Synergistic activation of the Diels-Alder reaction by an organic catalyst and substituents: a computational study

Supplementary material

Mats Linder[a] and Tore Brinck*[a]
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[a] *Physical Chemistry, Royal Institute of Technology (KTH), Stockholm, Sweden. Tel: +46 8 790 82 10; E-mail: tore@physchem.kth.se*

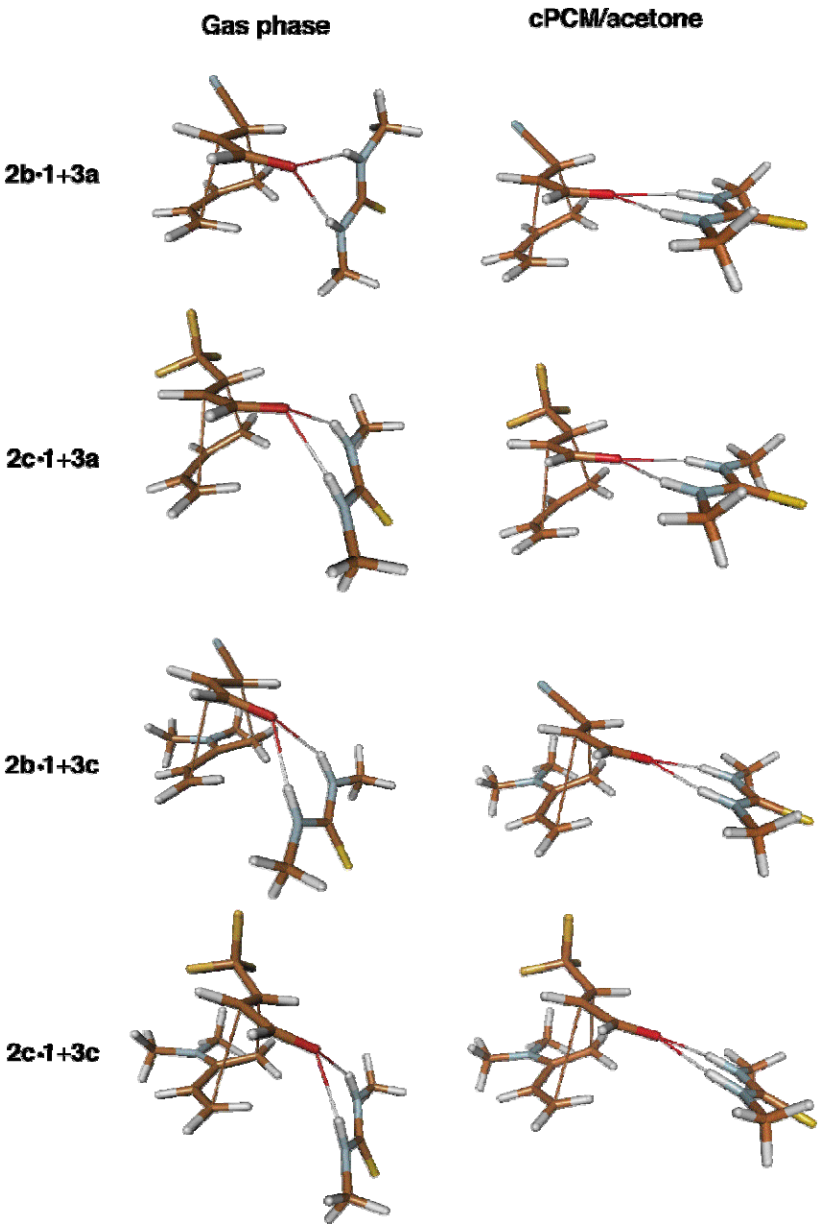

Fig. S1 Optimized TS geometries of four additional species, in gas phase and acetone, respectively. The loss of long-range interactions with the catalyst due to solvation is illustrated.

.xyz-files

3a+2b•1 gas phase

	C	0.959858	0.393574	-0.551592
	H	0.937909	0.875598	0.422123
5	H	1.923668	-0.036424	-0.810237
	C	0.097897	0.853183	-1.547716
	H	-0.670526	1.574059	-1.278369
	C	0.006033	0.231567	-2.806069
	H	-0.836619	0.492357	-3.443236
10	C	0.810159	-0.826647	-3.169586
	H	0.627444	-1.367006	-4.094094
	H	1.787353	-0.969962	-2.725359
	H	-0.804653	-2.488172	-1.749015
	C	0.149537	-2.323647	-1.261843
15	C	1.239366	-3.199372	-1.638942
	C	0.211607	-1.519364	-0.103770
	O	2.364483	-3.216372	-1.130267
	H	1.052476	-1.684755	0.566483
	H	1.011424	-3.896711	-2.468732
20	C	4.423643	-0.898546	0.599452
	N	4.390419	-0.982867	-0.768607
	H	3.996443	-1.833677	-1.157176
	N	3.646376	-1.825572	1.228177
	S	5.308500	0.272129	1.425101
25	C	5.294769	-0.228036	-1.623168
	H	6.345988	-0.481763	-1.438409
	H	5.044053	-0.456726	-2.663262
	H	5.174591	0.843414	-1.449368
	H	3.226519	-2.547094	0.649510
30	C	3.640664	-2.015648	2.669695
	H	3.329906	-1.100211	3.180186
	H	2.933791	-2.817678	2.900297
	H	4.633746	-2.287052	3.046568
	C	-1.022528	-1.176940	0.551463
35	N	-2.022191	-0.900590	1.078070

3a+2b•1 cPCM/acetone

	C	-0.690438	0.144480	-0.009891
	H	-1.088024	0.139694	1.002542
40	H	0.384472	0.291915	-0.070158
	C	-1.513814	0.569746	-1.055193
	H	-2.570864	0.730329	-0.851953
	C	-1.097941	0.541316	-2.401068
	H	-1.860172	0.648944	-3.171068
45	C	0.182822	0.197730	-2.778817
	H	0.427270	0.047959	-3.826965
	H	1.025624	0.322766	-2.109154
	H	-0.457594	-2.446076	-2.493262
	C	0.149972	-2.099081	-1.664584
50	C	1.584810	-2.133090	-1.832065
	C	-0.422213	-1.901091	-0.389618
	O	2.407495	-1.819547	-0.957499
	H	0.246223	-1.983359	0.465685
	H	1.943748	-2.454790	-2.825888
55	C	5.610720	-1.324641	0.491981
	N	5.401470	-1.705766	-0.791277
	H	4.435292	-1.823121	-1.093606
	N	4.482414	-1.157931	1.229432
	S	7.167859	-1.073389	1.136008
60	C	6.456285	-1.944765	-1.761683
	H	7.131754	-2.739685	-1.427128
	H	5.984068	-2.247223	-2.700235
	H	7.052584	-1.041825	-1.934339
	H	3.592359	-1.329744	0.772489
65	C	4.462418	-0.754306	2.625627
	H	4.915953	0.233670	2.761337
	H	3.418579	-0.716943	2.948422
	H	5.006288	-1.468363	3.253402
	C	-1.744259	-2.416234	-0.150978
70	N	-2.813056	-2.832525	0.047812

3a+2c•1 gas phase

	C	0.372549	-0.049480	0.162473
	H	0.045170	0.086343	1.188458
75	H	1.413591	-0.343140	0.060572
	C	-0.241430	0.701986	-0.834416
	H	-1.145485	1.253070	-0.586660
	C	0.103201	0.588018	-2.201879
	H	-0.569784	1.039452	-2.928275
80	C	1.133954	-0.189819	-2.656178
	H	1.281139	-0.342851	-3.721638
	H	1.948130	-0.506099	-2.014913
	H	-0.621360	-2.406442	-2.285102
	C	0.112001	-2.417398	-1.486937
85	C	1.392599	-3.016600	-1.766740
	C	-0.242403	-2.004419	-0.199981
	O	2.335598	-3.101009	-0.968671
	H	0.371282	-2.373782	0.617803
	H	1.514017	-3.418492	-2.790974
90	C	4.751057	-0.861822	0.237083
	N	4.750786	-1.343009	-1.039717
	H	4.160198	-2.146961	-1.231320
	N	3.756845	-1.370474	1.022431
	S	5.858968	0.284169	0.789049
95	C	5.787393	-1.026142	-2.006602
	H	6.774731	-1.374136	-1.679093
	H	5.526916	-1.513481	-2.950868
	H	5.850197	0.054072	-2.161401
	H	3.195692	-2.122551	0.633666
100	C	3.670348	-1.124231	2.451376
	H	3.570528	-0.054674	2.655646
	H	2.789153	-1.650317	2.831216
	H	4.560788	-1.482602	2.981595
	C	-1.710863	-1.959593	0.141258
105	F	-2.433540	-1.338246	-0.817449
	F	-2.205851	-3.211567	0.267242
	F	-1.955282	-1.326791	1.309881

3a+2c•1 cPCM/acetone

110	C	0.001605	0.017538	-0.014449
	H	0.015912	0.024544	1.072001
	H	0.985281	0.026080	-0.476449
	C	-1.074108	0.614979	-0.670649
	H	-1.952953	0.883818	-0.087718
115	C	-1.179540	0.671318	-2.082678
	H	-2.147438	0.938723	-2.503717
	C	-0.182615	0.264686	-2.930068
	H	-0.354581	0.202759	-4.001188
	H	0.846410	0.166811	-2.605187

H	-0.977647	-2.437199	-2.380944
C	-0.085626	-2.244195	-1.794359
C	1.183134	-2.377041	-2.459970
C	-0.168890	-2.003062	-0.416976
O	2.291256	-2.167123	-1.933484
H	0.719841	-2.210323	0.175922
H	1.139751	-2.679703	-3.521359
C	5.786420	-1.814690	-1.645574
N	5.145473	-2.102029	-2.804180
H	4.130955	-2.197429	-2.766446
N	4.979441	-1.703643	-0.559155
S	7.475930	-1.609674	-1.553693
C	5.802548	-2.266384	-4.089451
H	6.531535	-3.083731	-4.062292
H	5.032738	-2.497308	-4.830694
H	6.327684	-1.352583	-4.389453
H	3.981703	-1.830907	-0.700128
C	5.442358	-1.392720	0.782915
H	5.914341	-0.404597	0.825751
H	4.574050	-1.403658	1.447241
H	6.169866	-2.132976	1.132265
C	-1.431765	-2.426996	0.290582
F	-2.556955	-2.068402	-0.375004
F	-1.475926	-3.782901	0.426588
F	-1.533025	-1.922232	1.546023

3c+2b•1 gas phase

C	0.150127	-0.322282	0.450010
H	-0.127577	-0.391653	1.495287
H	1.214142	-0.421301	0.271365
C	-0.594176	0.513215	-0.406141
C	-0.152283	0.701654	-1.781746
H	-0.764688	1.327973	-2.422059
C	0.943062	0.132237	-2.323759
H	1.187689	0.315679	-3.365875
H	1.659075	-0.452945	-1.761560
H	-0.702979	-2.664559	-2.232427
C	0.028139	-2.684592	-1.431804
C	1.356637	-3.096697	-1.734815
C	-0.337843	-2.318816	-0.126727
O	2.321888	-3.082918	-0.943392
H	0.313303	-2.666533	0.671890
C	4.659478	-0.774353	0.170773
N	4.640952	-1.266056	-1.098314
H	4.034437	-2.062748	-1.279306
N	3.693757	-1.298133	0.981893
S	5.756915	0.399766	0.691234
C	5.626361	-0.915718	-2.104029
H	6.637467	-1.225372	-1.812513
H	5.349765	-1.418495	-3.035597
H	5.645295	0.165621	-2.267155
H	3.139578	-2.063162	0.605486
C	3.640773	-1.053533	2.411714
H	3.528055	0.014207	2.619944
H	2.778650	-1.594836	2.813806
H	4.549996	-1.396796	2.920222
H	1.522998	-3.446868	-2.771718
N	-1.777778	1.060557	-0.019148
C	-2.754011	1.583251	-0.976062
C	-2.161871	1.117404	1.392666
H	-2.815598	0.946229	-1.861034
H	-3.737863	1.582172	-0.503941
H	-2.519526	2.610417	-1.286719
H	-2.631711	0.184167	1.721576
H	-1.285399	1.322623	2.012816
H	-2.869901	1.937880	1.529856
C	-1.737139	-2.281891	0.205278
N	-2.869832	-2.214587	0.464098

3c+2b•1 cPCM/acetone

C	-0.018581	0.032397	-0.069505
H	0.059877	0.080548	1.009703
H	0.928591	0.000575	-0.591259
C	-1.128922	0.581503	-0.731301
C	-1.155448	0.614062	-2.196227
H	-2.068907	0.953790	-2.672103
C	-0.147283	0.230907	-3.004341
H	-0.272126	0.272256	-4.082773
H	0.826989	-0.080009	-2.646165
H	-0.942921	-2.840006	-2.239609
C	-0.070702	-2.631433	-1.627871
C	1.217225	-2.790634	-2.220982
C	-0.214733	-2.200452	-0.307926
O	2.307276	-2.503860	-1.676453
H	0.649671	-2.253526	0.348225
C	5.725861	-2.140714	-1.125016
N	5.188684	-2.536339	-2.303667
H	4.171280	-2.609337	-2.350796
N	4.822749	-1.899586	-0.140541
S	7.405385	-1.958453	-0.890155
C	5.957129	-2.844331	-3.496953
H	6.663252	-3.662400	-3.316307
H	5.253641	-3.144470	-4.278315
H	6.527246	-1.974344	-3.842344
H	3.839935	-2.032163	-0.364329
C	5.164768	-1.474208	1.205835
H	5.687853	-0.511434	1.200570
H	4.234380	-1.372738	1.771049
H	5.807984	-2.207483	1.704701
H	1.228287	-3.195552	-3.248921
N	-2.226235	1.006206	-0.050832
C	-3.466449	1.400929	-0.729982
C	-2.171152	1.142920	1.407691
H	-3.819706	0.612613	-1.401609
H	-4.237035	1.564959	0.023003
H	-3.339199	2.329920	-1.300444
H	-2.140727	0.165572	1.901448
H	-1.287377	1.719961	1.704328
H	-3.058705	1.676032	1.748515
C	-1.482695	-2.362403	0.342563
N	-2.514697	-2.499960	0.865178

3c+2c•1 gas phase

C	0.145269	-0.235037	0.453136
H	-0.120394	-0.286724	1.500692
H	1.194791	-0.395650	0.243265

C	-0.603206	0.550264	-0.426861
C	-0.193790	0.668273	-1.824556
H	-0.848868	1.226176	-2.485752
C	0.913254	0.122605	-2.362806
H	1.125827	0.260098	-3.419026
H	1.669305	-0.396489	-1.787137
H	-0.738847	-2.680725	-2.175252
C	0.020219	-2.695658	-1.399728
C	1.355165	-3.045624	-1.781447
C	-0.308638	-2.381792	-0.093656
O	2.353371	-3.020304	-1.039644
H	0.389019	-2.656591	0.690952
C	4.710952	-0.787717	0.202278
N	4.690206	-1.204269	-1.093953
H	4.075657	-1.981083	-1.323766
N	3.738304	-1.344909	0.980050
S	5.823249	0.339436	0.791879
C	5.684461	-0.810598	-2.074576
H	6.688657	-1.160067	-1.804440
H	5.398502	-1.245430	-3.037057
H	5.725866	0.278295	-2.166289
H	3.168170	-2.073942	0.559691
C	3.670912	-1.164862	2.418400
H	3.565767	-0.106652	2.674040
H	2.799421	-1.715437	2.786206
H	4.571429	-1.539745	2.919856
H	1.482540	-3.358451	-2.835843
N	-1.762692	1.169887	-0.047701
C	-2.775100	1.574880	-1.022274
C	-2.118875	1.289460	1.362639
H	-2.957574	0.782720	-1.755021
H	-3.712678	1.758571	-0.495159
H	-2.499236	2.496502	-1.551293
H	-2.583198	0.376020	1.752140
H	-1.226103	1.509914	1.954378
H	-2.817210	2.121094	1.482725
C	-1.751186	-2.459302	0.320149
F	-2.566326	-1.779291	-0.521714
F	-1.968455	-1.979848	1.569790
F	-2.180845	-3.741857	0.329386

3c+2c•1 cPCM/acetone

C	-1.580820	-1.043419	-0.570185
H	-1.784788	-1.013737	-1.632865
H	-0.537718	-1.141358	-0.300251
C	-2.552266	-1.467413	0.338692
C	-2.225067	-1.578554	1.766118
H	-3.029566	-1.865849	2.435536
C	-1.016425	-1.356863	2.316678
H	-0.878789	-1.468156	3.388482
H	-0.131202	-1.114656	1.740542
H	-1.595135	1.873633	1.815538
C	-0.893943	1.578763	1.040166
C	0.490379	1.495260	1.406974
C	-1.330304	1.285464	-0.233979
O	1.412343	1.088383	0.670410
H	-0.608683	1.209521	-1.041224
C	4.503147	-0.227285	-0.280496
N	4.282599	0.398815	0.900311
H	3.341507	0.754340	1.071345
N	3.422804	-0.293459	-1.099889
S	6.018412	-0.882040	-0.708257
C	5.285243	0.583098	1.935072
H	6.132270	1.174502	1.570011
H	4.812247	1.111248	2.767376
H	5.671722	-0.377978	2.292724
H	2.556744	0.121828	-0.767346
C	3.421354	-0.912140	-2.414473
H	3.663512	-1.979190	-2.354866
H	2.420160	-0.795760	-2.838224
H	4.148788	-0.434909	-3.080467
H	0.735919	1.821637	2.433462
N	-3.832748	-1.748630	-0.042004
C	-4.942970	-1.826266	0.912128
C	-4.171867	-1.945364	-1.450376
H	-4.878733	-1.031418	1.659948
H	-5.878320	-1.689058	0.365872
H	-4.981489	-2.798995	1.421269
H	-4.372175	-0.997068	-1.964626
H	-3.357610	-2.462292	-1.966348
H	-5.065290	-2.571546	-1.512798
C	-2.685700	1.757569	-0.673480
F	-3.663243	1.496888	0.229603
F	-3.079566	1.226658	-1.858833
F	-2.689397	3.112750	-0.859685