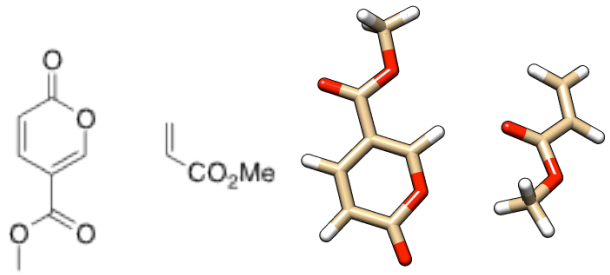
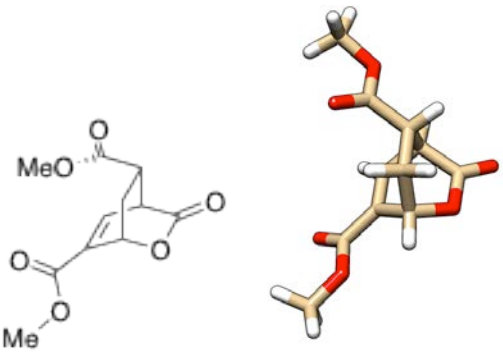


Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-2.193610	0.043717	-0.043599
6	C	-0.882693	-0.320515	0.050488
6	C	-2.785185	-2.291824	-0.359061
6	C	-3.166542	-0.991641	-0.257361
1	H	-3.492271	-3.096769	-0.519202
1	H	-0.046407	0.351699	0.208262
6	C	4.368712	1.119852	-0.588680
6	C	4.094021	2.387289	-0.912010
1	H	3.117126	2.811786	-0.699782
1	H	4.833189	3.021278	-1.390884
1	H	-4.210064	-0.702582	-0.333962
8	O	-0.489540	-1.597803	-0.048833
6	C	-1.393415	-2.676982	-0.254574
8	O	-0.912246	-3.784057	-0.318975
6	C	-2.642249	1.451339	0.066754
8	O	-1.621133	2.309696	0.269038
8	O	-3.807735	1.796031	-0.015393
6	C	-1.980619	3.699688	0.391536
1	H	-2.470159	4.047379	-0.521117
1	H	-2.653614	3.844613	1.239741
1	H	-1.040045	4.225608	0.550694
1	H	5.335498	0.667975	-0.787562
6	C	3.353890	0.255239	0.066061
8	O	2.218110	0.593639	0.359745
8	O	3.852173	-0.972849	0.302741
6	C	2.964807	-1.919338	0.938164
1	H	3.539794	-2.840717	1.018904
1	H	2.677891	-1.556205	1.928146
1	H	2.069338	-2.072253	0.333857

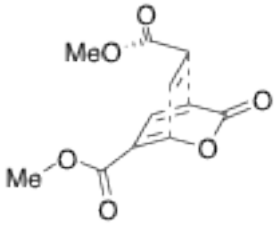
Sum of electronic and zero-point Energies= -877.557258

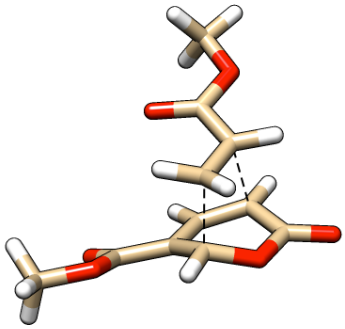


Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	1.142560	0.096278	-0.310257
6	C	0.910281	0.936558	0.926426
6	C	-1.027868	1.012379	-0.688941
6	C	0.111599	0.148299	-1.169230
1	H	-1.842880	1.120333	-1.400335
1	H	1.784396	1.024949	1.565910
6	C	-1.528166	0.434165	0.693565
1	H	-2.315835	1.105461	1.053981
6	C	-0.332323	0.410053	1.674904
1	H	-0.521774	1.054538	2.537678
1	H	-0.154096	-0.604870	2.037689
1	H	0.090434	-0.378921	-2.117056
8	O	0.599909	2.309116	0.506321
6	C	-0.442568	2.389480	-0.358077
8	O	-0.846473	3.446783	-0.778915
6	C	-2.183212	-0.933866	0.519563
8	O	-1.876330	-1.942974	1.119255
8	O	-3.183260	-0.878622	-0.383058
6	C	-3.900269	-2.110681	-0.614024
1	H	-3.219778	-2.880644	-0.984079
1	H	-4.367200	-2.454605	0.311502
1	H	-4.654686	-1.868405	-1.361373
6	C	2.352542	-0.722522	-0.561755
8	O	3.230526	-0.645671	0.464290
8	O	2.541423	-1.389188	-1.561267
6	C	4.441245	-1.414453	0.314010
1	H	4.204694	-2.475881	0.210719
1	H	4.993483	-1.080162	-0.567126
1	H	5.013958	-1.231484	1.222380

Sum of electronic and zero-point Energies= -877.566946



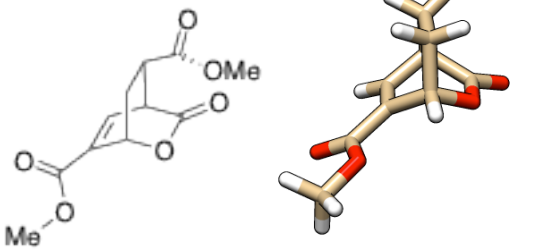


Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	1.167485	0.480289	-0.489518
6	C	0.939260	1.311096	0.639528
6	C	-1.026811	1.138528	-1.142783
6	C	0.116766	0.386703	-1.395922
1	H	-1.926300	1.029888	-1.737609
1	H	1.747817	1.510628	1.332708
6	C	-1.482095	0.087157	1.128353
1	H	-2.305476	0.777964	1.267627
6	C	-0.256300	0.260656	1.788237
1	H	-0.235800	0.993715	2.590332
1	H	0.347089	-0.628201	1.947890
1	H	0.153137	-0.348867	-2.192324
8	O	0.169884	2.448656	0.464369
6	C	-0.938777	2.374588	-0.366518
8	O	-1.710554	3.307735	-0.400854
6	C	-1.785973	-1.213267	0.503701
8	O	-0.966260	-2.099933	0.320517
8	O	-3.090156	-1.316272	0.160085
6	C	-3.487165	-2.565157	-0.437413
1	H	-2.948469	-2.728922	-1.374130
1	H	-3.282297	-3.395347	0.242756
1	H	-4.557045	-2.470513	-0.619839
6	C	2.331808	-0.428399	-0.593746
8	O	3.076298	-0.432670	0.536709
8	O	2.598065	-1.087332	-1.580171
6	C	4.230737	-1.297810	0.523105
1	H	3.923910	-2.333829	0.363817
1	H	4.918432	-0.997567	-0.270613

1	H	4.693173	-1.176737	1.502000

Sum of electronic and zero-point Energies= -877.512475

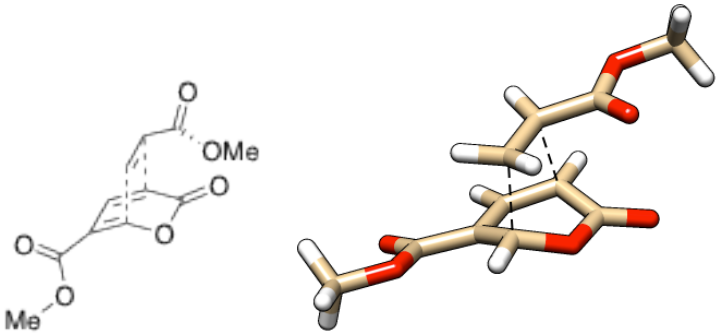


Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-1.542915	0.146029	0.319164
6	C	-0.849716	-0.110267	-1.002866
6	C	0.735879	0.676748	0.795757
6	C	-0.693260	0.572693	1.267545
1	H	1.422957	1.082934	1.534600
1	H	-1.532778	-0.318321	-1.822077
6	C	1.169251	-0.768370	0.319676
6	C	0.220406	-1.207024	-0.820254
1	H	0.780751	-1.317642	-1.751653
1	H	-0.262349	-2.161986	-0.595536
1	H	-0.994349	0.824206	2.279140
8	O	-0.136089	1.109157	-1.396392
6	C	0.730732	1.562040	-0.455815
8	O	1.412445	2.543142	-0.629782
6	C	-2.988685	-0.057086	0.572821
8	O	-3.633541	-0.499652	-0.531178
8	O	-3.538981	0.139272	1.639866
6	C	-5.051246	-0.719679	-0.385143
1	H	-5.240418	-1.475158	0.380926
1	H	-5.550209	0.210650	-0.104939
1	H	-5.392028	-1.063084	-1.361114
1	H	1.074009	-1.421539	1.192865
6	C	2.642611	-0.800793	-0.084308
8	O	3.068311	-1.078275	-1.185436
8	O	3.427529	-0.485999	0.964827
6	C	4.847766	-0.443286	0.704779
1	H	5.305578	-0.170252	1.654621
1	H	5.200289	-1.421420	0.370253

1	H	5.066231	0.304419	-0.060478

Sum of electronic and zero-point Energies= -877.565775

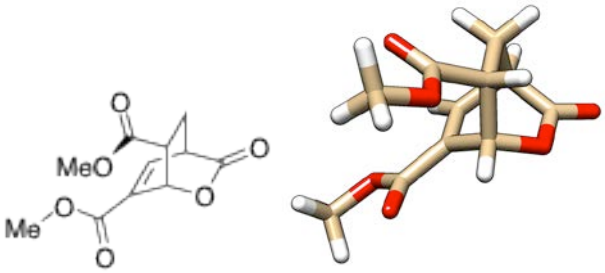


Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-1.574633	0.546777	0.146611
6	C	-0.901797	0.123696	-1.033135
6	C	0.569328	1.350157	0.806228
6	C	-0.775427	1.151465	1.110699
1	H	1.276143	1.712091	1.543488
1	H	-1.463348	-0.293573	-1.860373
6	C	1.054923	-1.105001	0.495775
6	C	0.068564	-1.499206	-0.418309
1	H	0.429064	-1.782650	-1.404828
1	H	-0.779511	-2.066765	-0.049821
1	H	-1.171779	1.349435	2.101757
8	O	0.131914	0.904556	-1.504060
6	C	0.976018	1.517139	-0.588956
8	O	1.935217	2.136708	-0.989870
6	C	-2.962961	0.148374	0.463248
8	O	-3.508228	-0.622441	-0.507439
8	O	-3.555993	0.473399	1.475667
6	C	-4.871282	-1.040475	-0.287436
1	H	-4.945263	-1.627946	0.630451
1	H	-5.525162	-0.168887	-0.211519
1	H	-5.131040	-1.644128	-1.156167
1	H	0.890664	-1.161190	1.564735
6	C	2.464236	-0.974023	0.052990
8	O	2.853082	-1.140444	-1.088417
8	O	3.278442	-0.662008	1.086933
6	C	4.672051	-0.497284	0.753062
1	H	5.166680	-0.255671	1.693250
1	H	5.073234	-1.421854	0.331084

1	H	4.790728	0.313277	0.030786

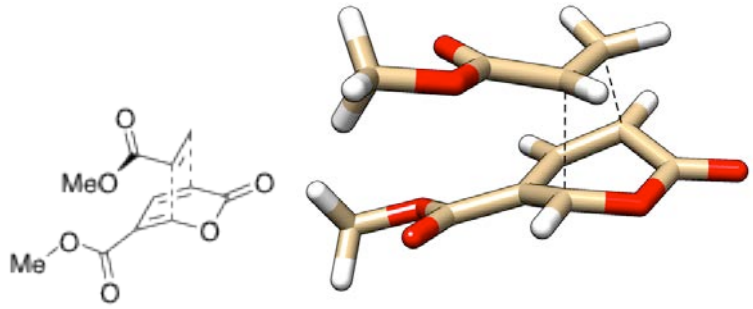
Sum of electronic and zero-point Energies= -877.508462



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-0.904820	-1.276875	0.953499
6	C	-2.133798	-0.404073	1.001121
6	C	-0.579036	0.174896	-0.900196
6	C	-0.068008	-0.963259	-0.049388
6	C	-1.652495	1.081160	1.175056
1	H	-2.524257	1.739503	1.220702
1	H	-1.103060	1.170142	2.114629
6	C	-0.742503	1.454122	-0.017013
1	H	-1.211589	2.205747	-0.658926
1	H	0.019506	0.353025	-1.790037
1	H	-2.854237	-0.691718	1.765237
1	H	-0.721058	-2.060653	1.679766
8	O	-1.921261	-0.149414	-1.372446
6	C	-2.792642	-0.472494	-0.376535
8	O	-3.945907	-0.743327	-0.607125
6	C	1.255141	-1.562917	-0.321747
8	O	2.026878	-1.139130	-1.165577
8	O	1.520293	-2.619848	0.472232
6	C	2.807422	-3.241463	0.284841
1	H	2.833865	-4.066732	0.995441
1	H	2.906286	-3.608606	-0.739156
1	H	3.607212	-2.526749	0.492251
6	C	0.619598	1.994378	0.401031
8	O	1.224882	2.596811	-0.639159
8	O	1.113977	1.889123	1.505046
6	C	2.564037	3.083416	-0.406123
1	H	2.868642	3.545682	-1.344048
1	H	2.564993	3.813282	0.406316
1	H	3.225428	2.252005	-0.153225

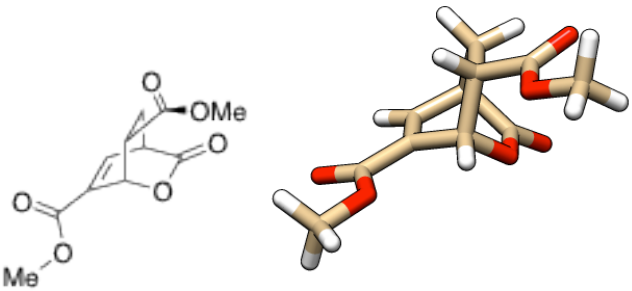
Sum of electronic and zero-point Energies= -877.567971



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-0.953998	-1.410660	0.820701
6	C	-2.210927	-0.791271	0.945998
6	C	-0.752883	-0.092257	-1.136308
6	C	-0.178356	-1.043192	-0.269301
6	C	-1.621127	1.282324	1.250123
1	H	-2.648495	1.630938	1.257386
1	H	-1.175200	1.084043	2.218652
6	C	-0.772550	1.674695	0.203824
1	H	-1.167507	2.277875	-0.606801
1	H	-0.215308	0.295038	-1.993139
1	H	-2.846661	-1.000193	1.799208
1	H	-0.545581	-2.022013	1.617161
8	O	-2.105688	-0.089923	-1.335250
6	C	-2.938151	-0.446675	-0.280986
8	O	-4.136123	-0.408291	-0.439473
6	C	1.254727	-1.381561	-0.436919
8	O	1.985024	-0.864100	-1.264643
8	O	1.654878	-2.336325	0.423679
6	C	3.045409	-2.709741	0.349135
1	H	3.171758	-3.496412	1.091932
1	H	3.286803	-3.077556	-0.650609
1	H	3.677819	-1.850869	0.584411
6	C	0.678379	1.799380	0.470399
8	O	1.291621	2.529992	-0.484567
8	O	1.260360	1.291993	1.415986
6	C	2.724972	2.642612	-0.375740
1	H	3.022335	3.312076	-1.182249
1	H	3.002284	3.058588	0.595444
1	H	3.184201	1.659796	-0.502815

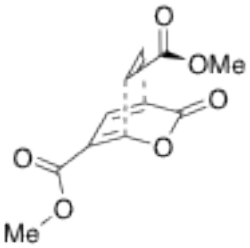
Sum of electronic and zero-point Energies= -877.512586

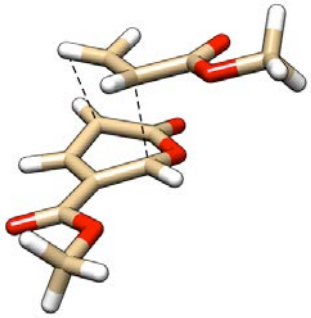


Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-1.381772	-0.484078	-0.164501
6	C	-0.081432	0.124218	0.313652
6	C	0.196452	-2.230055	-0.556152
6	C	-1.229072	-1.740470	-0.614496
1	H	0.322311	-3.270610	-0.851391
1	H	-0.197678	1.084398	0.806583
6	C	1.077779	-1.262942	-1.420090
6	C	0.909831	0.180050	-0.885554
1	H	0.470362	0.840765	-1.640907
1	H	-2.048237	-2.349606	-0.982294
8	O	0.519488	-0.760269	1.310981
6	C	0.668639	-2.048238	0.888187
8	O	1.142842	-2.897933	1.600160
6	C	-2.690255	0.210576	-0.154111
8	O	-2.588294	1.465848	0.340424
8	O	-3.734733	-0.275180	-0.545380
6	C	-3.816189	2.219457	0.399494
1	H	-4.238198	2.335443	-0.601412
1	H	-4.540672	1.710615	1.039267
1	H	-3.541365	3.186411	0.819109
1	H	0.765273	-1.338011	-2.464375
1	H	2.125822	-1.563605	-1.357236
6	C	2.238015	0.818770	-0.478473
8	O	2.039716	2.057682	0.014573
8	O	3.332037	0.310195	-0.598619
6	C	3.223333	2.766344	0.441013
1	H	2.867310	3.730361	0.802156
1	H	3.725092	2.214127	1.238458
1	H	3.909566	2.895189	-0.398874

Sum of electronic and zero-point Energies= -877.566249

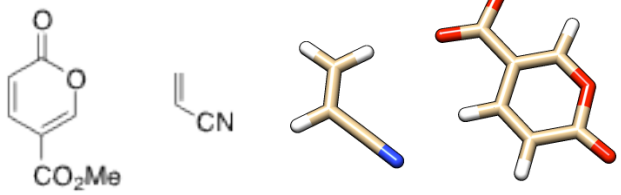




Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	1.374064	-0.668349	-0.130581
6	C	0.229478	-0.107933	-0.735057
6	C	-0.113142	-2.431721	0.466303
6	C	1.189346	-1.899821	0.480191
1	H	-0.332353	-3.367213	0.969082
1	H	0.238729	0.867613	-1.203771
6	C	-1.124819	-0.948155	1.689597
6	C	-0.916477	0.328651	1.145284
1	H	-0.158160	0.981235	1.562214
1	H	1.982883	-2.341857	1.074234
8	O	-0.706833	-0.927199	-1.293091
6	C	-0.941466	-2.175033	-0.719794
8	O	-1.768610	-2.903726	-1.209711
6	C	2.640125	0.082253	0.042893
8	O	2.580322	1.318878	-0.499448
8	O	3.625503	-0.360814	0.603025
6	C	3.773481	2.119783	-0.375596
1	H	4.022651	2.269585	0.677295
1	H	4.610307	1.630406	-0.878810
1	H	3.534268	3.067922	-0.855479
1	H	-0.559884	-1.248371	2.563449
1	H	-2.111347	-1.390417	1.583850
6	C	-2.058098	1.008805	0.484510
8	O	-1.777520	2.315047	0.244951
8	O	-3.113941	0.485425	0.184466
6	C	-2.833807	3.074865	-0.374548
1	H	-2.440488	4.085807	-0.477903
1	H	-3.084206	2.653953	-1.351210
1	H	-3.725885	3.070383	0.256302

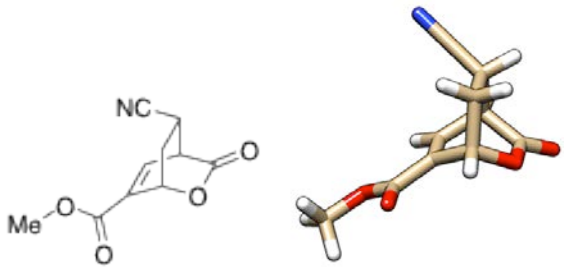
Sum of electronic and zero-point Energies= -877.507272



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	1.020971	0.526103	0.000023
6	C	2.337665	0.880305	-0.000233
6	C	1.696772	-1.805793	0.000238
6	C	0.705008	-0.877977	0.000254
1	H	1.488534	-2.868857	0.000425
1	H	2.695820	1.902983	-0.000424
6	C	-4.449812	-1.363279	-0.000012
6	C	-4.438853	-0.022124	-0.000428
1	H	-3.511358	0.542257	-0.000676
1	H	-5.375075	0.527022	-0.000572
1	H	-0.335275	-1.186399	0.000482
8	O	3.328916	-0.012853	-0.000279
6	C	3.094597	-1.426595	-0.000037
8	O	4.070445	-2.134694	-0.000080
6	C	-0.062042	1.532850	0.000093
8	O	0.403551	2.801264	0.000040
8	O	-1.250495	1.258133	0.000223
6	C	-0.591096	3.843999	0.000126
1	H	-1.217804	3.771346	-0.891688
1	H	-1.217685	3.771312	0.892020
1	H	-0.028746	4.776962	0.000104
1	H	-5.377912	-1.929067	0.000204
6	C	-3.246737	-2.139770	0.000080
7	N	-2.276952	-2.784096	0.000037

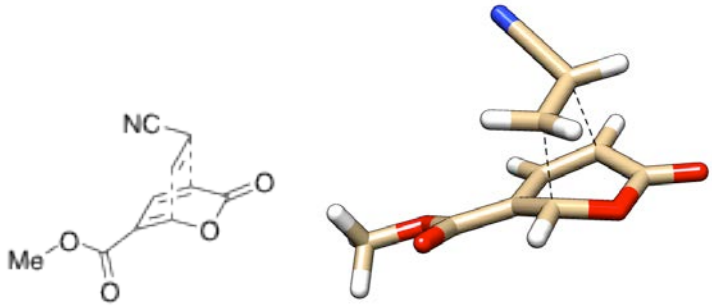
Sum of electronic and zero-point Energies= -741.954918



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-0.658246	-0.252276	0.033811
6	C	0.255390	-0.751152	1.128631
6	C	1.504234	-0.011237	-0.936679
6	C	0.007127	0.138207	-1.064877
1	H	2.059822	0.231734	-1.840581
1	H	-0.283832	-1.194542	1.962708
6	C	1.988468	0.855265	0.295730
1	H	3.059323	0.671235	0.432708
6	C	1.199332	0.389224	1.562746
1	H	1.890559	0.017402	2.323299
1	H	0.618900	1.204870	1.999241
1	H	-0.458973	0.528542	-1.961962
8	O	1.103195	-1.817789	0.589442
6	C	1.785498	-1.462538	-0.528390
8	O	2.535228	-2.219756	-1.093182
6	C	-2.120889	-0.192626	0.260393
8	O	-2.796588	0.229353	-0.824287
8	O	-2.645954	-0.488109	1.319627
6	C	-4.229531	0.323430	-0.678395
1	H	-4.649426	-0.655369	-0.436361
1	H	-4.483136	1.032905	0.112345
1	H	-4.593279	0.673149	-1.643528
6	C	1.828353	2.285439	0.018272
7	N	1.702082	3.418579	-0.204018

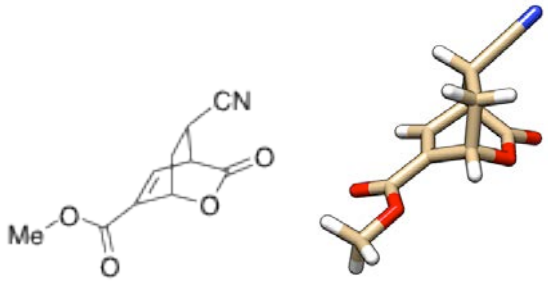
Sum of electronic and zero-point Energies= -741.964244



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-0.580848	-0.621609	-0.114611
6	C	0.304824	-1.055730	0.909670
6	C	1.412339	-0.138708	-1.326969
6	C	0.021151	-0.115197	-1.262227
1	H	1.951692	0.346260	-2.132441
1	H	-0.106229	-1.547426	1.784745
6	C	1.713444	1.310912	0.766388
1	H	2.786470	1.167435	0.692259
6	C	0.954435	0.596527	1.716779
1	H	1.526670	0.078203	2.481888
1	H	0.024699	1.036976	2.065332
1	H	-0.563911	0.393387	-2.020240
8	O	1.499309	-1.640295	0.535631
6	C	2.176792	-1.119646	-0.559696
8	O	3.299481	-1.507388	-0.794224
6	C	-2.013958	-0.473650	0.222892
8	O	-2.757550	-0.115740	-0.840310
8	O	-2.465119	-0.653579	1.342195
6	C	-4.169168	0.060197	-0.594706
1	H	-4.608010	-0.871671	-0.231518
1	H	-4.328100	0.849106	0.143625
1	H	-4.594363	0.339675	-1.557532
6	C	1.190155	2.475011	0.135934
7	N	0.749589	3.433633	-0.361881

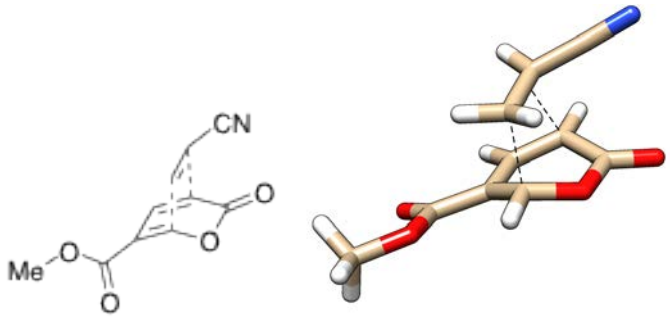
Sum of electronic and zero-point Energies= -741.908566



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-0.895102	0.146443	0.306487
6	C	-0.138391	-0.232510	-0.949790
6	C	1.378423	0.532291	0.920725
6	C	-0.084262	0.565516	1.291273
1	H	2.046112	0.926543	1.684635
1	H	-0.781702	-0.433482	-1.802536
6	C	1.708860	-0.975035	0.569893
6	C	0.820344	-1.401118	-0.642754
1	H	1.432460	-1.592840	-1.527287
1	H	0.256416	-2.308779	-0.414368
1	H	-0.434732	0.898017	2.262642
8	O	0.700398	0.896432	-1.352729
6	C	1.527094	1.347276	-0.370729
8	O	2.271171	2.279370	-0.536459
6	C	-2.368437	0.064023	0.463928
8	O	-2.964498	-0.402707	-0.655391
8	O	-2.970811	0.369526	1.474675
6	C	-4.403070	-0.511687	-0.604179
1	H	-4.701471	-1.198665	0.190788
1	H	-4.847752	0.468765	-0.420902
1	H	-4.697772	-0.894845	-1.580141
1	H	1.453909	-1.570462	1.452528
6	C	3.137920	-1.182224	0.317577
7	N	4.269167	-1.364724	0.128470

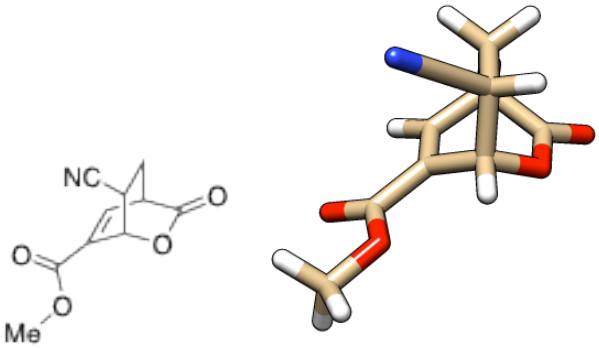
Sum of electronic and zero-point Energies= -741.961308



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	0.912839	-0.545767	0.101145
6	C	0.193251	0.029993	-0.984017
6	C	-1.235162	-1.230414	0.877867
6	C	0.139006	-1.157657	1.082733
1	H	-1.911400	-1.596766	1.641773
1	H	0.734492	0.445730	-1.826175
6	C	-1.489805	1.339799	0.777088
6	C	-0.548052	1.674828	-0.217521
1	H	-0.947550	2.066306	-1.149898
1	H	0.374660	2.143024	0.110094
1	H	0.593467	-1.467698	2.018806
8	O	-0.946396	-0.611888	-1.421258
6	C	-1.768227	-1.236114	-0.485675
8	O	-2.802142	-1.738538	-0.853885
6	C	2.351944	-0.291216	0.329755
8	O	2.884097	0.516579	-0.617031
8	O	2.988873	-0.751648	1.259123
6	C	4.293260	0.800726	-0.483314
1	H	4.492432	1.291346	0.471915
1	H	4.870255	-0.124669	-0.541784
1	H	4.534011	1.460027	-1.316186
1	H	-1.196422	1.310259	1.820649
6	C	-2.890711	1.403116	0.541179
7	N	-4.041350	1.490375	0.371396

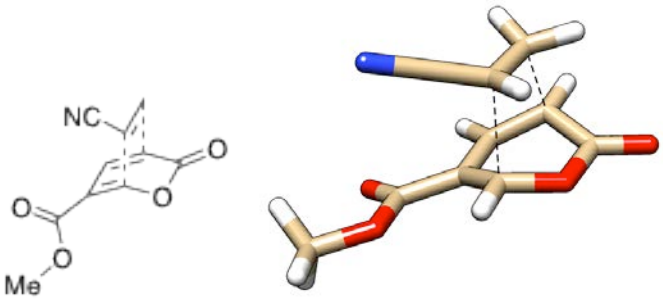
Sum of electronic and zero-point Energies= -741.903574



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-0.496976	-0.819274	1.277487
6	C	-1.920024	-0.416351	0.980665
6	C	-0.306824	0.167243	-0.874899
6	C	0.367497	-0.500849	0.301146
6	C	-1.943958	1.138022	0.780494
1	H	-2.961408	1.469268	0.558606
1	H	-1.625767	1.620695	1.706522
6	C	-0.987350	1.495370	-0.401729
1	H	-1.564436	1.874047	-1.252440
1	H	0.344750	0.318519	-1.731145
1	H	-2.640007	-0.736326	1.732406
1	H	-0.205473	-1.313047	2.198498
8	O	-1.402819	-0.667472	-1.347891
6	C	-2.291950	-1.020529	-0.374206
8	O	-3.256746	-1.700598	-0.616419
6	C	1.824098	-0.771062	0.394264
8	O	2.363562	-1.295732	1.348752
8	O	2.477762	-0.359197	-0.711910
6	C	3.908576	-0.549310	-0.707003
1	H	4.253683	-0.160366	-1.663885
1	H	4.356936	0.003150	0.121483
1	H	4.146786	-1.610583	-0.608363
6	C	0.002162	2.516336	-0.049978
7	N	0.787051	3.325865	0.228659

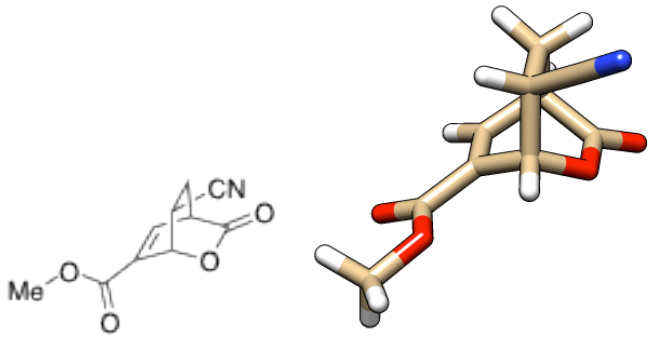
Sum of electronic and zero-point Energies= -741.963458



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-0.580862	-0.913522	1.246201
6	C	-1.930617	-0.559467	1.052529
6	C	-0.320295	-0.272513	-1.017382
6	C	0.273150	-0.748023	0.168044
6	C	-1.790049	1.550867	0.705191
1	H	-2.844860	1.653133	0.471918
1	H	-1.518397	1.783032	1.728712
6	C	-0.852702	1.799739	-0.319875
1	H	-1.218551	2.026348	-1.317046
1	H	0.254022	-0.059732	-1.909740
1	H	-2.640598	-0.629029	1.869483
1	H	-0.184570	-1.153070	2.227642
8	O	-1.610772	-0.607378	-1.315138
6	C	-2.515902	-0.794206	-0.274879
8	O	-3.661685	-1.071337	-0.536115
6	C	1.746410	-0.865102	0.339926
8	O	2.276688	-1.223333	1.373128
8	O	2.412562	-0.540272	-0.783457
6	C	3.853677	-0.544378	-0.687611
1	H	4.207159	-0.261107	-1.677916
1	H	4.177940	0.180948	0.061199
1	H	4.210081	-1.540183	-0.415928
6	C	0.429438	2.350251	-0.000918
7	N	1.478566	2.788050	0.255282

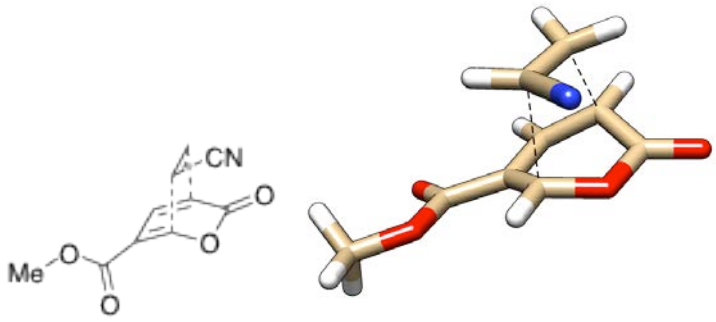
Sum of electronic and zero-point Energies= -741.906151



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	0.150108	-1.506153	0.803583
6	C	-1.354488	-1.425143	0.728547
6	C	-0.193558	0.503372	-0.419396
6	C	0.774030	-0.480761	0.201119
6	C	-1.811876	-0.093915	1.415151
1	H	-2.893068	0.017562	1.306686
1	H	-1.584091	-0.136492	2.482401
6	C	-1.059209	1.098141	0.738680
1	H	0.281785	1.272136	-1.022392
1	H	-1.868703	-2.290399	1.144279
1	H	0.672694	-2.321308	1.293202
8	O	-1.094575	-0.202296	-1.317305
6	C	-1.719972	-1.273645	-0.750015
8	O	-2.481995	-1.967511	-1.373188
6	C	2.250423	-0.340033	0.173642
8	O	3.026456	-1.138605	0.661337
8	O	2.631503	0.794031	-0.454341
6	C	4.054929	1.019108	-0.541896
1	H	4.164672	1.967410	-1.066025
1	H	4.490718	1.073171	0.458114
1	H	4.529101	0.209132	-1.100270
1	H	-0.377219	1.574603	1.450753
6	C	-1.970590	2.141880	0.257434
7	N	-2.683681	2.984590	-0.102838

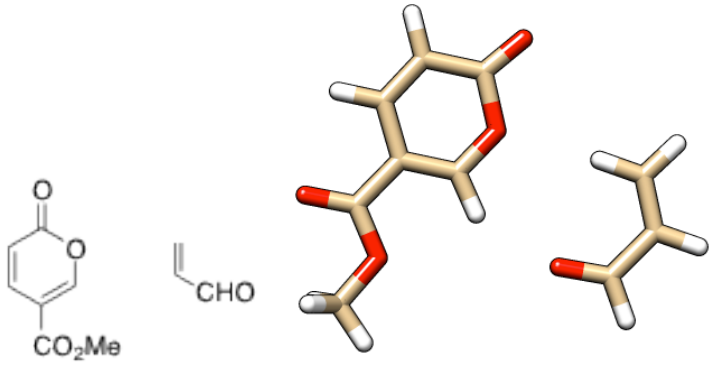
Sum of electronic and zero-point Energies= -741.961682



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	0.097879	-1.682625	0.576565
6	C	-1.311524	-1.650299	0.561949
6	C	-0.069757	0.256872	-0.772543
6	C	0.754815	-0.666045	-0.098976
6	C	-1.695839	0.146565	1.644835
1	H	-2.774914	0.120144	1.526453
1	H	-1.323733	-0.283110	2.566972
6	C	-0.977048	1.220363	1.075338
1	H	0.317520	1.123808	-1.292090
1	H	-1.882783	-2.393836	1.107164
1	H	0.649970	-2.364426	1.215422
8	O	-1.257658	-0.152568	-1.297347
6	C	-1.966147	-1.169344	-0.663541
8	O	-3.020411	-1.530958	-1.124362
6	C	2.217071	-0.465376	0.066117
8	O	2.944582	-1.235585	0.663054
8	O	2.645015	0.669462	-0.525779
6	C	4.059211	0.942966	-0.423117
1	H	4.353587	1.024891	0.625375
1	H	4.631553	0.144037	-0.899260
1	H	4.206807	1.888411	-0.943032
1	H	-0.035697	1.519008	1.525753
6	C	-1.660411	2.270454	0.383662
7	N	-2.189149	3.142442	-0.179859

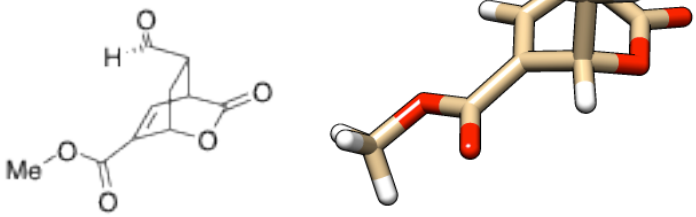
Sum of electronic and zero-point Energies= -741.903057



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-1.572745	0.470177	0.000186
6	C	-1.036990	2.840418	0.000856
6	C	-1.968631	1.851076	0.001079
1	H	-1.301524	3.890920	0.001496
6	C	4.121743	0.100047	-0.000914
1	H	-3.030422	2.076869	0.001944
8	O	0.693057	1.151693	-0.000991
6	C	0.378882	2.539203	-0.000362
8	O	1.312820	3.306979	-0.000837
6	C	-2.612130	-0.586328	0.000425
8	O	-2.089026	-1.829234	-0.000484
8	O	-3.808150	-0.355352	0.001352
6	C	-3.036088	-2.915402	-0.000311
1	H	-3.665564	-2.869934	0.891361
1	H	-3.667032	-2.868946	-0.890893
1	H	-2.431504	-3.821483	-0.001308
1	H	4.913122	0.843352	0.001050
1	H	3.097565	0.461582	-0.006629
6	C	3.349212	-2.254351	0.000966
8	O	2.145208	-2.043855	-0.003384
1	H	3.720529	-3.299772	0.003515
6	C	-0.238738	0.188027	-0.000810
1	H	0.201028	-0.802803	-0.001514
6	C	4.399676	-1.213002	0.003380
1	H	5.427384	-1.570811	0.008762

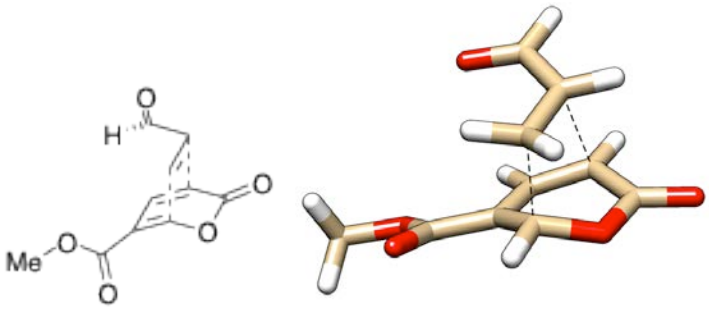
Sum of electronic and zero-point Energies= -763.026532



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-0.657422	-0.299639	0.040937
6	C	0.281227	-0.624462	1.178952
6	C	1.487422	-0.170094	-0.989577
6	C	-0.013708	-0.064213	-1.114061
1	H	2.024936	-0.058103	-1.930820
1	H	-0.236673	-0.955623	2.076003
6	C	1.967176	0.867845	0.104693
1	H	3.050279	0.720415	0.220507
6	C	1.218105	0.577225	1.423214
1	H	1.916394	0.325437	2.225862
1	H	0.638030	1.449930	1.735339
1	H	-0.502710	0.178671	-2.050690
8	O	1.131093	-1.752226	0.775003
6	C	1.800077	-1.543595	-0.384628
8	O	2.564496	-2.357102	-0.844869
6	C	1.798972	2.282532	-0.424036
8	O	1.174257	3.162320	0.126653
6	C	-2.117475	-0.229712	0.275494
8	O	-2.809935	0.055030	-0.845476
8	O	-2.632428	-0.403486	1.365851
6	C	-4.241059	0.152358	-0.693331
1	H	-4.649155	-0.794508	-0.332680
1	H	-4.493324	0.947509	0.011840
1	H	-4.620356	0.382989	-1.688047
1	H	2.312833	2.477534	-1.390547

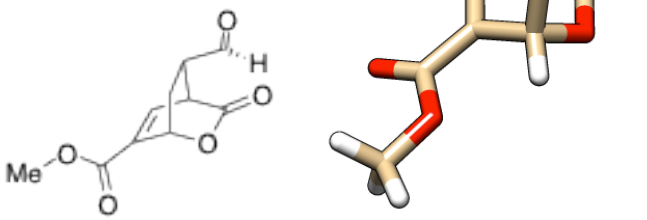
Sum of electronic and zero-point Energies= -763.037084



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-0.477794	-0.670861	-0.061761
6	C	0.434121	-0.903744	1.005535
6	C	1.467408	-0.253288	-1.371902
6	C	0.081978	-0.312811	-1.285443
1	H	1.968612	0.121771	-2.256948
1	H	0.051593	-1.327802	1.927785
6	C	1.620632	1.518873	0.617875
1	H	2.703674	1.467209	0.558593
6	C	0.914203	0.848328	1.633762
1	H	1.500349	0.486437	2.475163
1	H	-0.067692	1.240676	1.886534
1	H	-0.546157	0.029722	-2.099566
8	O	1.672849	-1.440762	0.701098
6	C	2.312141	-1.016786	-0.454810
8	O	3.470220	-1.325026	-0.632796
6	C	0.929857	2.455198	-0.267337
8	O	-0.288540	2.609438	-0.263965
6	C	-1.917040	-0.562021	0.268343
8	O	-2.685968	-0.415611	-0.825129
8	O	-2.349119	-0.606201	1.408057
6	C	-4.100278	-0.261654	-0.584727
1	H	-4.492505	-1.135431	-0.059659
1	H	-4.283227	0.634807	0.011626
1	H	-4.550233	-0.168116	-1.572120
1	H	1.568683	3.028617	-0.966726

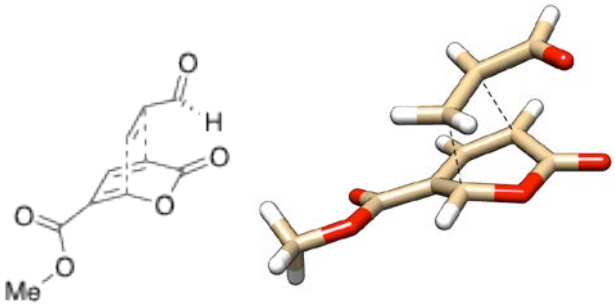
Sum of electronic and zero-point Energies= -762.985897



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-0.953231	0.227176	0.280018
6	C	-0.140290	-0.393888	-0.837171
6	C	1.286642	0.809895	0.860384
6	C	-0.187396	0.871191	1.175725
1	H	1.910851	1.392582	1.537706
1	H	-0.743769	-0.795404	-1.646787
6	C	1.691206	-0.716193	0.829092
6	C	0.840539	-1.428863	-0.246127
1	H	1.485705	-1.812033	-1.041415
1	H	0.283453	-2.272094	0.170558
1	H	-0.580463	1.393584	2.041675
8	O	0.678995	0.656451	-1.453426
6	C	1.461927	1.327168	-0.572740
8	O	2.212540	2.207391	-0.917547
6	C	-2.427555	0.138743	0.406560
8	O	-2.974588	-0.574572	-0.603552
8	O	-3.074978	0.636513	1.308096
6	C	-4.410441	-0.709605	-0.572766
1	H	-4.724019	-1.210588	0.345854
1	H	-4.882249	0.274036	-0.626420
1	H	-4.662544	-1.308124	-1.447193
1	H	1.477497	-1.109052	1.833456
6	C	3.195179	-0.884070	0.654918
8	O	3.718356	-1.643177	-0.130135
1	H	3.813447	-0.263085	1.337717

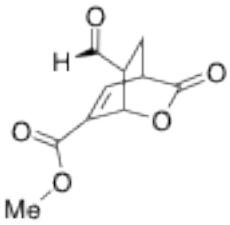
Sum of electronic and zero-point Energies= -763.034792

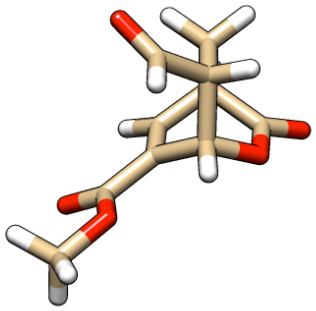


Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	0.946796	-0.575198	0.034239
6	C	0.178240	0.137873	-0.928464
6	C	-1.157083	-1.419157	0.774694
6	C	0.222459	-1.345038	0.939459
1	H	-1.791682	-1.924953	1.493434
1	H	0.678175	0.682910	-1.720554
6	C	-1.425482	1.157029	1.072166
6	C	-0.537557	1.651684	0.103619
1	H	-1.005104	2.145743	-0.746100
1	H	0.400682	2.085746	0.434621
1	H	0.718908	-1.782878	1.799958
8	O	-0.969734	-0.453220	-1.410535
6	C	-1.744289	-1.222321	-0.551567
8	O	-2.788511	-1.682825	-0.949180
6	C	2.390354	-0.330450	0.244773
8	O	2.877709	0.608916	-0.598625
8	O	3.067541	-0.905364	1.077198
6	C	4.286670	0.896434	-0.475412
1	H	4.512987	1.262575	0.528463
1	H	4.872952	-0.003672	-0.672539
1	H	4.490369	1.662254	-1.222675
1	H	-1.086354	0.952556	2.082954
6	C	-2.886609	1.184061	0.869745
8	O	-3.429779	1.594343	-0.143882
1	H	-3.489723	0.815411	1.723124

Sum of electronic and zero-point Energies= -762.978596

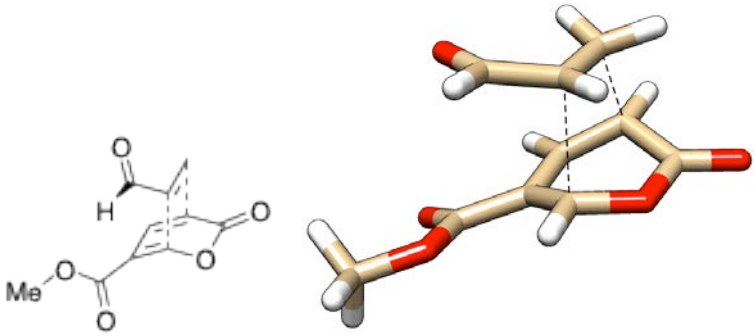




Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-0.447494	-0.739696	1.317292
6	C	-1.879039	-0.405739	0.985126
6	C	-0.290493	0.002106	-0.934142
6	C	0.406554	-0.513653	0.305390
6	C	-1.933748	1.116119	0.601131
1	H	-2.963283	1.391145	0.357465
1	H	-1.614949	1.717712	1.455831
6	C	-0.995595	1.355434	-0.600545
1	H	-1.564044	1.622839	-1.503091
1	H	0.355493	0.061783	-1.807117
1	H	-2.587971	-0.654400	1.773287
1	H	-0.140285	-1.114552	2.288008
8	O	-1.359129	-0.920997	-1.300582
6	C	-2.239511	-1.171820	-0.288337
8	O	-3.190597	-1.896413	-0.445597
6	C	1.867842	-0.728036	0.422949
8	O	2.423028	-1.197532	1.396721
8	O	2.522428	-0.323836	-0.691839
6	C	3.956180	-0.485668	-0.670478
1	H	4.302858	-0.117087	-1.635115
1	H	4.389268	0.095386	0.146708
1	H	4.214293	-1.539056	-0.541751
6	C	0.021173	2.467379	-0.407859
8	O	0.118784	3.154401	0.585842
1	H	0.697291	2.632689	-1.273756

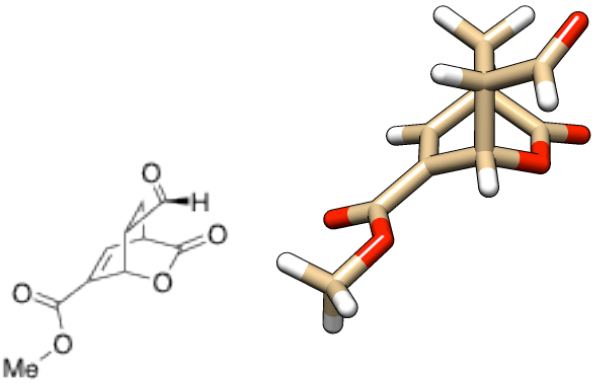
Sum of electronic and zero-point Energies= -763.035785



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-0.513134	-0.714299	1.317228
6	C	-1.877287	-0.431179	1.088038
6	C	-0.294247	-0.494183	-1.029266
6	C	0.322400	-0.722811	0.211035
6	C	-1.840398	1.551324	0.466242
1	H	-2.910932	1.600855	0.289998
1	H	-1.504768	1.944031	1.421061
6	C	-0.967136	1.717292	-0.627241
1	H	-1.366018	1.740429	-1.637529
1	H	0.258198	-0.418437	-1.956628
1	H	-2.572698	-0.404667	1.919980
1	H	-0.096982	-0.764310	2.317731
8	O	-1.581586	-0.890396	-1.240443
6	C	-2.466492	-0.924925	-0.166138
8	O	-3.602136	-1.287613	-0.355420
6	C	1.798046	-0.785272	0.378580
8	O	2.348425	-1.064268	1.424132
8	O	2.451380	-0.513412	-0.771219
6	C	3.892747	-0.519406	-0.689439
1	H	4.238650	-0.275220	-1.693053
1	H	4.229663	0.228706	0.031098
1	H	4.249329	-1.505878	-0.385294
6	C	0.364584	2.292996	-0.420949
8	O	0.890833	2.436984	0.676398
1	H	0.905742	2.586916	-1.343483

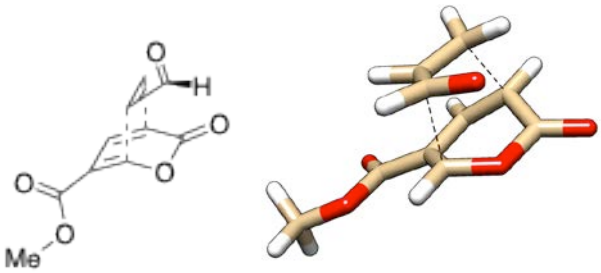
Sum of electronic and zero-point Energies= -762.982390



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	0.861165	-0.451644	0.220719
6	C	-0.113695	0.480301	-0.465207
6	C	-1.261012	-1.407041	0.756435
6	C	0.243600	-1.460428	0.858016
1	H	-1.767577	-2.258321	1.208649
1	H	0.365712	1.219090	-1.104255
6	C	-1.742088	-0.043572	1.365211
6	C	-1.040767	1.109390	0.611947
1	H	-0.401695	1.703283	1.281568
1	H	0.771525	-2.242616	1.393552
8	O	-0.976717	-0.297790	-1.351403
6	C	-1.602027	-1.342999	-0.733643
8	O	-2.342113	-2.080480	-1.333955
6	C	2.332983	-0.284370	0.214227
8	O	2.707908	0.823472	-0.467610
8	O	3.117565	-1.037526	0.758076
6	C	4.128309	1.067064	-0.537495
1	H	4.541824	1.186293	0.466456
1	H	4.628752	0.234888	-1.037394
1	H	4.235724	1.985383	-1.113381
1	H	-1.506235	-0.028386	2.431834
1	H	-2.826207	0.049081	1.260069
6	C	-1.993007	2.115091	-0.024450
8	O	-3.183923	2.168814	0.184894
1	H	-1.504351	2.848642	-0.701662

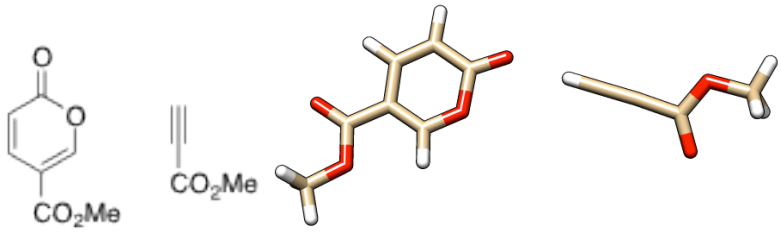
Sum of electronic and zero-point Energies= -763.035356



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	0.835912	-0.638634	-0.077965
6	C	0.014995	0.232246	-0.819487
6	C	-1.228239	-1.611747	0.611357
6	C	0.182319	-1.631074	0.636996
1	H	-1.793051	-2.349213	1.171384
1	H	0.407449	1.070947	-1.380216
6	C	-1.642169	0.176661	1.636925
6	C	-0.929388	1.251530	1.071936
1	H	0.024449	1.548016	1.498431
1	H	0.735504	-2.278286	1.309852
8	O	-1.167457	-0.200808	-1.320343
6	C	-1.870048	-1.202743	-0.648685
8	O	-2.898705	-1.616761	-1.118514
6	C	2.292937	-0.414331	0.090863
8	O	2.720791	0.685994	-0.567100
8	O	3.022099	-1.137522	0.742266
6	C	4.131081	0.974799	-0.462082
1	H	4.410147	1.126346	0.582922
1	H	4.715916	0.151133	-0.877093
1	H	4.281599	1.885713	-1.039918
1	H	-1.306182	-0.230216	2.583815
1	H	-2.716889	0.155954	1.473800
6	C	-1.624657	2.277265	0.276314
8	O	-2.765305	2.174911	-0.147106
1	H	-1.026784	3.189264	0.066370

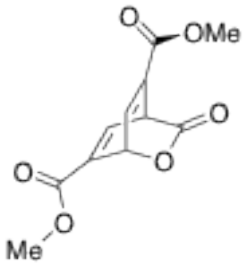
Sum of electronic and zero-point Energies= -762.977825

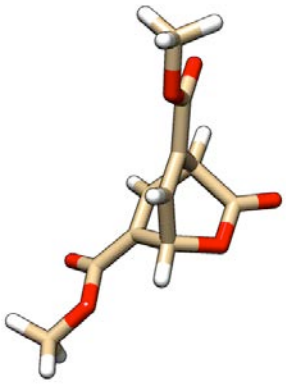


Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	3.238583	-1.695287	-0.009663
6	C	1.968479	-2.177669	-0.036946
6	C	2.398557	0.548780	-0.010161
6	C	3.479910	-0.278692	0.004637
6	C	-3.314805	-0.372340	-0.097506
6	C	-4.445744	0.058569	-0.077435
1	H	2.450650	1.630566	-0.001253
1	H	1.746114	-3.237592	-0.047511
1	H	4.096239	-2.360426	0.003058
8	O	1.139536	0.093987	-0.037174
6	C	0.827268	-1.287701	-0.054168
8	O	-0.346726	-1.584327	-0.081285
6	C	4.873566	0.229349	0.034803
8	O	5.851961	-0.493454	0.048114
8	O	4.933332	1.577219	0.045931
6	C	6.257786	2.150754	0.075592
1	H	6.102837	3.228788	0.079765
1	H	6.787572	1.831206	0.975546
1	H	6.822654	1.843106	-0.806978
6	C	-5.770231	0.636542	-0.068770
8	O	-6.711582	-0.291588	0.206278
8	O	-6.011195	1.809511	-0.281678
6	C	-8.068759	0.193564	0.235135
1	H	-8.679124	-0.679216	0.464111
1	H	-8.182588	0.959686	1.005867
1	H	-8.342554	0.614939	-0.735093
1	H	-2.312068	-0.757057	-0.112109

Sum of electronic and zero-point Energies= -876.312972

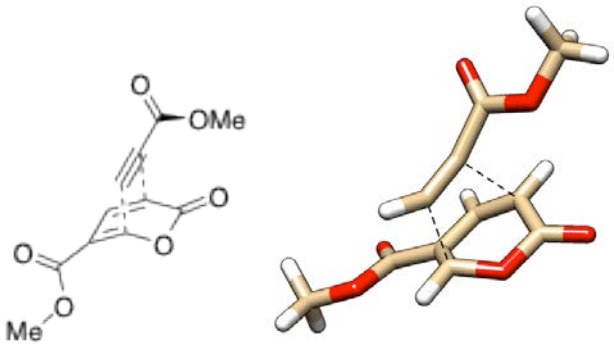




Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-1.434009	0.083452	0.301764
6	C	-0.761710	0.158188	-1.065221
6	C	0.696062	1.075393	0.757608
6	C	-0.657251	0.603569	1.264037
1	H	1.343572	1.515324	1.511028
1	H	-1.395764	-0.139690	-1.894207
6	C	1.357036	-0.062367	-0.022757
6	C	0.568231	-0.571027	-0.979240
1	H	-0.961002	0.725077	2.297516
8	O	-0.445069	1.580693	-1.303539
6	C	0.340304	2.119050	-0.334266
8	O	0.697606	3.269073	-0.352514
6	C	2.739180	-0.475716	0.314978
8	O	3.386641	0.008180	1.225002
8	O	3.192987	-1.456342	-0.492168
6	C	4.529458	-1.925330	-0.217830
1	H	5.245240	-1.106207	-0.316328
1	H	4.587170	-2.336409	0.792644
1	H	4.720738	-2.698003	-0.961393
6	C	-2.790559	-0.455621	0.543836
8	O	-3.346959	-0.936552	-0.592353
8	O	-3.342997	-0.477500	1.626762
6	C	-4.674048	-1.485416	-0.457180
1	H	-4.667344	-2.322050	0.245071
1	H	-5.364343	-0.718693	-0.098602
1	H	-4.951452	-1.819368	-1.456213
1	H	0.829349	-1.385442	-1.643424

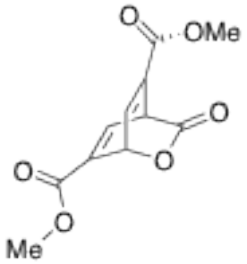
Sum of electronic and zero-point Energies= -876.352679

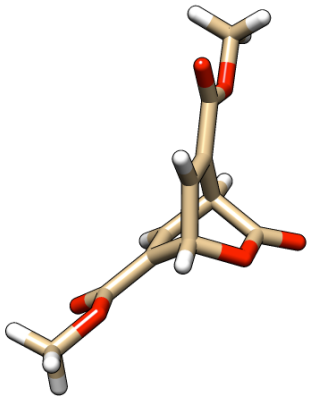


Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-1.509918	0.436029	0.383729
6	C	-1.016805	0.921361	-0.851695
6	C	0.676929	0.926407	1.196720
6	C	-0.592037	0.422310	1.435948
1	H	1.470850	0.845353	1.930020
1	H	-1.672137	1.016447	-1.709088
6	C	1.117142	-0.776047	-0.703309
6	C	0.091764	-0.634011	-1.400190
1	H	-0.837438	-0.085373	2.363047
8	O	-0.084657	1.928989	-0.845305
6	C	0.893226	1.923290	0.146276
8	O	1.786355	2.735880	0.091895
6	C	2.360985	-1.268432	-0.148704
8	O	2.444723	-2.293064	0.504269
8	O	3.393634	-0.464511	-0.457985
6	C	4.682831	-0.870381	0.048807
1	H	4.656256	-0.946189	1.138275
1	H	4.968852	-1.835679	-0.375274
1	H	5.370061	-0.087628	-0.268311
6	C	-2.810373	-0.257293	0.507553
8	O	-3.444183	-0.371624	-0.683736
8	O	-3.266176	-0.672200	1.556185
6	C	-4.729317	-1.027170	-0.649884
1	H	-5.417922	-0.473715	-0.007698
1	H	-5.079287	-1.028503	-1.681451
1	H	-4.624372	-2.047099	-0.273520
1	H	-0.459000	-1.041737	-2.230085

Sum of electronic and zero-point Energies= -876.265906

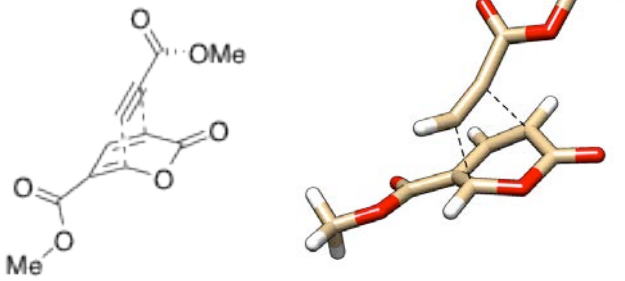




Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-1.425909	0.036044	0.317437
6	C	-0.875326	0.315064	-1.077034
6	C	0.823113	0.753387	0.716190
6	C	-0.518796	0.301352	1.269254
1	H	1.565844	1.001893	1.467678
1	H	-1.606881	0.231303	-1.874261
6	C	1.299671	-0.265939	-0.325215
6	C	0.378794	-0.517955	-1.265180
1	H	-0.716416	0.248252	2.333792
8	O	-0.444486	1.729315	-1.085709
6	C	0.474087	2.008866	-0.126875
8	O	0.943435	3.108240	0.025165
6	C	2.645447	-0.891106	-0.322177
8	O	3.020738	-1.710227	-1.139228
8	O	3.404459	-0.449364	0.702625
6	C	4.738265	-0.993777	0.777944
1	H	4.696648	-2.077749	0.906026
1	H	5.293038	-0.758101	-0.132876
1	H	5.195037	-0.517305	1.644300
6	C	-2.800943	-0.430809	0.602702
8	O	-3.504584	-0.635769	-0.534294
8	O	-3.249367	-0.618421	1.717355
6	C	-4.860427	-1.096348	-0.359456
1	H	-4.869189	-2.054124	0.165688
1	H	-5.436040	-0.365414	0.212654
1	H	-5.261169	-1.202415	-1.366725
1	H	0.509723	-1.209209	-2.089138

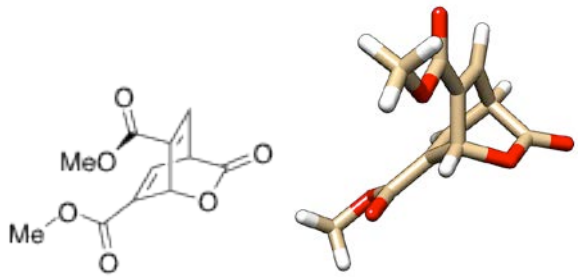
Sum of electronic and zero-point Energies= -876.352354



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-1.509941	0.435844	0.383704
6	C	-1.016799	0.921142	-0.851708
6	C	0.676938	0.926101	1.196699
6	C	-0.592055	0.422068	1.435923
1	H	1.470867	0.844982	1.929984
1	H	-1.672089	1.016211	-1.709134
6	C	1.117207	-0.776264	-0.703236
6	C	0.091854	-0.634283	-1.400155
1	H	-0.837486	-0.085607	2.363019
8	O	-0.084618	1.928733	-0.845318
6	C	0.893250	1.923024	0.146283
8	O	1.786368	2.735628	0.091937
6	C	2.361199	-1.268433	-0.148744
8	O	2.445258	-2.293222	0.503945
8	O	3.393546	-0.464123	-0.457806
6	C	4.682904	-0.869653	0.048858
1	H	4.656055	-0.947053	1.138202
1	H	4.969829	-1.834116	-0.376521
1	H	5.369607	-0.085914	-0.266965
6	C	-2.810499	-0.257287	0.507560
8	O	-3.444401	-0.371415	-0.683696
8	O	-3.266312	-0.672166	1.556197
6	C	-4.729690	-1.026662	-0.649851
1	H	-4.625114	-2.046459	-0.273031
1	H	-5.418295	-0.472744	-0.008063
1	H	-5.079434	-1.028329	-1.681495
1	H	-0.458860	-1.042036	-2.230068

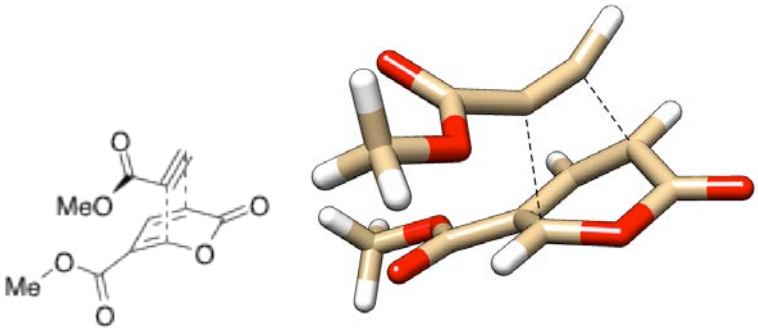
Sum of electronic and zero-point Energies= -876.265905



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-1.327861	1.164946	0.896401
6	C	-0.128697	2.104676	0.902261
6	C	0.158674	0.166469	-0.664103
6	C	-1.166913	0.113063	0.080813
6	C	1.134309	1.301942	1.176519
6	C	1.281834	0.248335	0.360737
1	H	0.274912	-0.607073	-1.415649
1	H	-0.249023	2.987244	1.525579
1	H	-2.220236	1.380264	1.471515
8	O	0.169178	1.452542	-1.398407
6	C	0.016922	2.525475	-0.590832
8	O	-0.002954	3.660779	-0.995360
6	C	-2.118786	-0.990213	-0.167993
8	O	-1.901076	-1.909678	-0.936481
8	O	-3.250667	-0.867987	0.556033
6	C	-4.232947	-1.906739	0.364975
1	H	-5.062847	-1.640816	1.018513
1	H	-4.555243	-1.936364	-0.678310
1	H	-3.816610	-2.877786	0.642502
6	C	2.432672	-0.681929	0.433347
8	O	2.373050	-1.625300	-0.529515
8	O	3.322202	-0.610822	1.260426
6	C	3.449123	-2.585172	-0.540694
1	H	4.403954	-2.079029	-0.699859
1	H	3.480951	-3.127506	0.406968
1	H	3.224560	-3.259086	-1.366250
1	H	1.851725	1.598763	1.932838

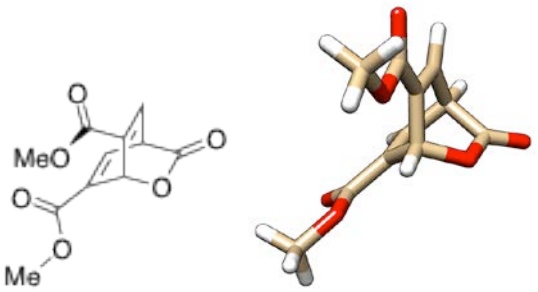
Sum of electronic and zero-point Energies= -876.353643



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-1.294985	1.601138	0.586754
6	C	-0.199389	2.454895	0.766133
6	C	0.111182	0.481072	-0.956406
6	C	-1.131138	0.544237	-0.303812
6	C	1.250729	0.993442	1.592462
6	C	1.299776	-0.028048	0.876558
1	H	0.372396	-0.331096	-1.622860
1	H	-0.231561	3.256500	1.495526
1	H	-2.163939	1.659130	1.232257
8	O	0.798507	1.617298	-1.240556
6	C	0.710871	2.693032	-0.359970
8	O	1.365754	3.684322	-0.576848
6	C	-2.041653	-0.619045	-0.427734
8	O	-1.794017	-1.608910	-1.092919
8	O	-3.179447	-0.453276	0.276067
6	C	-4.125330	-1.540648	0.205631
1	H	-4.967170	-1.229001	0.822582
1	H	-4.440234	-1.701761	-0.827785
1	H	-3.676035	-2.456741	0.595061
6	C	1.733584	-1.406883	0.674466
8	O	2.457746	-1.544835	-0.454077
8	O	1.457471	-2.316422	1.431168
6	C	2.939336	-2.878765	-0.728487
1	H	3.492948	-2.794306	-1.662608
1	H	3.591681	-3.219138	0.078735
1	H	2.099246	-3.568718	-0.833900
1	H	1.556649	1.593169	2.426730

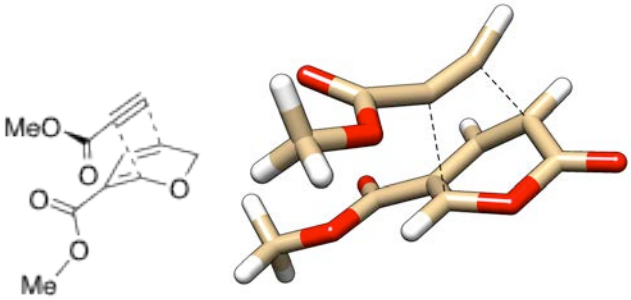
Sum of electronic and zero-point Energies= -876.265491



Standard orientation:

Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	1.239681	1.436533	-1.018066
6	C	0.000032	2.289033	-0.791364
6	C	0.000000	0.179929	0.569783
6	C	1.234870	0.294818	-0.315444
6	C	-1.239637	1.436570	-1.018077
6	C	-1.234870	0.294862	-0.315442
1	H	-0.000013	-0.669414	1.242932
1	H	0.000049	3.238649	-1.320512
1	H	2.053515	1.762203	-1.655583
8	O	0.000033	1.378343	1.440513
6	C	0.000013	2.538676	0.746562
8	O	0.000134	3.622937	1.272653
6	C	2.333024	-0.697145	-0.368086
8	O	3.319744	-0.595781	-1.072137
8	O	2.105950	-1.739853	0.461014
6	C	3.125117	-2.760028	0.480632
1	H	2.773217	-3.505508	1.192578
1	H	3.242356	-3.196341	-0.513924
1	H	4.078287	-2.334826	0.802753
6	C	-2.333058	-0.697062	-0.368078
8	O	-2.106021	-1.739773	0.461027
8	O	-3.319771	-0.595670	-1.072135
6	C	-3.125223	-2.759913	0.480649
1	H	-2.773363	-3.505387	1.192620
1	H	-4.078386	-2.334671	0.802739
1	H	-3.242455	-3.196246	-0.513899
1	H	-2.053458	1.762264	-1.655600

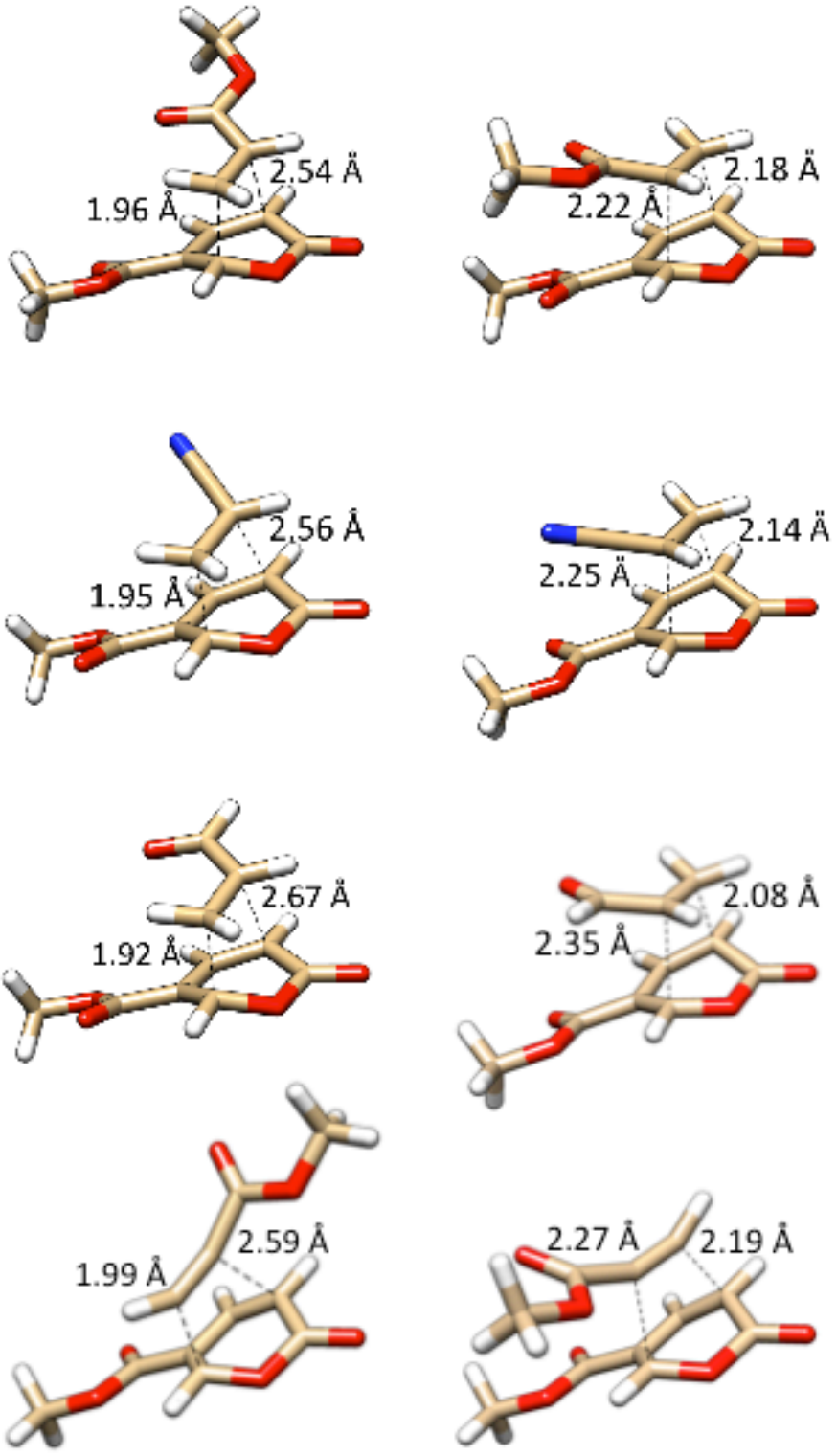
Sum of electronic and zero-point Energies= -876.352966

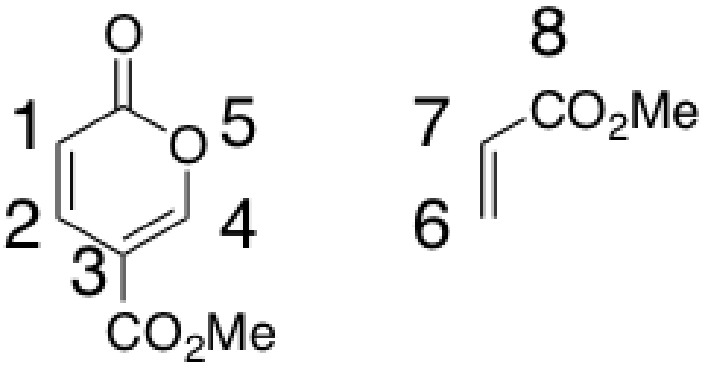


Standard orientation:

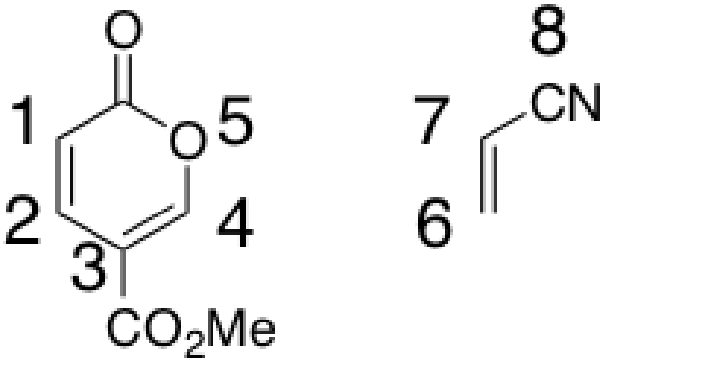
Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
6	C	-1.326959	-1.743496	0.713695
6	C	-2.430877	-0.881488	0.709436
6	C	-0.424723	-0.251328	-0.888248
6	C	-0.254724	-1.403195	-0.104315
6	C	-1.474776	0.928304	1.489012
6	C	-0.437715	1.201949	0.850343
1	H	0.356141	0.152270	-1.519405
1	H	-3.272418	-1.051798	1.371573
1	H	-1.227556	-2.543165	1.440074
8	O	-1.660028	0.104156	-1.330634
6	C	-2.767750	-0.172645	-0.531848
8	O	-3.860626	0.183614	-0.900548
6	C	1.052986	-2.090909	0.034821
8	O	1.232454	-3.073021	0.728766
8	O	2.017384	-1.506205	-0.707040
6	C	3.333292	-2.088865	-0.601230
1	H	3.964445	-1.494918	-1.260967
1	H	3.688394	-2.030704	0.429851
1	H	3.310672	-3.132879	-0.921007
6	C	0.784281	1.970626	0.668246
8	O	0.699933	2.790679	-0.400388
8	O	1.763611	1.870109	1.381655
6	C	1.856039	3.620290	-0.644287
1	H	1.606653	4.202140	-1.530586
1	H	2.038635	4.276011	0.210040
1	H	2.738885	3.001283	-0.820095
1	H	-2.200122	1.131652	2.252269

Sum of electronic and zero-point Energies= -876.265577

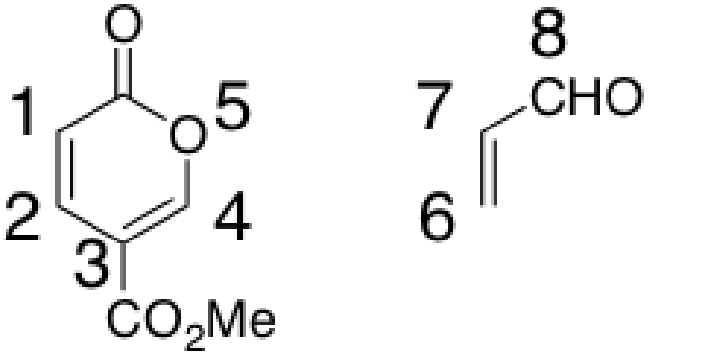




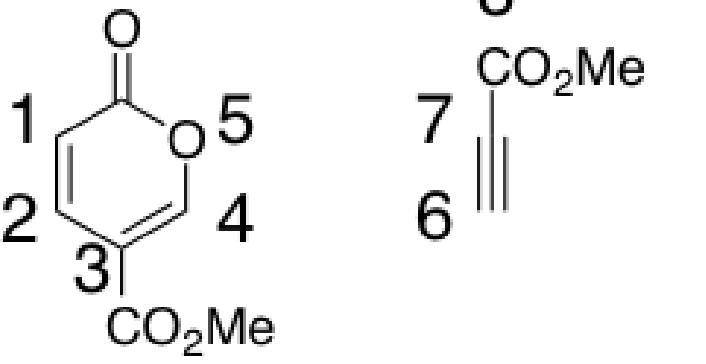
Atom #	Sum of Coefficients
1	-0.56
2	-0.26
3	0.57
4	0.44
5	-0.39
6	1.02
7	-0.70
8	-0.53



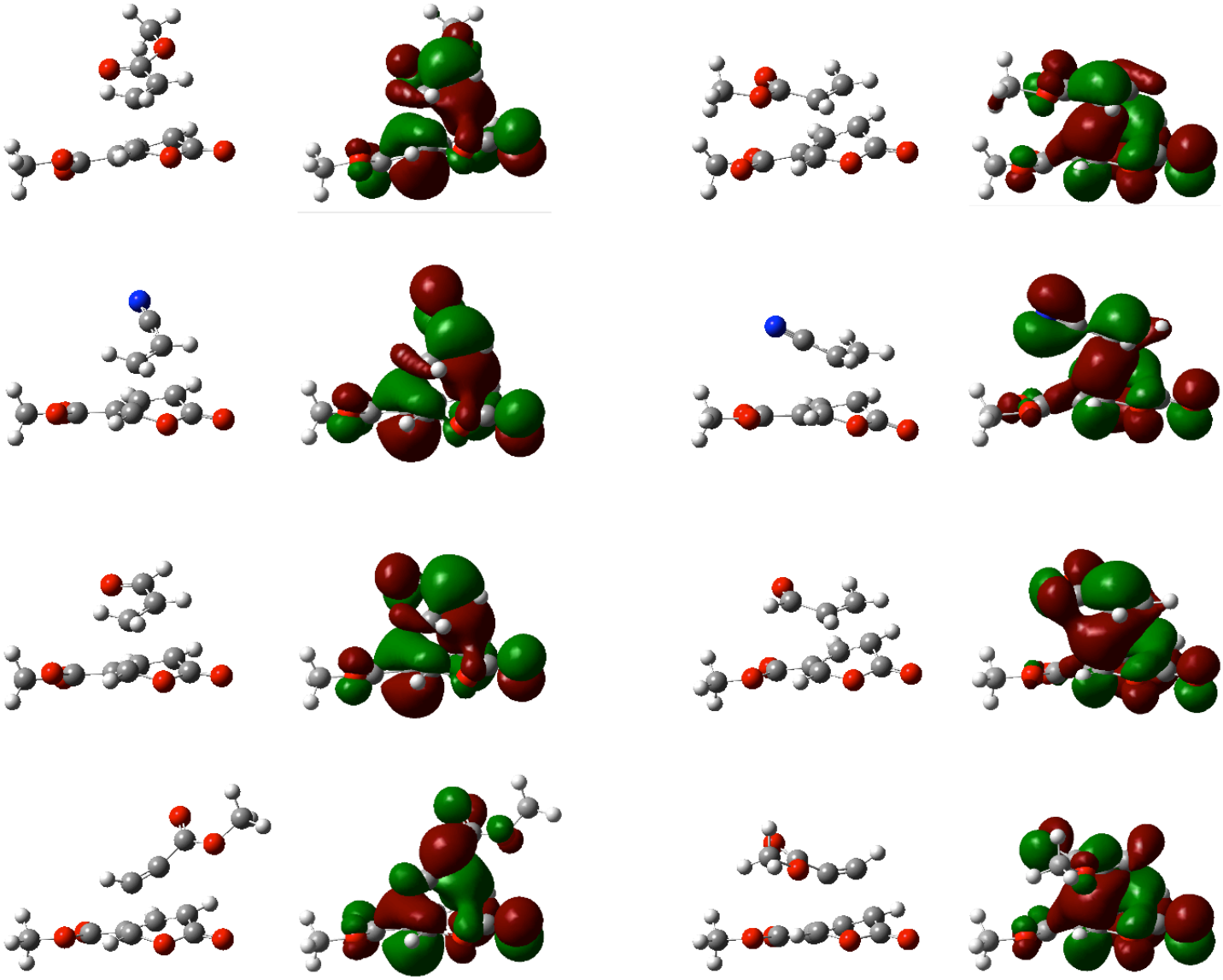
Atom #	Sum of Coefficients
1	-0.56
2	-0.26
3	0.57
4	0.44
5	-0.39
6	1.22
7	-0.99
8	-0.37



Atom #	Sum of Coefficients
1	-0.56
2	-0.26
3	0.57
4	0.44
5	-0.39
6	1.00
7	-0.55
8	-0.83



Atom #	Sum of Coefficients
1	-0.56
2	-0.26
3	0.57
4	0.44
5	-0.39
6	-1.00
7	0.87
8	0.78



Kohn-Sham HOMO orbitals for transition states forming para (left) and meta (right) regioisomers.