C	1.016398	-2.422540	-0.624120
C	-2.222630	-0.781110	-3.434870
C	-1.582220	-1.940930	-3.032960
C	-2.229690	-2.841720	-2.077450
C	-3.484330	-2.534760	-1.577100
C	-4.161860	-1.309690	-2.004280
C	-3.615730	0.991508	-2.709040
C	-2.331140	1.563759	-3.113480
C	-1.467230	0.467765	-3.557530
C	-0.114400	0.490052	-3.263440
C	0.563053	-0.731460	-2.830920
C	-0.150840	-1.914360	-2.726100
C	-1.197220	-3.369920	-1.184120
C	-1.475080	-3.566930	0.156562
C	-2.802170	-3.247430	0.685378
C	-3.778370	-2.743130	-0.158060
C	-4.637610	-1.646820	0.291470
C	-4.875460	-0.761260	-0.849710
C	-4.938760	0.609065	-0.661710

C	-4.292320	1.510080	-1.617400
C	-1.792880	2.625606	-2.406550
C	-2.507640	3.173561	-1.252020
C	-3.723010	2.631156	-0.868220
C	-4.017180	2.422851	0.550877
C	-4.767960	1.172965	0.678428
C	-4.541400	0.335487	1.758112
C	-4.474400	-1.113510	1.559273
C	-3.441980	-1.645280	2.449512
C	-2.630250	-2.683720	2.025761
C	0.085523	-2.788560	-1.585010
C	-0.485030	-3.192870	1.168595
C	-3.548790	-0.457520	-2.907810
C	3.620057	1.247704	1.266153
H	3.619195	1.508375	2.365983
C	3.750383	-1.094740	0.906607
O	4.486171	0.107996	1.136893
C	4.207579	2.377927	0.480066
C	4.081615	3.683339	0.972811
C	4.917308	2.147788	-0.703340
C	4.637040	4.750204	0.269916
H	3.544715	3.868965	1.915227
C	5.475095	3.219817	-1.399900
H	5.044702	1.115228	-1.073900
C	5.332588	4.520177	-0.917880
H	4.530070	5.774429	0.656326
H	6.031066	3.033235	-2.330720
C	3.879597	-1.945810	2.090769
N	4.011627	-2.622850	3.024385
C	4.423440	-1.760330	-0.299890
O	4.920251	-1.187430	-1.267070
O	4.456976	-3.116610	-0.213890
C	5.103746	-3.836900	-1.280170
H	4.805661	-3.396960	-2.267160
H	4.675347	-4.869260	-1.164080
C	6.601048	-3.827630	-1.103710
H	7.070490	-4.471310	-1.885480
H	6.995438	-2.787170	-1.205360
H	6.881594	-4.217990	-0.096130
H	5.771743	5.364337	-1.469810

Energy = 1.433136910912
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3030.45217648

trans-**4b**

-AM1-

C	-1.155890	-0.404790	-2.344960
C	-1.150220	-1.715120	-1.669260
C	-1.578770	-1.817810	-0.371770
C	-2.309330	-0.717650	0.395169
C	-2.316490	0.688641	-0.327650
C	-1.582360	0.706153	-1.667440
C	0.015075	-0.349350	-3.216110
C	0.744852	-1.610370	-3.090100
C	0.022743	-2.450090	-2.135210
C	0.728163	-3.262650	-1.262190
C	-0.815230	-2.644370	0.547696
C	-1.547380	-0.740500	1.720404
C	-1.098940	0.369152	2.386122
C	-1.105150	1.680751	1.713017
C	-1.558390	1.779580	0.424187
C	-0.813800	2.605203	-0.512180
C	-0.830140	1.940622	-1.808160
C	0.275325	2.020669	-2.642310
C	0.714087	0.837301	-3.370210
C	2.129167	-1.618500	-3.115100
C	2.866155	-0.361990	-3.266680
C	2.177986	0.832748	-3.392940
C	2.642339	2.024104	-2.679470
C	1.464926	2.761751	-2.218650
C	1.480335	3.393546	-0.988050
C	0.307228	3.318721	-0.114790
C	0.773107	3.217627	1.261773
C	0.083320	2.408387	2.150380
C	-0.797410	-1.978390	1.842782
C	2.942364	0.305657	3.215674
C	2.251582	-0.885720	3.357869
C	2.693543	-2.079410	2.634111
C	3.803967	-2.017210	1.808473
C	4.535143	-0.757940	1.660438
C	4.112067	1.673309	1.675775
C	2.935176	2.413019	2.132931
C	2.208419	1.566004	3.081136
C	0.823801	1.564824	3.087967
C	0.091351	0.307270	3.230369
C	0.787485	-0.882960	3.368433
C	1.502154	-2.811300	2.200604

C	1.486077	-3.443440	0.970301
C	2.660824	-3.382250	0.099022
C	3.787153	-2.686400	0.506369
C	4.508043	-1.840590	-0.446110
C	4.971234	-0.649070	0.267257
C	4.966939	0.582435	-0.365610
C	4.526400	1.776215	0.358154
C	2.237068	3.218211	1.249062
C	2.674575	3.326772	-0.144100
C	3.787724	2.625500	-0.577390
C	3.771153	1.956329	-1.879570
C	4.499388	0.693549	-1.748430
C	4.059708	-0.433320	-2.423160
C	4.064190	-1.735500	-1.753910
C	2.873239	-2.469180	-2.183470
C	2.192157	-3.271160	-1.283590
C	0.326212	-2.064200	2.651290
C	0.293302	-3.362820	0.124594
C	4.116614	0.371063	2.344969
C	-3.825040	1.005506	-0.529010
H	-4.124330	0.674558	-1.568280
C	-3.823910	-1.037250	0.617917
O	-4.553300	0.175310	0.396738
C	-4.228350	2.424514	-0.294490
C	-4.289050	3.298763	-1.387600
C	-4.586210	2.880680	0.978534
C	-4.678360	4.623334	-1.199780
H	-4.030550	2.940558	-2.395640
C	-4.980790	4.205982	1.159691
H	-4.567460	2.186309	1.832797
C	-5.023070	5.078943	0.073303
H	-4.718130	5.308355	-2.059580
H	-5.261210	4.559336	2.163054
C	-4.104700	-1.467080	1.984029
N	-4.348630	-1.816580	3.063461
C	-4.339110	-2.066140	-0.394450
O	-4.653310	-1.833590	-1.560940
O	-4.457930	-3.320160	0.113043
C	-4.976090	-4.346110	-0.755010
H	-4.624760	-5.285920	-0.249000
H	-4.511720	-4.249870	-1.770710
C	-6.480340	-4.277350	-0.829390
H	-6.799560	-3.325390	-1.319620

H	-6.861720	-5.138910	-1.427830
H	-6.927870	-4.319310	0.192490
H	-5.332190	6.124723	0.218165

Energy = 1.433349744252
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3030.45678420

Reaction of C_{60} with **3c** (R = OCH_3)

trans-epoxide (**3c**)
-AM1-

C	-0.306219	-0.625737	0.916700
H	-0.623802	-1.652275	1.214097
C	-1.391400	0.304228	0.426592
O	-0.847110	0.407513	1.755887
C	1.094743	-0.505061	0.491360
C	1.919032	0.515624	0.973636
C	1.615719	-1.459334	-0.396656
C	3.252167	0.596848	0.576958
H	1.507931	1.259364	1.675788
C	2.939333	-1.391227	-0.805806
H	0.969701	-2.267986	-0.772475
C	3.760182	-0.355663	-0.315035
H	3.885898	1.405650	0.966040
H	3.359573	-2.128963	-1.503988
C	-1.116840	1.399792	-0.457875
N	-0.906947	2.279588	-1.186141
C	-2.793582	-0.227451	0.383249
O	-3.152927	-1.353705	0.727195
O	-3.701869	0.665713	-0.091211
C	-5.073502	0.238329	-0.180023
H	-5.626236	1.216052	-0.216628
H	-5.350483	-0.334315	0.743125
C	-5.302499	-0.581539	-1.424616
H	-4.732907	-1.540810	-1.365130
H	-6.390265	-0.811930	-1.522232
H	-4.967587	-0.023432	-2.331564
C	5.909973	0.667485	-0.322759
H	6.027829	0.622573	0.787089
H	6.882483	0.449576	-0.833015
H	5.513751	1.663584	-0.636363
O	5.058168	-0.378517	-0.778884

Energy = -0.102602203732

-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -858.783318107

TS1
-AM1-

C	0.107271	-0.787427	-0.485661
H	0.683667	-1.637791	-0.077612
C	1.720776	0.518217	-0.334755
O	0.774559	0.093465	-1.294900
C	-1.286296	-0.622147	-0.247317
C	-2.006794	0.447230	-0.818138
C	-1.965456	-1.549695	0.578214
C	-3.366578	0.591581	-0.582093
H	-1.472718	1.172914	-1.456485
C	-3.318714	-1.418988	0.818985
H	-1.405239	-2.384398	1.030652
C	-4.025909	-0.339677	0.237102
H	-3.912265	1.433234	-1.032458
H	-3.860598	-2.132765	1.457057
C	1.359760	1.591494	0.485358
N	1.073927	2.481705	1.182082
C	3.041350	-0.037785	-0.477994
O	3.348309	-1.090727	-1.056728
O	4.028976	0.684790	0.141622
C	5.363512	0.165103	0.069260
H	5.991284	1.074876	0.271555
H	5.567055	-0.226770	-0.961359
C	5.586232	-0.904581	1.110244
H	4.948231	-1.793956	0.887051
H	6.657820	-1.215575	1.103366
H	5.325119	-0.524558	2.126662
C	-6.111617	0.786462	-0.003790
H	-6.100709	0.747250	-1.119758
H	-7.143603	0.603864	0.391035
H	-5.712230	1.762169	0.364381
O	-5.360410	-0.298672	0.540611

Energy = -0.056581082854
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -858.744586862

INT1
-AM1-

C	0.254736	1.063114	0.008594

H	0.097910	2.150383	0.100438
C	-2.044835	0.700797	-0.109719
O	-0.757471	0.234794	-0.103556
C	1.574748	0.487262	0.006562
C	2.681426	1.346605	0.123423
C	1.781917	-0.901449	-0.109180
C	3.973314	0.836106	0.125809
H	2.525563	2.433402	0.214172
C	3.065186	-1.422904	-0.108085
H	0.911688	-1.573924	-0.201108
C	4.166916	-0.549657	0.009998
H	4.828785	1.520038	0.217970
H	3.240924	-2.505108	-0.197635
C	-2.338013	2.060860	0.001368
N	-2.615537	3.190299	0.092213
C	-3.008333	-0.367609	-0.241986
O	-2.785404	-1.580974	-0.341750
O	-4.306569	0.076312	-0.262501
C	-5.331950	-0.921138	-0.377301
H	-5.034907	-1.689275	-1.138077
H	-6.209377	-0.324121	-0.746827
C	-5.617797	-1.561188	0.958815
H	-6.483935	-2.257923	0.861549
H	-4.725170	-2.136421	1.306135
H	-5.860381	-0.784710	1.723024
C	6.535317	-0.317173	0.117721
H	6.517014	0.233562	1.089147
H	7.393350	-1.036097	0.085314
H	6.583765	0.395750	-0.740573
O	5.395412	-1.165058	0.000916

Energy = -0.082638789701
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -858.765573228

TS2
-AM1-

C	-4.167609	-0.225927	-0.241731
C	-3.680917	-0.195690	1.079163
C	-2.331052	0.024150	1.301312
C	-1.448533	0.218091	0.218723
C	-1.949950	0.183299	-1.101924
C	-3.294663	-0.035245	-1.337242
C	-0.057431	0.431482	0.483183

O	0.753916	0.654682	-0.526552
C	2.103680	0.881113	-0.201485
C	2.931273	-0.268295	-0.332842
O	4.281232	-0.013934	-0.265754
C	5.158466	-1.139521	-0.387357
C	5.301810	-1.861957	0.930398
C	2.449482	2.182865	0.138061
N	2.755411	3.271372	0.427126
O	2.558053	-1.447301	-0.482718
H	0.333690	0.431739	1.521902
H	-1.944003	0.047116	2.333741
H	-1.251901	0.329257	-1.945726
H	-4.359123	-0.345518	1.931620
H	-3.699617	-0.066118	-2.360192
H	6.126528	-0.663889	-0.702630
H	4.788227	-1.833172	-1.186588
H	4.325212	-2.319773	1.221051
H	6.067623	-2.667704	0.835327
H	5.616811	-1.154411	1.733948
C	-6.397312	-0.638125	0.494372
H	-6.121835	-1.549868	1.077179
H	-6.433895	0.262012	1.154104
H	-7.373395	-0.783728	-0.035540
O	-5.476408	-0.433820	-0.577958

Energy = -0.072735687988
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -858.740486902

INT2
-AM1-

C	0.006289	-0.220297	-0.129451
H	0.486772	-1.209481	-0.252935
C	2.072407	0.915883	-0.087014
O	0.698168	0.888892	-0.037916
C	-1.428865	-0.089367	-0.058525
C	-2.206339	-1.257562	-0.151177
C	-2.065316	1.157123	0.098242
C	-3.592361	-1.189150	-0.089213
H	-1.713444	-2.235708	-0.273650
C	-3.446360	1.239705	0.161342
H	-1.454359	2.072424	0.170556
C	-4.214511	0.059726	0.067129
H	-4.186795	-2.110788	-0.163129

H	-3.955715	2.206919	0.283782
C	2.571423	2.223404	0.018443
N	3.010936	3.298460	0.105120
C	2.882681	-0.253736	-0.226526
O	2.511252	-1.439863	-0.324406
O	4.228871	0.004417	-0.261343
C	5.108748	-1.122485	-0.385204
H	6.053039	-0.648722	-0.768730
H	4.701915	-1.846099	-1.138466
C	5.324975	-1.790452	0.950299
H	4.369717	-2.243962	1.310456
H	6.092421	-2.593743	0.846221
H	5.675152	-1.049525	1.708137
O	-5.573132	0.247965	0.140454
C	-6.385963	-0.919903	0.050514
H	-6.163872	-1.618349	0.893195
H	-7.426387	-0.514260	0.134829
H	-6.237118	-1.426541	-0.933572

Energy = -0.085174195646
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -858.768273326

TS3
-AM1-

C	-0.557946	-0.095437	2.673967
C	-0.212611	1.319449	2.510342
C	-0.643186	2.010247	1.393106
C	-1.481445	1.351507	0.376545
C	-1.804980	-0.003100	0.530511
C	-1.310869	-0.734607	1.705913
C	0.586690	-0.772136	3.282619
C	1.639927	0.221848	3.497442
C	1.144822	1.513795	3.020167
C	2.005190	2.391604	2.382300
C	0.269105	2.930947	0.716836
C	-1.021298	1.834637	-0.936311
C	-0.948364	0.978837	-2.019364
C	-1.293998	-0.436065	-1.858698
C	-1.686196	-0.908988	-0.619897
C	-1.188327	-2.199546	-0.146343
C	-0.955382	-2.091525	1.292637
C	0.125834	-2.737273	1.870004
C	0.919763	-2.059097	2.893493

C	2.967486	-0.123797	3.309525
C	3.318700	-1.483574	2.895946
C	2.323163	-2.424516	2.693972
C	2.395343	-3.331513	1.547118
C	1.036610	-3.525733	1.038132
C	0.815588	-3.628157	-0.324780
C	-0.328927	-2.948200	-0.933764
C	0.086607	-2.445262	-2.242316
C	-0.382345	-1.221201	-2.690080
C	0.035583	2.822336	-0.722862
C	2.906794	0.354006	-3.344719
C	2.575553	1.640226	-2.953253
C	-0.557946	-0.095437	2.673967
C	-0.212611	1.319449	2.510342
C	-0.643186	2.010247	1.393106
C	-1.481445	1.351507	0.376545
C	-1.804980	-0.003100	0.530511
C	-1.310869	-0.734607	1.705913
C	0.586690	-0.772136	3.282619
C	1.639927	0.221848	3.497442
C	1.144822	1.513795	3.020167
C	2.005190	2.391604	2.382300
C	0.269105	2.930947	0.716836
C	-1.021298	1.834637	-0.936311
C	-0.948364	0.978837	-2.019364
C	-1.293998	-0.436065	-1.858698
C	-1.686196	-0.908988	-0.619897
C	-1.188327	-2.199546	-0.146343
C	-0.955382	-2.091525	1.292637
C	0.125834	-2.737273	1.870004
C	0.919763	-2.059097	2.893493
C	2.967486	-0.123797	3.309525
C	3.318700	-1.483574	2.895946
C	2.323163	-2.424516	2.693972
C	2.395343	-3.331513	1.547118
C	1.036610	-3.525733	1.038132
C	0.815588	-3.628157	-0.324780
C	-0.328927	-2.948200	-0.933764
C	0.086607	-2.445262	-2.242316
C	-0.382345	-1.221201	-2.690080
C	0.035583	2.822336	-0.722862
C	2.906794	0.354006	-3.344719
H	2.575553	1.640226	-2.953253

C	-0.557946	-0.095437	2.673967
O	-0.212611	1.319449	2.510342
C	-0.643186	2.010247	1.393106
C	-1.481445	1.351507	0.376545
C	-1.804980	-0.003100	0.530511
C	-1.310869	-0.734607	1.705913
H	0.586690	-0.772136	3.282619
C	1.639927	0.221848	3.497442
H	1.144822	1.513795	3.020167
C	2.005190	2.391604	2.382300
H	0.269105	2.930947	0.716836
H	-1.021298	1.834637	-0.936311
C	-0.948364	0.978837	-2.019364
N	-1.293998	-0.436065	-1.858698
C	-1.686196	-0.908988	-0.619897
O	-1.188327	-2.199546	-0.146343
O	-0.955382	-2.091525	1.292637
C	0.125834	-2.737273	1.870004
H	0.919763	-2.059097	2.893493
H	2.967486	-0.123797	3.309525
C	3.318700	-1.483574	2.895946
H	2.323163	-2.424516	2.693972
H	2.395343	-3.331513	1.547118
H	1.036610	-3.525733	1.038132
C	0.815588	-3.628157	-0.324780
H	-0.328927	-2.948200	-0.933764
H	0.086607	-2.445262	-2.242316
H	-0.382345	-1.221201	-2.690080
O	0.035583	2.822336	-0.722862

Energy = 1.477957777952
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3144.92851206

TS4
-AM1-

C	0.834333	0.727611	-2.255278
C	0.433281	2.022373	-1.698291
C	0.70972	2.321658	-0.377283
C	1.439501	1.366591	0.474101
C	1.813814	0.126318	-0.057163
C	1.484836	-0.192240	-1.453113
C	-0.211639	0.289444	-3.178496
C	-1.259437	1.311835	-3.195374

C	-0.859866	2.382169	-2.280712
C	-1.813197	3.023579	-1.507774
C	-0.300803	2.992591	0.439028
C	0.816068	1.417909	1.807632
C	0.639625	0.264852	2.549693
C	1.040715	-1.031067	1.995866
C	1.588744	-1.094118	0.727585
C	1.186415	-2.164805	-0.183446
C	1.121448	-1.606602	-1.532871
C	0.133852	-2.025644	-2.409441
C	-0.552571	-1.050903	-3.256016
C	-2.589856	0.939132	-3.286655
C	-2.949605	-0.477725	-3.36634
C	-1.959060	-1.445145	-3.351578
C	-2.140657	-2.666346	-2.564888
C	-0.846404	-3.025840	-1.982980
C	-0.784552	-3.554620	-0.704896
C	0.261151	-3.113617	0.219857
C	-0.319282	-3.043712	1.560125
C	0.059625	-2.028096	2.422533
C	-0.235405	2.433885	1.789178
C	-3.32589	-0.703439	3.137533
C	-2.986525	0.636897	3.212442
C	-3.674294	1.614482	2.367083
C	-4.664708	1.198837	1.493024
C	-5.023433	-0.218176	1.414098
C	-3.972201	-2.436939	1.658576
C	-2.678059	-2.79750	2.239830
C	-2.277970	-1.725671	3.153216
C	-0.947691	-1.351785	3.241964
C	-0.588459	0.064864	3.319946
C	-1.579901	1.031504	3.306751
C	-2.692362	2.612428	1.939421
C	-2.754376	3.141313	0.661615
C	-3.801675	2.702649	-0.262256
C	-4.730162	1.757997	0.141800
C	-5.129255	0.686594	-0.772337
C	-5.310737	-0.534774	0.014031
C	-4.932061	-1.758876	-0.510863
C	-4.244407	-2.736482	0.334279
C	-1.725684	-3.438301	1.465449
C	-2.013324	-3.754607	0.065263
C	-3.237558	-3.413471	-0.484626

C	-3.302976	-2.854272	-1.836025
C	-4.350252	-1.831701	-1.852173
C	-4.178319	-0.676395	-2.596010
C	-4.578773	0.617745	-2.041115
C	-3.597382	1.616205	-2.468208
C	-3.219912	2.629837	-1.603681
C	-1.397650	2.250591	2.519486
C	-1.525018	3.338062	-0.108794
C	-4.372671	-1.142797	2.213543
C	4.339801	0.396962	-0.138478
H	4.012653	0.780520	-1.124570
C	3.680311	2.388618	0.903618
O	4.303367	1.149900	0.945185
C	5.019161	-0.869960	-0.014716
C	5.254068	-1.618874	-1.182220
C	5.447911	-1.372142	1.230218
C	5.900703	-2.845983	-1.114647
H	4.924479	-1.229119	-2.159299
C	6.094546	-2.593411	1.311759
H	5.263861	-0.782816	2.144241
C	6.321459	-3.335846	0.132529
H	6.076407	-3.420423	-2.035287
H	6.433797	-2.997298	2.277094
C	3.446418	2.899358	2.195187
N	3.223890	3.338240	3.250448
C	3.847136	3.228218	-0.259197
O	4.261569	2.880636	-1.380079
O	3.477916	4.530962	-0.071463
C	3.593450	5.415458	-1.197833
H	2.895872	6.251242	-0.918650
H	3.235159	4.901049	-2.127013
C	5.011917	5.903637	-1.357024
H	5.682938	5.051435	-1.624394
H	5.054021	6.667995	-2.168981
H	5.378967	6.361843	-0.407646
O	6.968307	-4.531604	0.319251
C	7.207335	-5.319357	-0.845465
H	7.866480	-4.770707	-1.560831
H	7.728129	-6.223695	-0.439013
H	6.242802	-5.602624	-1.331917

Energy = 1.474997831633
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3144.93025186

cis-**4c**
-AM1-

C	0.301322	0.094263	-2.869714
C	0.039634	1.507963	-2.544305
C	0.630553	2.074435	-1.445937
C	1.765913	1.443362	-0.636745
C	2.046656	-0.069725	-0.984230
C	1.129547	-0.643009	-2.066729
C	-0.934713	-0.476345	-3.398630
C	-1.958967	0.567447	-3.405973
C	-1.353951	1.789714	-2.877965
C	-2.103497	2.639580	-2.080452
C	-0.168096	2.939597	-0.595417
C	1.261772	1.680252	0.786785
C	1.258098	0.739931	1.783013
C	1.522501	-0.673766	1.460441
C	1.763485	-1.037995	0.162357
C	1.136117	-2.246418	-0.346636
C	0.746095	-2.001973	-1.728333
C	-0.414704	-2.570150	-2.232556
C	-1.285270	-1.782292	-3.095106
C	-3.272887	0.254360	-3.101563
C	-3.639310	-1.124471	-2.770382
C	-2.673061	-2.116086	-2.769360
C	-2.655597	-3.120402	-1.703997
C	-1.257941	-3.405044	-1.374841
C	-0.887965	-3.637072	-0.062196
C	0.345198	-3.047652	0.463503
C	0.106998	-2.658559	1.847082
C	0.678772	-1.491493	2.327824
C	0.220994	2.694203	0.786187
C	-2.437393	0.126846	3.511570
C	-2.097606	1.431925	3.198253
C	-2.972978	2.230413	2.338133
C	-4.142632	1.680878	1.839529
C	-4.502480	0.301925	2.173130
C	-3.413816	-1.857722	2.664316
C	-2.016786	-2.145865	2.990666
C	-1.410775	-0.917858	3.509759
C	-0.102107	-0.601568	3.186509
C	0.258268	0.774359	2.847265
C	-0.71209	1.763351	2.860297
C	-2.126621	3.053398	1.472440

C	-2.496369	3.286214	0.159988
C	-3.734731	2.709931	-0.366541
C	-4.533881	1.927156	0.450344
C	-5.135508	0.700349	-0.074318
C	-5.116999	-0.303965	0.990616
C	-4.871103	-1.632082	0.686027
C	-3.996690	-2.431047	1.546312
C	-1.277855	-2.993885	2.183293
C	-1.893627	-3.599544	1.000896
C	-3.215663	-3.325891	0.691084
C	-3.607038	-3.079713	-0.698151
C	-4.629604	-2.032582	-0.701202
C	-4.645548	-1.082382	-1.708819
C	-4.905517	0.321994	-1.386692
C	-4.059927	1.148189	-2.248995
C	-3.492211	2.309878	-1.754021
C	-0.729430	2.756299	1.794487
C	-1.488629	3.234157	-0.901180
C	-3.673850	-0.453316	2.986402
C	3.520304	-0.108759	-1.469398
H	3.532845	-0.272323	-2.587680
C	3.123044	2.163824	-0.910668
O	4.105693	1.187239	-1.258844
C	4.382677	-1.129667	-0.799016
C	4.551406	-2.379369	-1.403400
C	5.062315	-0.837517	0.392229
C	5.362638	-3.347912	-0.816421
H	4.041363	-2.608220	-2.351969
C	5.878945	-1.788805	0.988568
H	4.955905	0.162918	0.849664
C	6.024191	-3.051449	0.382050
H	5.477432	-4.326833	-1.301316
H	6.415413	-1.570975	1.923044
C	3.005362	3.112801	-2.019184
N	2.940435	3.874065	-2.893094
C	3.672989	2.869461	0.334832
O	4.324155	2.351533	1.239396
O	3.393646	4.199499	0.364854
C	3.900602	4.962669	1.476052
H	3.748939	4.389443	2.427350
H	3.244495	5.874784	1.457430
C	5.352796	5.311740	1.270054
H	5.693442	5.982500	2.094614

H	5.977136	4.385110	1.274673
H	5.498000	5.834173	0.294212
C	7.025419	-5.209974	0.464128
H	7.490861	-5.118489	-0.547145
H	7.719097	-5.729349	1.173115
H	6.049890	-5.750252	0.399943
O	6.851131	-3.926793	1.054797

Energy = 1.372315527721
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3144.97283191

trans-**4c**
-AM1-

C	0.787414	0.834773	-2.342586
C	0.415526	2.104508	-1.692178
C	0.787252	2.343476	-0.395084
C	1.784813	1.499913	0.395837
C	2.184841	0.137671	-0.299717
C	1.496374	-0.104179	-1.64196
C	-0.314996	0.444427	-3.217461
C	-1.364410	1.458125	-3.118749
C	-0.909861	2.480415	-2.177097
C	-1.819585	3.082605	-1.322818
C	-0.182663	2.943945	0.505103
C	1.033593	1.335341	1.717185
C	0.901200	0.156810	2.402143
C	1.274029	-1.113973	1.754420
C	1.748935	-1.106464	0.469605
C	1.268838	-2.121167	-0.453866
C	1.113896	-1.500178	-1.762263
C	0.080859	-1.895510	-2.59943
C	-0.65944	-0.891185	-3.351742
C	-2.697345	1.084838	-3.149774
C	-3.059123	-0.328312	-3.280349
C	-2.067912	-1.289751	-3.380765
C	-2.193568	-2.550352	-2.646550
C	-0.863127	-2.927704	-2.166684
C	-0.71577	-3.517999	-0.924255
C	0.38339	-3.108451	-0.047625
C	-0.105171	-3.115653	1.324754
C	0.327274	-2.132669	2.200559
C	-0.028847	2.321186	1.812629
C	-3.009453	-0.879129	3.213209

C	-2.674103	0.458542	3.335455
C	-3.420358	1.471985	2.587065
C	-4.463161	1.092592	1.758086
C	-4.818624	-0.321553	1.631128
C	-3.743726	-2.542082	1.694871
C	-2.413187	-2.921644	2.171129
C	-1.956136	-1.891194	3.105986
C	-0.625306	-1.509185	3.118644
C	-0.268090	-0.096429	3.239995
C	-1.265813	0.858697	3.352277
C	-2.472020	2.495676	2.144660
C	-2.618824	3.086537	0.902548
C	-3.723309	2.68962	0.027645
C	-4.618753	1.718011	0.443477
C	-5.070458	0.690251	-0.495650
C	-5.194953	-0.570192	0.238462
C	-4.846414	-1.763779	-0.370640
C	-4.10151	-2.777704	0.377734
C	-1.512399	-3.518951	1.305841
C	-1.890198	-3.767653	-0.086820
C	-3.149126	-3.407126	-0.538202
C	-3.304956	-2.781792	-1.852889
C	-4.353429	-1.765895	-1.749082
C	-4.234134	-0.573393	-2.443426
C	-4.602624	0.688706	-1.799303
C	-3.655249	1.714062	-2.237796
C	-3.229259	2.687828	-1.350586
C	-1.140295	2.108657	2.614576
C	-1.441980	3.322441	0.063614
C	-4.112300	-1.279935	2.338945
C	3.724687	0.244222	-0.489408
H	3.928789	0.629691	-1.532823
C	3.151393	2.227038	0.618893
O	4.187393	1.257480	0.425352
C	4.500561	-1.003314	-0.229100
C	4.826957	-1.835138	-1.305116
C	4.945588	-1.330977	1.059213
C	5.563520	-3.000239	-1.103258
H	4.502082	-1.572555	-2.324040
C	5.686093	-2.484534	1.278801
H	4.715522	-0.658767	1.901219
C	5.990905	-3.324942	0.190481
H	5.804215	-3.645512	-1.959169

H	6.040107	-2.751015	2.284799
C	3.289719	2.742268	1.977340
N	3.417110	3.165072	3.050576
C	3.374016	3.339534	-0.411491
O	3.750378	3.181784	-1.572107
O	3.139812	4.586912	0.071790
C	3.364561	5.699987	-0.814149
H	2.763774	6.516059	-0.328568
H	2.954472	5.461699	-1.829818
C	4.830555	6.045769	-0.880467
H	5.403623	5.209433	-1.350116
H	4.966581	6.968056	-1.494250
H	5.239383	6.227350	0.142367
O	6.723945	-4.447747	0.512677
C	7.056902	-5.315010	-0.566006
H	7.688363	-4.783406	-1.318540
H	7.637701	-6.133627	-0.069816
H	6.133017	-5.721052	-1.044766

Energy = 1.372533914140
-B3LYP/6-31G*//AM1-
E(RB+HF-LYP) = -3144.97836252