Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Insights into the catalytic activity of boron doped thiazoles in Diels-Alder reaction

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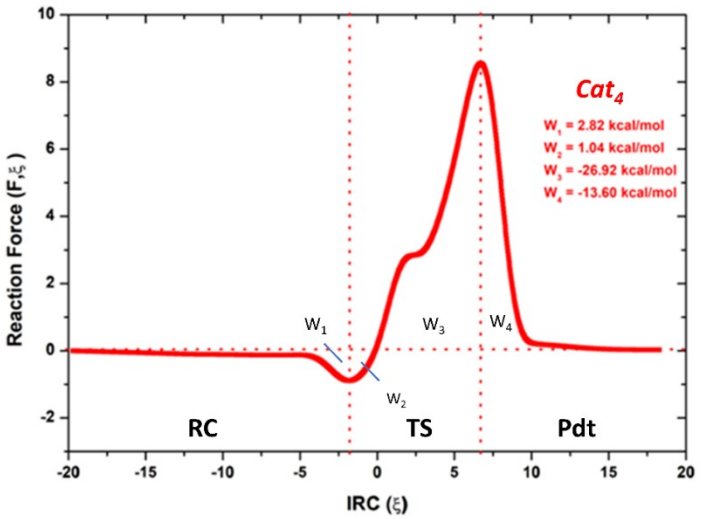

Figure S1: The reaction force profile along with IRC of Reaction 5 in presence Cat_4. (Where red dotted lines separated the reaction profile with three regions i.e., reactant complex (RC), transition state (TS) and product (Pdt).

Table S1: Calculated hardness, electrophilicity for individual reactant and product along with $\Delta\eta$, $\Delta\omega$ of our studied reactions (in eV unit).

Reactions	Hardness (η,eV)		Electrophilicity (ω,eV)		Δη	Δω
	Reactant	Product	Reactant	Product		
Reaction-1 (Without catalyst)	7.264	8.847	1.311	0.850	1.583	-0.461
Reaction-2 (BF_3/Cat_1)	5.919	7.320	2.307	1.710	1.401	-0.309
Reaction-3 (Cat_2)	3.650	4.404	2.039	1.439	0.754	-0.685
Reaction-4 (Cat_3)	3.675	4.501	2.585	1.792	0.826	-0.966
Reaction-5 (Cat_4)	4.007	4.215	3.295	3.126	0.208	-2.918

Calculated Hirschfield charges of *Cat2-Cat4*

Cat2

Atom	**1(B):**	**0.12258249**
Atom	2(N):	-0.23354058
Atom	3(S):	0.00984371
Atom	4(C):	0.03916888
Atom	5(C):	-0.00750246
Atom	6(H):	-0.04649601
Atom	7(H):	0.05448844
Atom	8(H):	0.06145553

Cat3

Atom	**1(B):**	**0.23751472**
Atom	2(N):	-0.24811939
Atom	3(S):	0.01804743
Atom	4(C):	0.16299239
Atom	5(C):	0.10136857
Atom	6(F):	-0.06066222
Atom	7(F):	-0.07664482
Atom	8(F):	-0.13449668

Cat4

Atom	**1(B):**	**0.25585645**
Atom	2(N):	-0.20195685
Atom	3(S):	0.07780713
Atom	4(C):	0.10670277
Atom	5(C):	0.03329478
Atom	6(C):	0.07198360
Atom	7(N):	-0.14484069
Atom	8(C):	0.05968041
Atom	9(N):	-0.13898099
Atom	10(F):	-0.11954662

Cartesian Coordinates of TS (Reaction 1 i.e., Without Catalyst)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.959537	0.446288	0.127071
2	6	0	-0.863690	0.017554	0.995800
3	6	0	-0.336358	-1.251486	0.821385
4	1	0	-0.643400	0.607890	1.874949
5	1	0	0.269632	-1.690308	1.602998
6	1	0	-0.912568	-1.943673	0.217132
7	8	0	-2.259157	-0.120287	-0.902723
8	1	0	-2.502353	1.359005	0.442022
9	6	0	2.058813	-0.367647	-0.177534
10	6	0	1.795919	0.991842	0.079906
11	6	0	0.606582	1.573152	-0.260055
12	6	0	1.094420	-1.207472	-0.696498
13	1	0	2.966981	-0.801662	0.228400
14	1	0	2.493057	1.539713	0.705639
15	1	0	0.375767	2.582834	0.060533
16	1	0	1.326557	-2.258733	-0.825127
17	1	0	0.321176	-0.829828	-1.357668
18	1	0	0.001518	1.183671	-1.067547

Cartesian Coordinates of TS (Reaction 2 i.e., BF_3/*Cat*$_1$Catalyst)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.390921	-1.214539	1.157757
2	6	0	-0.644004	-0.308486	1.463886
3	6	0	-0.735364	1.059272	1.204828
4	1	0	-1.433207	-0.766120	2.048841
5	1	0	-1.394891	1.625926	1.850112
6	1	0	0.131129	1.590682	0.831992
7	8	0	1.458100	-1.094130	0.497753
8	1	0	0.264600	-2.211718	1.589004
9	5	0	1.963952	0.129738	-0.318013
10	9	0	0.920056	0.433137	-1.204254
11	9	0	3.082864	-0.297891	-0.951198
12	9	0	2.173165	1.163393	0.570599
13	6	0	-2.919522	0.623895	-0.408132
14	6	0	-2.851734	-0.787115	-0.549642
15	6	0	-1.691414	-1.445524	-0.805318
16	6	0	-1.820445	1.451323	-0.499570
17	1	0	-3.863244	1.045503	-0.073196
18	1	0	-3.747702	-1.358215	-0.329919
19	1	0	-1.667469	-2.529527	-0.812094
20	1	0	-1.969426	2.518090	-0.376552
21	1	0	-0.963010	1.164681	-1.095480

22	1	0	-0.796737	-0.935661	-1.143842

Cartesian Coordinates of TS (Reaction 3 i.e., *Cat$_2$* Catalyst)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.551645	-1.297390	1.292546
2	6	0	-1.558441	-0.333960	1.485162
3	6	0	-1.498249	1.037679	1.212962
4	1	0	-2.425108	-0.727677	2.002671
5	1	0	-2.232982	1.656641	1.714711
6	1	0	-0.512923	1.473457	1.024911
7	8	0	0.542691	-1.272343	0.663328
8	1	0	-0.734504	-2.260211	1.779414
9	6	0	-3.243352	0.961228	-0.785177
10	6	0	-3.526690	-0.429765	-0.858679
11	6	0	-2.559889	-1.378900	-0.899056
12	6	0	-1.968843	1.481530	-0.687637
13	1	0	-4.084964	1.632226	-0.637395
14	1	0	-4.562813	-0.735981	-0.760489
15	1	0	-2.816128	-2.430834	-0.846124
16	1	0	-1.848304	2.558121	-0.652185
17	1	0	-1.110645	0.948480	-1.076617
18	1	0	-1.525613	-1.142076	-1.118350
19	5	0	1.152551	-0.264370	-0.345870
20	7	0	1.267993	1.126464	0.181229
21	16	0	3.011301	-0.875512	-0.642392
22	6	0	2.499490	1.544501	0.227181
23	6	0	3.548340	0.675446	-0.161226
24	1	0	2.732116	2.553873	0.569696
25	1	0	4.597873	0.934583	-0.157479
26	1	0	0.518621	-0.399272	-1.366825

Cartesian Coordinates of TS (Reaction 4 i.e., *Cat$_3$* Catalyst)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.169246	-0.935214	1.667553
2	6	0	-2.047272	0.150557	1.592433
3	6	0	-1.854095	1.385690	0.971200
4	1	0	-2.948673	0.001412	2.174702
5	1	0	-2.496972	2.195254	1.294527
6	1	0	-0.856593	1.654653	0.627614
7	8	0	-0.062892	-1.196080	1.094688
8	1	0	-1.461370	-1.718832	2.370660
9	6	0	-3.776842	1.011202	-0.864298
10	6	0	-4.201980	-0.333717	-0.616799
11	6	0	-3.354827	-1.382030	-0.543161
12	6	0	-2.471395	1.399986	-1.022306
13	1	0	-4.539547	1.783626	-0.807238
14	1	0	-5.254273	-0.487002	-0.401501

15	1	0	-3.725317	-2.366565	-0.281347
16	1	0	-2.259799	2.441589	-1.234595
17	1	0	-1.698864	0.694757	-1.305689
18	1	0	-2.309604	-1.307403	-0.820876
19	5	0	0.606424	-0.536505	-0.100401
20	7	0	0.970978	0.887961	0.117118
21	16	0	2.309803	-1.555817	-0.354246
22	6	0	2.231145	1.053617	0.050027
23	6	0	3.092272	-0.049305	-0.185857
24	9	0	2.800757	2.251962	0.196151
25	9	0	4.407071	0.093798	-0.276171
26	9	0	-0.254299	-0.764394	-1.177359

Cartesian Coordinates of TS (Reaction 5 i.e., *Cat*$_4$ Catalyst)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.531937	-0.714078	1.723367
2	6	0	-2.323023	0.419762	1.520769
3	6	0	-2.074325	1.525039	0.710618
4	1	0	-3.207662	0.430010	2.146257
5	1	0	-2.633245	2.425977	0.930423
6	1	0	-1.091453	1.658549	0.267002
7	8	0	-0.462417	-1.132082	1.167507
8	1	0	-1.859338	-1.375546	2.527788
9	6	0	-4.183285	0.977978	-0.924700
10	6	0	-4.612702	-0.309630	-0.463922
11	6	0	-3.782809	-1.361644	-0.304307
12	6	0	-2.891040	1.301191	-1.240357
13	1	0	-4.925646	1.771771	-0.920331
14	1	0	-5.650070	-0.403958	-0.160807
15	1	0	-4.152231	-2.293572	0.108270
16	1	0	-2.673962	2.298516	-1.604557
17	1	0	-2.157948	0.538950	-1.472956
18	1	0	-2.756639	-1.351093	-0.653328
19	5	0	0.246130	-0.640798	-0.069279
20	7	0	0.797100	0.740377	0.068594
21	16	0	1.837544	-1.826568	-0.269585
22	6	0	2.077721	0.779537	0.010999
23	6	0	2.829702	-0.446155	-0.162653
24	6	0	2.789372	2.040816	0.116172
25	7	0	3.344968	3.042469	0.199876
26	6	0	4.236229	-0.493604	-0.235656
27	7	0	5.388653	-0.531120	-0.293737
28	9	0	-0.638032	-0.810137	-1.130353