

# Solvent Effects on the 9-Hydroxymethylanthracene + *N*-Ethylmaleimide Diels–Alder Reaction. A Theoretical Study

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## Index

Table S1. Cartesian Coordinates of 9-hydroxymethylanthracene, according to B3LYP/6-31+G( <i>d</i> ) calculations.	page S2
Table S2. Cartesian Coordinates of <i>N</i> -ethyl maleimide, according to B3LYP/6-31+G( <i>d</i> ) calculations.	page S2
Table S3. Cartesian Coordinates of the transition state presenting a hydrogen bond, according to B3LYP/6-31+G( <i>d</i> ) calculations.	page S3
Table S4. Cartesian Coordinates of the transition state lacking a hydrogen bond, according to B3LYP/6-31+G( <i>d</i> ) calculations.	page S4
Table S5. Energy values (Hartrees) of the stationary points studied in this work, according to B3LYP/6-31+G( <i>d</i> ) calculations.	page S5
Table S6. Solvation terms (kcal mol <sup>-1</sup> ) of the stationary points studied in this work, according to B3LYP/6-31+G( <i>d</i> ) calculations.	page S5

## Supplementary Information

**Table S1.** Cartesian Coordinates of 9-hydroxymethylanthracene, according to B3LYP/6-31+G(*d*) calculations.

C	-3.652890	0.078419	-0.083611
C	-3.596390	-1.340075	0.038550
C	-2.503399	0.825388	-0.161142
C	-1.209241	0.207968	-0.127209
C	-1.160156	-1.228820	0.017896
C	-2.381198	-1.971623	0.091594
C	-0.004011	0.949328	-0.226590
C	1.247261	0.288794	-0.127256
C	1.281851	-1.151886	0.027079
C	0.082646	-1.867896	0.085136
C	2.512332	0.969340	-0.163615
C	3.700524	0.289495	-0.065383
C	3.722786	-1.128508	0.073036
C	2.543277	-1.823304	0.117616
C	-0.078855	2.448369	-0.434412
O	-0.452588	3.177905	0.746527
H	-4.619746	0.574756	-0.106256
H	-4.517682	-1.913774	0.096878
H	-2.576705	1.905455	-0.215698
H	-2.322051	-3.053053	0.193876
H	0.117288	-2.950821	0.191193
H	2.542195	2.048826	-0.261554
H	4.637881	0.839370	-0.092326
H	4.673653	-1.649749	0.145010
H	2.541969	-2.905648	0.227004
H	-0.850476	2.693909	-1.168343
H	0.861531	2.839812	-0.833595
H	0.105624	2.877742	1.481471

**Table S2.** Cartesian Coordinates of *N*-ethyl maleimide, according to B3LYP/6-31+G(*d*) calculations.

C	1.951567	0.672183	0.251652
C	1.954134	-0.665461	0.251876
C	0.561476	1.147663	-0.068072
N	-0.214564	-0.000878	-0.248314
C	0.565868	-1.146388	-0.067603
C	-1.641482	-0.003658	-0.568384
C	-2.530796	-0.001987	0.677295
O	0.167312	2.294731	-0.162688
O	0.176113	-2.295002	-0.161688
H	2.763259	1.364624	0.437020
H	2.768473	-1.354725	0.437478
H	-1.827518	-0.893379	-1.176545
H	-1.830332	0.882470	-1.180932
H	-3.585892	-0.004122	0.379555
H	-2.350254	0.890370	1.285961
H	-2.347790	-0.891030	1.290078

**Table S3.** Cartesian Coordinates of the transition state presenting a hydrogen bond, according to B3LYP/6-31+G(*d*) calculations.

C	-4.439177	-1.578344	-0.180623
C	-4.588160	-0.310880	-0.779767
C	-3.239489	-1.919245	0.421902
C	-2.174138	-0.995111	0.466375
C	-2.309835	0.281882	-0.147118
C	-3.540720	0.596307	-0.778595
C	-0.883906	-1.318952	1.020435
C	-0.118030	-0.241946	1.585870
C	-0.248061	1.046113	0.982770
C	-1.162955	1.171237	-0.128916
C	0.790224	-0.437339	2.651492
C	1.515682	0.627865	3.153148
C	1.379481	1.908485	2.574134
C	0.535560	2.115284	1.497477
C	-1.262871	2.451659	-0.957830
O	-0.068975	3.176718	-1.153965
H	-5.266035	-2.283447	-0.188644
H	-5.532876	-0.040605	-1.244111
H	-3.113088	-2.895949	0.883929
H	-3.686640	1.565540	-1.243561
H	-0.751506	-2.307994	1.455106
H	0.893190	-1.430207	3.082026
H	2.189354	0.480526	3.993307
H	1.948072	2.743619	2.975239
H	0.462549	3.093551	1.039505
H	-1.953916	3.143964	-0.455212
H	-1.718702	2.199818	-1.926163
H	0.589627	2.610135	-1.608857
C	0.095230	-1.590599	-0.846813
C	0.066996	-0.373563	-1.550849
C	1.512151	-1.812408	-0.404705
N	2.227898	-0.667620	-0.773456
C	1.424423	0.206705	-1.507923
O	1.982367	-2.773101	0.179337
O	1.827465	1.260755	-1.998242
C	3.627872	-0.421919	-0.434693
C	4.595682	-0.972474	-1.485468
H	-0.503964	-2.457227	-1.097590
H	-0.616666	-0.108800	-2.345568
H	3.804988	-0.889029	0.538146
H	3.743111	0.660264	-0.329692
H	4.424103	-0.500938	-2.458847
H	4.481767	-2.056428	-1.591423
H	5.628743	-0.764966	-1.182266

**Table S4.** Cartesian Coordinates of the transition state lacking a hydrogen bond, according to B3LYP/6-31+G(*d*) calculations.

C	-4.258991	-1.887291	0.137790
C	-4.475162	-0.768594	-0.693018
C	-3.046154	-2.038908	0.789252
C	-2.035717	-1.062078	0.655813
C	-2.243941	0.069029	-0.182682
C	-3.481713	0.182259	-0.864458
C	-0.727253	-1.206118	1.240795
C	-0.007931	-0.011611	1.587226
C	-0.214471	1.129225	0.760182
C	-1.137200	0.993372	-0.345096
C	0.943947	0.034838	2.632057
C	1.643661	1.201315	2.882353
C	1.436202	2.338814	2.071160
C	0.538860	2.303016	1.018401
C	-1.248311	2.119714	-1.354786
O	-1.871550	3.296437	-0.817311
H	-5.043050	-2.629067	0.263640
H	-5.426653	-0.651426	-1.204959
H	-2.866051	-2.904906	1.422465
H	-3.670006	1.025652	-1.522774
H	-0.528226	-2.100853	1.827758
H	1.108633	-0.852104	3.238398
H	2.354564	1.244066	3.703370
H	1.984831	3.254137	2.277690
H	0.378719	3.187901	0.412963
H	-1.782451	1.777146	-2.249755
H	-0.255510	2.435860	-1.678159
H	-2.735899	3.058851	-0.445370
C	0.268443	-1.711307	-0.603400
C	0.125976	-0.634887	-1.499266
C	1.700359	-1.732414	-0.158158
N	2.311843	-0.613340	-0.725918
C	1.438998	0.051043	-1.602288
O	2.252233	-2.541786	0.569369
O	1.750211	1.008284	-2.295319
C	3.696318	-0.215809	-0.484942
C	4.685578	-0.916564	-1.420404
H	-0.260996	-2.652390	-0.684969
H	-0.576392	-0.581895	-2.319989
H	3.919740	-0.448973	0.560100
H	3.740081	0.868479	-0.618543
H	4.469167	-0.676648	-2.466848
H	4.644265	-2.002864	-1.289346
H	5.706201	-0.583330	-1.197333

**Table S5.** Energy values (Hartrees) of the stationary points studied in this work, according to B3LYP/6-31+G(*d*) calculations.

<i>Structure</i>	<i>9-hydroxymethylanthracene</i>	<i>N-ethylmaleimide</i>	<i>TS having HB</i>	<i>TS lacking HB</i>
E(gas-phase)	-654.070919	-438.079648	-1092.122973	-1092.118038
G(gas-phase)	-653.882126	-437.988137	-1091.816337	-1091.813180
E(SCRF)	-654.089997	-438.093403	-1092.146087	-1092.147597
E(SCRF)+ non electrostatic terms	-654.076719	-438.080329	-1092.121424	-1092.123652

**Table S6.** Solvation terms (kcal mol<sup>-1</sup>) of the stationary points studied in this work, according to B3LYP/6-31+G(*d*) calculations.

<i>Structure</i>	<i>9-hydroxymethylanthracene</i>	<i>N-ethylmaleimide</i>	<i>TS having HB</i>	<i>TS lacking HB</i>
Electrostatics	-11.97	-8.63	-14.50	-18.55
Cavitation	28.44	20.32	41.13	40.69
Dispersion	-21.85	-12.96	-27.52	-27.62
Repulsion	1.73	0.84	1.86	1.95