Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Theoretical and Experimental Exploration of the Photochemistry of Resveratrol: Beyond the Simple Double Bond Isomerization

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1 Cartesian Coordinates

trans-resveratrol
SCF Energy: -766.359299573
Num. Imaginary Frequencies: 0

C	-3.653505	1.247422	-0.055520
C	-2.269053	1.077196	-0.074440
C	-1.718986	-0.213151	-0.021050
C	-2.587999	-1.319284	0.042431
C	-3.970533	-1.133821	0.060328
C	-4.516872	0.150444	0.012433
H	-1.645200	1.960991	-0.140838
H	-2.176221	-2.326101	0.083127
H	-5.596683	0.271984	0.025181
O	-4.122993	2.531617	-0.110561
H	-5.092304	2.511777	-0.096381
O	-4.851248	-2.179219	0.124158
H	-4.348259	-3.007811	0.152742
C	-0.274731	-0.468496	-0.030501
H	-0.005760	-1.522930	-0.073629
C	0.709148	0.452795	0.022101
H	0.432514	1.503849	0.092407
C	2.152561	0.212490	0.008159
C	3.026998	1.303713	0.155484
C	2.735694	-1.062740	-0.149146
C	4.409950	1.142297	0.154186
H	2.612331	2.301764	0.275975
C	4.111202	-1.238724	-0.152303
H	2.101234	-1.934627	-0.277475
C	4.959525	-0.133454	0.000905
H	5.060930	2.007057	0.271495
H	4.551627	-2.223212	-0.275511
O	6.305794	-0.367163	-0.010864
H	6.772968	0.475263	0.102651

cis-resveratrol
SCF Energy: -766.382563076
Num. Imaginary Frequencies: 0

C	-0.717133	-2.162642	-0.385191
C	0.630429	-2.090058	-0.381080
H	-1.129167	-3.147537	-0.604767
H	1.153079	-3.036507	-0.515116
C	1.534069	-0.930708	-0.247012
C	-1.746716	-1.144622	-0.115610
C	1.233190	0.324171	-0.799030
C	2.148174	1.374392	-0.688483
C	3.371142	1.200428	-0.037471
C	3.674643	-0.051359	0.497266
C	2.772359	-1.114486	0.388579
H	0.294921	0.473379	-1.324017
O	1.898548	2.611369	-1.213967
H	4.075647	2.019553	0.040866
O	4.884229	-0.183540	1.120088
H	3.024682	-2.086897	0.805856
C	-3.010122	-1.273135	-0.724297
C	-4.038411	-0.370332	-0.481901
C	-3.831896	0.688747	0.407914
C	-2.593735	0.823435	1.047647
C	-1.570125	-0.082541	0.788749
H	-3.184263	-2.099292	-1.408946
H	-5.005571	-0.473397	-0.962322
O	-4.871120	1.548912	0.620724
H	-2.435426	1.631956	1.758742
H	-0.623433	0.028772	1.304799
H	4.973278	-1.090409	1.440892
H	1.028866	2.600880	-1.634900
H	-4.601077	2.217826	1.263676

cycloaddition-ts1
SCF Energy: -916.659313848
Num. Imaginary Frequencies: 1
Imaginary Frequency: -509.8907

C	0.782408	1.448070	-1.227228
C	-0.598408	1.528610	-0.908563
O	-0.613951	2.620102	0.611647
O	-1.289103	3.684849	0.432823
H	1.132151	2.152738	-1.978188
H	-1.142358	2.262041	-1.501134
C	-1.448004	0.370355	-0.493759
C	1.810266	0.686859	-0.577303
C	-1.121619	-0.930153	-0.901634
C	-1.974020	-1.994473	-0.585793
C	-3.150387	-1.781098	0.131043
C	-3.473662	-0.481367	0.525361
C	-2.637414	0.594498	0.213044
H	-0.214842	-1.109615	-1.470587
O	-1.699597	-3.278901	-0.961935
H	-3.805589	-2.608972	0.373814
O	-4.636057	-0.318186	1.221909
H	-2.900567	1.599710	0.525802
C	3.114946	0.671448	-1.139353
C	4.157197	-0.025418	-0.555198
C	3.938761	-0.727986	0.639611
C	2.667851	-0.712585	1.234089
C	1.624974	-0.020241	0.639029
H	3.293815	1.220470	-2.059876
H	5.148073	-0.036804	-0.996338
O	4.995709	-1.395626	1.177207
H	2.503273	-1.237840	2.172565
H	0.657852	-0.002324	1.126102
H	-4.742520	0.617131	1.440428
H	-0.863906	-3.292417	-1.446632
H	4.721267	-1.821145	2.000753

cycloaddition-int
SCF Energy: -916.668378834
Num. Imaginary Frequencies: 0

C	0.818575	1.329211	-1.324731
C	-0.567489	1.615700	-0.853939
O	-0.421112	2.539109	0.320291
O	-1.229981	3.580454	0.239224
H	1.115267	1.805279	-2.254587
H	-1.091919	2.227171	-1.592860
C	-1.450723	0.441679	-0.452455
C	1.815265	0.619710	-0.613590
C	-1.294060	-0.793063	-1.088158
C	-2.160452	-1.847742	-0.775808
C	-3.175849	-1.685200	0.165940
C	-3.321453	-0.447752	0.793246
C	-2.468529	0.620188	0.489426
H	-0.498692	-0.934877	-1.814148
O	-2.051093	-3.074706	-1.365411
H	-3.839464	-2.506615	0.407682
O	-4.327245	-0.331725	1.708723
H	-2.598955	1.579478	0.979367
C	3.110804	0.459665	-1.191603
C	4.120858	-0.225061	-0.546348
C	3.886286	-0.781916	0.722430
C	2.627485	-0.634779	1.326221
C	1.613644	0.048521	0.676731
H	3.301057	0.890976	-2.170589
H	5.101240	-0.342567	-0.995668
O	4.915620	-1.447149	1.314792
H	2.449038	-1.057646	2.312734
H	0.653992	0.159787	1.166953
H	-4.328246	0.567820	2.061812
H	-1.310717	-3.060161	-1.985945
H	4.631719	-1.771471	2.180116

cycloaddition-ts2
SCF Energy: -916.653799375
Num. Imaginary Frequencies: 1
Imaginary Frequency: -606.7183

C	0.855080	1.469265	-1.167861
C	-0.560371	1.782862	-0.694961
O	-0.341380	2.579151	0.485003
O	0.713441	3.373707	0.046032
C	-1.498073	0.629773	-0.387160
H	-1.028241	2.425516	-1.454372
H	1.123806	1.825971	-2.157568
C	1.748969	0.564278	-0.542890
C	-1.519638	-0.496152	-1.214919
C	-2.440007	-1.520722	-0.964826
C	-3.334664	-1.435307	0.102320
C	-3.301627	-0.307214	0.921279
C	-2.391929	0.731122	0.682024
H	-0.819924	-0.583528	-2.042496
O	-2.504522	-2.644300	-1.738592
H	-4.040923	-2.234315	0.292839
O	-4.191507	-0.264186	1.955541
H	-2.375350	1.606782	1.323489
C	2.988357	0.253494	-1.172093
C	3.910377	-0.590501	-0.586134
C	3.630014	-1.162026	0.666753
C	2.418455	-0.872893	1.315386
C	1.494127	-0.029236	0.724666
H	3.210485	0.697726	-2.138431
H	4.852347	-0.826043	-1.069459
O	4.567614	-1.989783	1.197797
H	2.206646	-1.315925	2.286139
H	0.568509	0.194890	1.239622
H	4.266621	-2.306274	2.060442
H	-4.070834	0.564137	2.438304
H	-1.836723	-2.586116	-2.434260

diotropic-ts
SCF Energy: -916.617873361
Num. Imaginary Frequencies: 1
Imaginary Frequency: -1060.0659

C	-3.064876	0.761727	-0.819442
C	-1.933408	0.465437	-0.028630
C	-2.032649	-0.583584	0.910868
C	-3.201780	-1.321739	1.033159
C	-4.309292	-1.017977	0.227970
C	-4.235445	0.030424	-0.700492
C	-0.712465	1.214762	-0.160648
C	0.569518	1.223529	0.048218
C	1.683444	0.283196	-0.018986
C	2.964625	0.704256	0.364796
C	4.031904	-0.198591	0.326770
C	3.836518	-1.514836	-0.093485
C	2.558839	-1.925104	-0.483065
C	1.480708	-1.038200	-0.453253
O	-5.481604	-1.700917	0.304232
O	-0.716666	3.615995	-0.145636
O	0.612397	3.682286	-0.169999
H	-0.952423	2.513965	-0.462210
H	0.902166	2.376244	0.202455
H	3.119322	1.728648	0.692564
O	5.297854	0.152653	0.692701
H	4.667469	-2.209276	-0.124635
O	2.427057	-3.220685	-0.892686
H	0.492116	-1.358985	-0.768384
H	-1.179943	-0.810187	1.542265
H	-3.263097	-2.128749	1.759962
H	-5.104901	0.252682	-1.309276
H	-3.010671	1.576169	-1.535249
H	-5.415554	-2.384276	0.984858
H	5.307517	1.084891	0.946881
H	1.511853	-3.375578	-1.160802

dioxetane
SCF Energy: -916.717331933
Num. Imaginary Frequencies: 0

C	0.764487	2.099869	-0.591027
C	-0.749819	1.938992	-0.909642
C	-1.456199	0.660852	-0.535347
H	-1.007940	2.228294	-1.935262
H	1.249960	2.696859	-1.374639
C	1.643567	0.956871	-0.197516
C	-1.438051	-0.415321	-1.428296
C	-2.077413	-1.609671	-1.079660
C	-2.747316	-1.732552	0.139351
C	-2.766979	-0.646383	1.012898
C	-2.119666	0.552516	0.686427
H	-0.927640	-0.329603	-2.385435
O	-2.089054	-2.699226	-1.903055
H	-3.249081	-2.657145	0.398136
O	-3.438821	-0.807103	2.190845
H	-2.139269	1.404682	1.358437
C	2.650534	0.515577	-1.067937
C	3.464032	-0.563769	-0.743116
C	3.290390	-1.212521	0.484773
C	2.303301	-0.770956	1.373834
C	1.486244	0.301843	1.030399
H	2.801616	1.026818	-2.015754
H	4.242841	-0.908705	-1.414642
O	4.117532	-2.261044	0.762567
H	2.174768	-1.268423	2.332745
H	0.725679	0.645611	1.721466
H	3.895326	-2.619707	1.632006
H	-3.392705	0.018459	2.690905
H	-1.582503	-2.497226	-2.700431
O	-1.010477	3.033913	0.006855
O	0.386607	2.959461	0.522991

diphenylacetylene
SCF Energy: -765.139238818
Num. Imaginary Frequencies: 0

C	0.832597	-0.008164	0.000220
C	-0.384204	-0.006233	0.000445
C	-1.808915	-0.002684	0.000242
C	2.256037	-0.009214	0.000049
C	-2.511038	1.216484	-0.000401
C	-3.907865	1.207893	-0.000791
C	-4.619103	0.006690	-0.000480
C	-3.915729	-1.199088	0.000428
C	-2.518730	-1.216912	0.000802
H	-1.961395	2.152981	-0.000373
O	-4.642229	2.359794	-0.001247
H	-5.702347	0.010314	-0.000779
O	-4.657351	-2.346113	0.001151
H	-1.975407	-2.157069	0.001957
C	2.982638	-1.218819	-0.001656
C	4.370002	-1.221563	-0.001700
C	5.070783	-0.008954	0.000043
C	4.368278	1.201915	0.001710
C	2.978078	1.199905	0.001665
H	2.441380	-2.159140	-0.002897
H	4.930443	-2.150251	-0.003017
O	6.433502	-0.071737	-0.000397
H	4.910316	2.145172	0.003185
H	2.436728	2.140116	0.003157
H	-4.060905	-3.106114	0.000998
H	-4.040843	3.115897	-0.001353
H	6.793680	0.825009	-0.000384