Supporting Information

Experimental and theoretical insights into binary Zn-SBA-15/KI catalysts for the selective coupling of CO_2 and epoxides into cyclic carbonates under mild conditions

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The Cartesian coordinates of optimized geometries of stable points calculated at B3LYP/6-31G(d) level of theory

Fig. 5	**A**		
Si	-0.19214	4.14271	-2.06384
H	-0.10027	5.42783	-2.78968
H	-1.46736	3.44235	-2.34267
O	1.06031	3.18053	-2.51655
O	-0.09838	4.47775	-0.45349

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Si	2.13498	2.22705	-3.30491
H	2.06193	2.51036	-4.7557
H	3.48595	2.48875	-2.76101
Si	-0.0662	4.10859	1.14382
H	-0.45496	5.26232	1.95922
O	-1.10978	2.85579	1.46308
H	-1.07326	2.16141	0.76247
O	1.7605	0.63257	-3.0941
O	1.47188	3.66589	1.56533
Si	2.61144	2.58586	1.06069
H	3.3119	2.06876	2.25707
H	3.54285	3.21568	0.10352
Si	1.90415	-0.88555	-2.51599
H	1.12775	-1.79996	-3.3611
O	3.47444	-1.36127	-2.47282
O	1.31229	-0.9703	-0.9659
O	1.88538	1.32164	0.26597
Si	0.85321	0.06365	0.21266
O	-0.66485	0.66023	-0.06281
H	-1.42023	0.02961	0.06452
O	0.81887	-0.72619	1.65927
Si	4.63072	-1.85551	-1.39333
H	5.04685	-0.70012	-0.56232
H	5.75754	-2.40077	-2.17675
Si	1.81293	-1.75538	2.52556
H	3.01871	-0.99749	2.93323
H	1.01146	-2.19382	3.68593
O	2.24995	-3.05757	1.641
Si	2.94383	-3.92253	0.41831

H	3.63884	-5.0767	1.02471
H	1.87342	-4.34735	-0.51211
O	4.05947	-3.02929	-0.39352
C	-4.08391	-0.93247	0.81441
H	-4.48564	-0.4471	-0.07311
H	-4.60064	-0.74838	1.75588
C	-3.25841	-2.13958	0.67785
H	-3.05806	-2.48539	-0.33702
C	-3.14299	-3.1694	1.76765
H	-3.37179	-2.73315	2.74564
H	-3.85091	-3.98443	1.57518
H	-2.13447	-3.59933	1.78811
O	-2.63102	-0.84396	0.93656
K	-1.64028	0.66482	3.15256
I	-4.15309	-0.44722	4.8882

Fig. 5	**TS_{A-1}**		
Si	-0.58253	3.83152	-1.7626
H	-0.66419	5.08373	-2.54397
H	-1.8486	3.06787	-1.78871
O	0.63675	2.89878	-2.35528
O	-0.23829	4.25413	-0.20148
Si	1.54463	1.99088	-3.37747
H	1.04166	2.14929	-4.75979
H	2.95606	2.41771	-3.24984
Si	0.07041	3.94745	1.37423
H	-0.25727	5.09574	2.22454
O	-0.83063	2.6379	1.88183
H	-0.86705	1.95958	1.16149

O	1.43252	0.39188	-2.98633
O	1.67658	3.59915	1.56566
Si	2.79845	2.61672	0.85488
H	3.77671	2.23413	1.89745
H	3.44504	3.29026	-0.28867
Si	1.77178	-1.08527	-2.3918
H	0.94648	-2.09348	-3.06415
O	3.36112	-1.45432	-2.57448
O	1.44183	-1.12818	-0.76083
O	2.06886	1.24753	0.27104
Si	1.08139	-0.04074	0.39969
O	-0.48041	0.47126	0.32781
H	-1.21049	-0.18589	0.59013
O	1.27867	-0.7448	1.89374
Si	4.72071	-1.78606	-1.69103
H	5.25192	-0.53009	-1.11096
H	5.69432	-2.42365	-2.6008
Si	2.49327	-1.6332	2.62628
H	3.6874	-0.76911	2.7697
H	1.93157	-2.00824	3.94545
O	2.86485	-2.98664	1.79573
Si	3.48965	-3.80763	0.49867
H	4.37052	-4.86464	1.0371
H	2.35993	-4.3649	-0.27662
O	4.39204	-2.811	-0.44424
C	-3.80451	-0.43927	1.123
H	-3.76921	0.29035	0.32715
H	-4.35267	-0.19032	2.02114
C	-3.30702	-1.78643	0.92548

H	-3.06652	-2.0617	-0.10244
C	-3.77835	-2.93135	1.78048
H	-3.9798	-2.59728	2.8043
H	-4.7122	-3.32062	1.36254
H	-3.03341	-3.73504	1.80587
O	-2.28881	-0.91948	1.51661
K	-1.0177	0.35631	3.38019
I	-6.69255	-0.54893	0.10899

Fig. 5 **Int_{A-1}**

Si	-0.60219	-3.59026	-2.04032
H	-0.62324	-4.80641	-2.88438
H	0.78367	-3.18435	-1.70967
O	-1.34269	-2.37685	-2.85735
O	-1.42443	-3.95291	-0.65718
Si	-1.87242	-1.14708	-3.80053
H	-1.54908	-1.46086	-5.21169
H	-3.33088	-0.9902	-3.60654
Si	-1.78865	-3.59346	0.90705
H	-1.98732	-4.83046	1.67561
O	-0.58333	-2.71237	1.61133
H	-0.31965	-1.92678	1.01446
O	-1.10464	0.26282	-3.42972
O	-3.20718	-2.7379	0.94042
Si	-3.89322	-1.4919	0.09099
H	-4.84991	-0.83205	1.01331
H	-4.5813	-2.00163	-1.11497
Si	-0.81568	1.68164	-2.67357
H	0.59536	2.0375	-2.87734

O	-1.76282	2.88048	-3.29201
O	-1.1664	1.59361	-1.06396
O	-2.75147	-0.41139	-0.4051
Si	-1.401	0.42071	0.07526
O	-0.13952	-0.49545	0.39467
H	1.27066	0.0382	1.12631
O	-1.83092	1.23812	1.49158
Si	-2.97141	3.86341	-2.73233
H	-4.16519	3.05159	-2.39328
H	-3.26962	4.84032	-3.80109
Si	-2.83176	2.53217	1.78074
H	-4.15757	2.29343	1.16413
H	-2.9313	2.63018	3.25798
O	-2.2158	3.95003	1.22892
Si	-1.66205	4.9106	0.00328
H	-1.85948	6.31086	0.43723
H	-0.22985	4.61357	-0.22871
O	-2.51158	4.69832	-1.38769
C	3.57376	-1.07771	0.78785
H	2.8367	-1.35691	0.03444
H	3.63693	-1.85747	1.54854
C	3.24033	0.28688	1.40331
H	3.30514	1.05631	0.62083
C	4.13202	0.67578	2.57445
H	4.08102	-0.08769	3.36079
H	5.17423	0.78107	2.26137
H	3.79541	1.62904	2.99437
O	1.89996	0.20612	1.88743
K	-0.27949	-0.46981	3.17737

I	5.48794	-1.12245	-0.26993

Fig. 5	**Int_{A-2}**		
Si	2.42348	-2.61528	2.96829
H	3.11086	-3.27128	4.10391
H	0.96053	-2.84334	3.0162
O	2.72343	-1.00489	3.0404
O	3.04607	-3.26902	1.58865
Si	2.85922	0.6107	3.27098
H	2.8906	0.87689	4.72798
H	4.09624	1.08712	2.61298
Si	2.94541	-3.52689	-0.03376
H	3.47298	-4.85794	-0.3656
O	1.38487	-3.4254	-0.5598
H	0.9401	-2.57041	-0.22866
O	1.55549	1.4097	2.65758
O	3.88168	-2.39897	-0.80733
Si	4.16033	-0.77064	-0.69251
H	4.61611	-0.32608	-2.03228
H	5.18179	-0.4874	0.339
Si	0.66302	2.27214	1.59562
H	-0.71162	2.35828	2.10528
O	1.26695	3.79568	1.42139
O	0.67598	1.58207	0.09634
O	2.7865	0.03554	-0.26532
Si	1.16302	0.15173	-0.57359
O	0.3121	-1.12539	-0.1495
H	-1.29307	-1.27261	-0.51492
O	1.01215	0.35425	-2.24473

Si	1.92352	4.70848	0.20738
H	3.23838	4.14888	-0.18923
H	2.0585	6.08809	0.72106
Si	1.39322	1.59859	-3.27635
H	2.80814	1.99622	-3.08886
H	1.15675	1.06534	-4.64062
O	0.42304	2.90769	-3.07831
Si	-0.16905	4.15157	-2.16521
H	-0.531	5.2366	-3.10319
H	-1.3513	3.67048	-1.41427
O	0.95421	4.7477	-1.12455
C	-3.59294	-0.83894	0.71614
H	-2.74869	-0.82725	1.40577
H	-4.10119	-1.80221	0.76969
C	-3.1359	-0.52311	-0.71344
H	-2.70589	0.48844	-0.73683
C	-4.24083	-0.63287	-1.75616
H	-4.68752	-1.63416	-1.73618
H	-5.03108	0.09999	-1.57348
H	-3.82893	-0.45468	-2.7554
O	-2.12349	-1.47895	-1.04278
K	-0.05157	-2.27525	-2.64952
I	-4.99167	0.62803	1.53799
C	-2.83494	-4.25601	-1.4702
O	-2.00751	-4.26196	-2.30348
O	-3.67211	-4.29869	-0.66171

Fig. 5	**TS_{A-2}**		
Si	-1.83752	2.3534	-2.3625

H	-2.59093	2.88652	-3.51848
H	-2.74248	1.85938	-1.29912
O	-0.86874	1.12642	-2.86861
O	-0.91918	3.58919	-1.76921
Si	-0.32239	-0.2934	-3.48207
H	-1.36624	-0.88387	-4.34918
H	0.926	-0.02712	-4.23191
Si	0.0951	4.16451	-0.61046
H	-0.03761	5.62136	-0.49201
O	-0.24812	3.48197	0.85915
H	-0.34181	2.48821	0.78434
O	-0.0164	-1.37315	-2.26945
O	1.65516	3.81964	-1.04029
Si	2.54601	2.53002	-1.56493
H	3.94545	2.76953	-1.14385
H	2.43907	2.38234	-3.0317
Si	1.00034	-2.20324	-1.29363
H	0.32596	-3.42121	-0.82928
O	2.37708	-2.60641	-2.09698
O	1.40891	-1.29209	0.02555
O	2.00007	1.12543	-0.88646
Si	1.41512	0.30534	0.41186
O	-0.02211	0.86334	0.89644
H	-0.81439	0.17101	1.50999
O	2.48474	0.53252	1.67768
Si	4.02078	-2.44057	-2.02635
H	4.3952	-1.0522	-2.38591
H	4.60483	-3.41972	-2.96639
Si	4.08873	0.19245	1.96049

H	4.92377	0.95266	1.00126
H	4.33915	0.63024	3.35438
O	4.4279	-1.40209	1.84
Si	4.52267	-2.88497	1.12018
H	5.77632	-3.51858	1.58127
H	3.33238	-3.67353	1.50889
O	4.59708	-2.7558	-0.5169
C	-3.77213	-0.54581	1.1086
H	-3.56946	0.47142	0.7728
H	-4.39257	-0.53449	2.00144
C	-2.46511	-1.31742	1.31999
H	-1.94913	-1.39986	0.35634
C	-2.61871	-2.70309	1.93833
H	-3.11328	-2.63736	2.90985
H	-3.20408	-3.35298	1.28098
H	-1.62939	-3.151	2.07588
O	-1.57849	-0.50434	2.12626
K	0.75736	2.3288	3.18763
I	-5.01113	-1.40278	-0.47652
C	-1.98083	0.04446	3.62704
O	-1.08862	0.81468	3.96153
O	-3.01422	-0.4267	4.02386

Fig. 5	**Int_{A-3}**		
Si	-0.76996	-3.80387	-1.99609
H	-0.82369	-4.93947	-2.94218
H	0.58749	-3.6115	-1.43807
O	-1.23695	-2.43836	-2.77805
O	-1.81854	-4.14582	-0.76848

Si	-1.38825	-1.0928	-3.70194
H	-0.75067	-1.33353	-5.01546
H	-2.8279	-0.78022	-3.84232
Si	-2.5285	-3.89744	0.68674
H	-3.02106	-5.1564	1.2562
O	-1.4477	-3.22664	1.75465
H	-0.86141	-2.56138	1.31443
O	-0.61878	0.18777	-3.00517
O	-3.82261	-2.88195	0.4971
Si	-4.11052	-1.43318	-0.24414
H	-5.10185	-0.70311	0.57966
H	-4.59032	-1.63685	-1.62586
Si	-0.315	1.53121	-2.13453
H	1.12791	1.79165	-2.13785
O	-1.11672	2.83097	-2.73631
O	-0.83604	1.33362	-0.57015
O	-2.71159	-0.55272	-0.33514
Si	-1.44348	0.16965	0.39972
O	-0.338	-0.98202	0.77682
H	0.5857	-0.67176	1.08988
O	-1.9686	0.86172	1.81169
Si	-2.25231	3.93549	-2.24878
H	-3.57131	3.26566	-2.14324
H	-2.26941	5.01801	-3.25354
Si	-2.76598	2.26711	2.23346
H	-4.11393	2.24643	1.618
H	-2.84213	2.23564	3.71186
O	-1.96572	3.60896	1.7622
Si	-1.21084	4.64456	0.71767

H	-1.40832	6.01118	1.24352
H	0.21987	4.27833	0.64259
O	-1.8805	4.58104	-0.78243
C	4.26447	-0.49434	0.87823
H	4.02093	-1.55559	0.91935
H	4.84201	-0.2048	1.75095
C	2.99496	0.34661	0.70584
H	2.58121	0.14346	-0.28821
C	3.19394	1.85162	0.86987
H	3.57805	2.07657	1.86667
H	3.89488	2.22879	0.11836
H	2.23558	2.36478	0.73375
O	1.9716	-0.15752	1.59355
K	-1.18783	-1.27196	3.7202
I	5.61789	-0.30921	-0.8384
C	2.16285	-0.12193	3.06563
O	3.24617	0.2702	3.47047
O	1.12145	-0.53087	3.62246

Fig. 5	**TS_{A-3}**		
Si	-1.04058	-3.77626	-2.1449
H	-1.21275	-4.86743	-3.12707
H	0.3635	-3.64203	-1.69635
O	-1.54097	-2.36244	-2.81397
O	-1.98826	-4.1408	-0.84112
Si	-1.68039	-1.00214	-3.72079
H	-1.01894	-1.21341	-5.02656
H	-3.11952	-0.69211	-3.87272
Si	-2.56194	-3.92995	0.67615

H	-3.03435	-5.19233	1.25334
O	-1.36725	-3.31888	1.66181
H	-0.80704	-2.6655	1.17875
O	-0.93167	0.26653	-2.97826
O	-3.83372	-2.87063	0.64136
Si	-4.16818	-1.41353	-0.06216
H	-5.13208	-0.71041	0.81371
H	-4.69139	-1.59126	-1.43094
Si	-0.69056	1.64132	-2.13929
H	0.67362	2.12664	-2.36266
O	-1.77486	2.79815	-2.56057
O	-0.88657	1.34764	-0.51165
O	-2.78155	-0.51287	-0.18117
Si	-1.43934	0.15682	0.45319
O	-0.32021	-1.03455	0.67546
H	0.62488	-0.75898	0.84429
O	-1.79172	0.76684	1.95328
Si	-2.98644	3.73554	-1.93276
H	-4.18428	2.89268	-1.70157
H	-3.25606	4.81772	-2.90056
Si	-2.6207	2.08872	2.55587
H	-4.0449	1.96248	2.16792
H	-2.44543	2.00617	4.02376
O	-2.01164	3.50189	2.01589
Si	-1.65944	4.64194	0.86745
H	-2.02586	5.95782	1.43024
H	-0.21731	4.54916	0.55372
O	-2.5481	4.39957	-0.49278
C	4.5717	-0.09334	1.2848

H	4.88341	-1.12379	1.34232
H	5.24392	0.65946	1.65883
C	3.27725	0.27674	0.58098
H	3.22681	-0.20405	-0.39381
C	3.05015	1.77809	0.4746
H	3.09323	2.24317	1.46578
H	3.82394	2.22051	-0.15864
H	2.07066	1.98331	0.03134
O	2.17753	-0.32887	1.34143
K	-0.84475	-1.47101	3.65211
I	6.15293	0.00095	-0.98398
C	2.46668	-0.45357	2.70217
O	3.66632	-0.18627	2.99346
O	1.53291	-0.8129	3.43104

Fig. 5	**Pro_A**		
Si	-4.26824	-2.55869	-1.30155
H	-5.55968	-3.21307	-1.60805
H	-3.28914	-2.72662	-2.39779
O	-4.5313	-0.95782	-1.05219
O	-3.68186	-3.26515	0.06988
Si	-4.91612	0.63455	-1.06147
H	-6.00476	0.86433	-2.03771
H	-5.31876	1.03321	0.30561
Si	-2.55385	-3.56717	1.21974
H	-2.71065	-4.91635	1.7738
O	-1.02658	-3.4324	0.58164
H	-0.97654	-2.6988	-0.07767
O	-3.63069	1.54993	-1.53747

O	-2.73795	-2.48302	2.45747
Si	-2.91619	-0.84658	2.59492
H	-2.21808	-0.42212	3.83026
H	-4.34624	-0.47763	2.62096
Si	-2.21296	2.3539	-1.50535
H	-1.63007	2.35841	-2.85121
O	-2.41444	3.89767	-0.97958
O	-1.1637	1.64299	-0.43323
O	-2.23974	-0.08731	1.28728
Si	-0.93014	0.24356	0.3706
O	-0.70659	-1.03917	-0.64342
H	0.07561	-1.00489	-1.26638
O	0.40491	0.38815	1.33089
Si	-1.83667	4.84411	0.25327
H	-2.41285	4.38413	1.53995
H	-2.226	6.23722	-0.04814
Si	1.07515	1.63455	2.22329
H	0.04871	2.11426	3.18067
H	2.24632	1.06202	2.91218
O	1.55762	2.88315	1.27821
Si	1.29617	4.09954	0.19156
H	2.2941	5.15284	0.4805
H	1.4515	3.56065	-1.17716
O	-0.19641	4.76885	0.36142
C	6.30181	-0.53114	-0.36534
H	6.45909	-0.87826	-1.38716
H	7.25885	-0.2548	0.09087
C	5.24395	0.58293	-0.25899
H	4.57294	0.56565	-1.12335

C	5.78197	1.97311	0.01187
H	6.42019	1.9824	0.90212
H	6.3717	2.31582	-0.84597
H	4.95987	2.67898	0.1626
O	4.44767	0.13015	0.87362
K	1.58126	-2.44301	1.03922
I	2.3279	-1.43922	-2.153
C	4.68276	-1.17184	1.09666
O	5.73688	-1.61721	0.39691
O	4.02319	-1.86239	1.84478

Fig. 6	**B**		
Si	2.75744	4.01228	2.00843
H	4.2015	4.08774	2.31024
H	2.08899	5.32405	2.19371
O	2.6356	3.61169	0.3915
O	2.08266	2.86309	2.96468
Si	1.61133	3.41025	-0.86028
H	0.37693	4.20979	-0.7232
H	2.32948	3.71602	-2.11597
Si	0.62442	2.05276	3.0006
H	-0.0496	2.39017	4.26731
O	-0.25226	2.41684	1.69417
O	1.08866	1.79132	-1.00646
O	0.98374	0.43438	3.06729
Si	1.74015	-0.96888	2.71158
H	1.04766	-2.06334	3.43251
H	3.176	-0.90706	3.06192
Si	1.91467	0.60329	-1.90694

H	1.721	0.88393	-3.33444
O	3.49995	0.67825	-1.52617
O	1.25631	-0.83189	-1.5087
O	1.68679	-1.29631	1.0755
Si	0.55334	-1.40826	-0.11644
O	-0.78878	-0.57844	0.18764
O	0.17535	-2.99562	-0.39658
Si	4.72678	-0.18879	-0.80973
H	4.74434	0.10946	0.63943
H	5.97731	0.23432	-1.47352
Si	1.17792	-4.31253	-0.61742
H	1.16519	-5.11733	0.62762
H	0.64094	-5.07824	-1.76286
O	2.7086	-3.83188	-0.96056
Si	4.24598	-3.35589	-0.59916
H	4.47235	-3.48867	0.86078
H	5.1665	-4.21234	-1.37659
O	4.51268	-1.79873	-1.06009
Zn	-0.62969	1.30392	0.26466
C	-3.48899	2.38236	0.10457
H	-4.37246	1.76045	-0.0346
H	-3.23974	2.69002	1.11763
C	-2.95518	3.14887	-1.02763
H	-2.3136	3.99709	-0.79079
C	-3.62162	3.15185	-2.37439
H	-4.28485	4.02163	-2.44971
H	-2.87849	3.22237	-3.17661
H	-4.21679	2.24421	-2.5113
O	-2.33462	1.87061	-0.6522

K	-2.86063	-2.08411	-0.45033
I	-5.74578	-0.69245	-1.02925

Fig. 6	**TS_{B-1}**		
Si	1.8838	4.39546	0.78395
H	3.26659	4.84662	1.04562
H	0.95656	5.54686	0.64309
O	1.91817	3.59827	-0.68204
O	1.41525	3.40409	2.00226
Si	0.99576	2.90376	-1.8352
H	-0.37871	3.44389	-1.86584
H	1.66936	3.08486	-3.14028
Si	0.17057	2.30911	2.21599
H	-0.64993	2.78271	3.34552
O	-0.66228	2.14478	0.84178
O	0.83795	1.22266	-1.62382
O	0.86965	0.88462	2.69689
Si	2.00864	-0.28773	2.6146
H	1.63937	-1.35029	3.57953
H	3.3551	0.25795	2.89863
Si	1.94995	0.09356	-2.2417
H	1.73515	-0.02888	-3.69004
O	3.45905	0.65002	-1.95561
O	1.65888	-1.32542	-1.50273
O	2.10055	-0.95033	1.08843
Si	1.09097	-1.70688	0.01895
O	-0.43224	-1.21297	0.14594
O	1.24336	-3.3378	0.17465
Si	4.81768	0.39786	-1.03079

H	4.64242	1.05314	0.28402
H	5.94449	0.9834	-1.78801
Si	2.5508	-4.35575	0.24331
H	2.68048	-4.85883	1.63242
H	2.31095	-5.46358	-0.70786
O	3.93687	-3.58619	-0.19649
Si	5.22801	-2.59421	0.04466
H	5.33968	-2.25722	1.4854
H	6.43029	-3.30786	-0.43878
O	5.09591	-1.20976	-0.83683
Zn	-0.80153	0.62283	-0.22093
C	-3.83168	1.83242	-0.33199
H	-4.89506	1.70944	-0.18124
H	-3.23162	2.21044	0.48978
C	-3.18562	1.59896	-1.63029
H	-2.47001	2.39039	-1.89446
C	-4.10012	1.29656	-2.80554
H	-4.63058	2.20148	-3.12522
H	-3.51011	0.92714	-3.65096
H	-4.83868	0.53454	-2.53391
O	-2.54471	0.4338	-1.11519
K	-2.80173	-2.15015	-0.20623
I	-5.00075	-0.43742	1.56568

Fig. 6	**Int_{B-1}**		
Si	0.88573	4.49132	0.88981
H	2.11302	5.25972	1.18896
H	-0.29701	5.38463	0.78848
O	1.12074	3.79779	-0.6079

O	0.67897	3.36646	2.065
Si	0.40543	2.928	-1.79221
H	-1.05354	3.14704	-1.85732
H	1.06306	3.27587	-3.07242
Si	-0.36331	2.06894	2.24722
H	-1.29068	2.3958	3.34945
O	-1.11409	1.75716	0.85966
O	0.62624	1.25762	-1.58685
O	0.56174	0.80218	2.79213
Si	1.90642	-0.12511	2.69662
H	1.72352	-1.27625	3.61467
H	3.1169	0.65183	3.04791
Si	1.95077	0.37031	-2.15874
H	1.84134	0.23902	-3.61824
O	3.32234	1.18131	-1.78993
O	1.88913	-1.09519	-1.45408
O	2.16666	-0.70023	1.15614
Si	1.34301	-1.60328	0.03829
O	-0.24604	-1.41918	0.11868
O	1.80849	-3.18095	0.17925
Si	4.65141	1.17813	-0.79538
H	4.28923	1.75702	0.51723
H	5.68209	1.98709	-1.48133
Si	3.28144	-3.89197	0.43915
H	3.41737	-4.20169	1.88454
H	3.32838	-5.12601	-0.3764
O	4.52325	-2.91596	-0.02848
Si	5.58034	-1.69063	0.28233
H	5.54832	-1.35739	1.72845

H	6.92255	-2.15378	-0.13414
O	5.23438	-0.34789	-0.60384
Zn	-0.98717	0.3216	-0.33334
C	-4.39747	0.84512	-0.24843
H	-5.24976	1.51342	-0.38357
H	-3.76086	1.19001	0.56642
C	-3.58704	0.63095	-1.53253
H	-3.24473	1.66619	-1.74775
C	-4.43627	0.18733	-2.72728
H	-5.26723	0.87815	-2.91488
H	-3.80804	0.14691	-3.62278
H	-4.85555	-0.81165	-2.55596
O	-2.50275	-0.22458	-1.34886
K	-2.33433	-2.69305	-0.62715
I	-5.30672	-1.00782	0.56938

Fig. 6	**Int_{B-2}**		
Si	-2.01491	4.63637	0.04377
H	-3.37619	5.18914	0.2103
H	-0.9873	5.70638	0.1232
O	-1.76718	3.60473	1.32959
O	-1.94564	3.85566	-1.39745
Si	-0.65686	2.66347	2.07347
H	0.72361	3.15682	1.89656
H	-1.02381	2.58586	3.50628
Si	-0.79789	2.85607	-2.09438
H	-0.21209	3.58157	-3.24012
O	0.29054	2.41899	-0.9938
O	-0.66758	1.0662	1.50104

O	-1.62754	1.57551	-2.7507
Si	-2.73463	0.37809	-2.60716
H	-2.59608	-0.5027	-3.7934
H	-4.10481	0.92932	-2.5075
Si	-1.6711	-0.17451	2.06232
H	-1.25835	-0.56033	3.41723
O	-3.21063	0.36684	2.10492
O	-1.46659	-1.43104	1.03939
O	-2.50861	-0.5298	-1.22894
Si	-1.28543	-1.46868	-0.62415
O	0.16769	-0.92906	-1.02581
O	-1.53013	-3.03797	-1.06973
Si	-4.72995	0.28541	1.44587
H	-4.80952	1.18473	0.27437
H	-5.66583	0.70061	2.51337
Si	-2.68722	-4.16032	-0.68803
H	-2.90768	-4.98837	-1.89702
H	-2.20812	-4.99211	0.44097
O	-4.10207	-3.45659	-0.24346
Si	-5.37817	-2.43221	-0.10689
H	-5.66286	-1.80941	-1.42232
H	-6.53109	-3.22919	0.36862
O	-5.09859	-1.25844	1.01363
Zn	0.73116	0.76382	-0.25108
C	4.69204	0.52762	1.23703
H	4.4439	-0.16163	2.04367
H	5.43764	1.24982	1.57245
C	3.44307	1.19427	0.65771
H	3.08041	1.76873	1.53848

C	3.75906	2.21367	-0.44334
H	2.84453	2.73984	-0.73334
H	4.49592	2.95409	-0.10764
H	4.1591	1.70778	-1.33004
O	2.49453	0.24592	0.26856
K	2.53876	-1.88099	-1.26624
I	5.8112	-0.75078	-0.18898
C	1.89726	-1.99703	2.19683
O	2.11137	-2.77595	1.34541
O	1.68939	-1.26475	3.07937

Fig. 6 **TS_{B-2}**

Si	-0.99505	4.6329	-0.7044
H	-2.23867	5.30634	-1.13481
H	0.10113	5.6123	-0.49161
O	-1.32311	3.91107	0.75762
O	-0.57837	3.53171	-1.84799
Si	-0.74592	2.91802	1.92386
H	0.69759	3.11269	2.15421
H	-1.53974	3.15242	3.1499
Si	0.52122	2.28538	-1.9882
H	1.55394	2.70448	-2.95747
O	1.14906	1.90119	-0.55177
O	-0.96743	1.28633	1.50783
O	-0.2875	1.01636	-2.68749
Si	-1.61762	0.0674	-2.82681
H	-1.28807	-1.01829	-3.78272
H	-2.78427	0.85368	-3.28662
Si	-2.29561	0.34388	1.97975

H	-2.29685	0.18026	3.43675
O	-3.66457	1.1173	1.52228
O	-2.14549	-1.09726	1.22959
O	-2.05791	-0.60383	-1.37167
Si	-1.39591	-1.54817	-0.18583
O	0.19266	-1.33928	-0.05334
O	-1.80323	-3.12492	-0.44404
Si	-4.88281	1.10654	0.39621
H	-4.40933	1.75264	-0.84913
H	-6.01147	1.84836	0.99831
Si	-3.24055	-3.93647	-0.26406
H	-3.25276	-5.01726	-1.2774
H	-3.32113	-4.49339	1.10598
O	-4.5276	-2.9496	-0.50744
Si	-5.55836	-1.73563	-0.90531
H	-5.32035	-1.3292	-2.31146
H	-6.93427	-2.24813	-0.71946
O	-5.37907	-0.43036	0.08231
Zn	0.79291	0.39805	0.502
C	4.20456	0.94438	0.00181
H	5.05465	1.62334	0.07804
H	3.41603	1.37421	-0.61471
C	3.67259	0.552	1.37557
H	3.30061	1.50199	1.79793
C	4.72912	-0.01156	2.32381
H	5.56292	0.69399	2.4137
H	4.31335	-0.17009	3.32289
H	5.12167	-0.96627	1.9601
O	2.56815	-0.34128	1.20442

K	2.26512	-2.86139	0.25243
I	4.96821	-0.748	-1.18751
C	1.86501	-0.91352	2.65828
O	2.21692	-2.05833	2.83884
O	1.13952	-0.03241	3.06827

Fig. 6	**Int_{B-3}**		
Si	-3.20483	-4.28119	0.60501
H	-4.67081	-4.4648	0.67158
H	-2.50235	-5.58835	0.53859
O	-2.89952	-3.46951	-0.81942
O	-2.73203	-3.4211	1.91927
Si	-1.6856	-2.97172	-1.7973
H	-0.47672	-3.80697	-1.67475
H	-2.20202	-2.94788	-3.18466
Si	-1.29763	-2.6772	2.35697
H	-0.76725	-3.39219	3.53479
O	-0.28499	-2.64767	1.11149
O	-1.20886	-1.37745	-1.44862
O	-1.71904	-1.16273	2.90133
Si	-2.53811	0.24424	2.79961
H	-2.10354	1.1145	3.91889
H	-4.00264	0.02695	2.82846
Si	-1.85468	0.0271	-2.12927
H	-1.34477	0.20238	-3.4931
O	-3.48891	-0.11106	-2.17396
O	-1.41993	1.27209	-1.17004
O	-2.23409	1.04521	1.36579
Si	-0.94472	1.41857	0.41673

O	0.38604	0.56893	0.6704
O	-0.59811	3.04685	0.56366
Si	-4.83861	0.4858	-1.41478
H	-5.04559	-0.22688	-0.13387
H	-5.96902	0.2775	-2.34487
Si	-1.66024	4.32272	0.70232
H	-1.95595	4.56183	2.13544
H	-0.98031	5.49073	0.09492
O	-3.05603	4.03926	-0.11591
Si	-4.59635	3.44675	-0.19755
H	-5.0743	3.13667	1.17246
H	-5.42473	4.49103	-0.83915
O	-4.68417	2.1018	-1.13692
Zn	0.41209	-1.2676	0.07702
C	4.88401	-1.11102	0.42067
H	5.63229	-1.69273	0.95977
H	3.92253	-1.1786	0.92428
C	4.78177	-1.54223	-1.04109
H	4.31733	-2.53674	-1.00467
C	6.10984	-1.60996	-1.7818
H	6.79363	-2.29983	-1.27541
H	5.94693	-1.96836	-2.80215
H	6.5814	-0.62369	-1.8341
O	3.93333	-0.66586	-1.7961
K	2.07011	2.29481	-0.49356
I	5.50129	0.98237	0.71171
C	2.58353	-0.66283	-1.55199
O	1.94203	0.25217	-2.08684
O	2.13907	-1.57948	-0.77231

Fig. 6	**TS_{B-3}**		
Si	-2.58137	-4.07601	1.43839
H	-4.01996	-4.41343	1.42885
H	-1.73553	-5.28312	1.60632
O	-2.23829	-3.41041	-0.0512
O	-2.31484	-2.99858	2.65064
Si	-1.01535	-2.97885	-1.04792
H	0.25393	-3.63016	-0.68121
H	-1.4229	-3.22709	-2.44305
Si	-1.0573	-1.99378	3.08505
H	-0.58923	-2.39763	4.42395
O	0.10821	-2.01981	1.97234
O	-0.713	-1.29221	-0.94016
O	-1.71891	-0.47373	3.26808
Si	-2.80259	0.63797	2.74852
H	-2.72314	1.79992	3.66855
H	-4.17389	0.08781	2.68406
Si	-1.51578	-0.1464	-1.90865
H	-0.91837	-0.14577	-3.24748
O	-3.09599	-0.54522	-1.98836
O	-1.29898	1.30819	-1.19127
O	-2.4518	1.16953	1.20495
Si	-1.12757	1.73579	0.40286
O	0.25212	1.14693	0.98091
O	-1.08096	3.39098	0.46514
Si	-4.61976	-0.08961	-1.50664
H	-4.89045	-0.63933	-0.16021
H	-5.55508	-0.62028	-2.51952

Si	-2.12636	4.51821	-0.18535
H	-2.34909	5.54684	0.85835
H	-1.48917	5.10856	-1.38429
O	-3.54538	3.82873	-0.61088
Si	-4.96193	2.99939	-0.73495
H	-5.51577	2.78367	0.62337
H	-5.87294	3.80978	-1.57167
O	-4.74736	1.55158	-1.48394
Zn	0.57358	-0.71557	0.75066
C	2.86762	-1.87303	-1.50136
H	2.35079	-1.27691	-2.23856
H	2.40809	-2.80605	-1.21706
C	4.36498	-1.67866	-1.30238
H	4.84871	-1.45445	-2.25015
C	5.05273	-2.82154	-0.57545
H	5.0213	-3.71372	-1.20639
H	6.09633	-2.56394	-0.37365
H	4.55254	-3.0383	0.37557
O	4.51962	-0.44618	-0.50225
K	2.01217	2.80177	1.72081
I	3.16723	-3.43644	-3.9513
C	3.43957	-0.13931	0.20496
O	3.41023	0.79133	0.99931
O	2.41125	-0.94013	-0.06356

Fig. 6	**Pro_B**		
Si	1.48465	4.78543	0.96425
H	2.78095	5.44991	1.21085
H	0.39125	5.77273	0.78374

O	1.64708	3.9499	-0.47283
O	1.16326	3.77578	2.21701
Si	0.83723	3.13824	-1.63265
H	-0.59226	3.50859	-1.69212
H	1.51336	3.36448	-2.92829
Si	0.18981	2.43721	2.41287
H	-0.57219	2.62616	3.6593
O	-0.73448	2.23057	1.09961
O	0.86932	1.45198	-1.38262
O	1.19622	1.13982	2.62419
Si	2.15149	-0.17842	2.72765
H	1.56588	-1.13867	3.69213
H	3.52501	0.21287	3.11223
Si	2.04328	0.41817	-2.0582
H	1.83182	0.36041	-3.5095
O	3.52248	1.02799	-1.72785
O	1.83043	-1.04636	-1.38353
O	2.29023	-0.92633	1.24214
Si	1.27633	-1.55062	0.101
O	-0.25193	-1.08125	0.27904
O	1.37887	-3.19841	0.09771
Si	4.91833	0.68093	-0.89002
H	4.80369	1.22752	0.48041
H	6.02203	1.31468	-1.64162
Si	2.72499	-4.17772	0.1858
H	2.90486	-4.61478	1.59089
H	2.47986	-5.32728	-0.71195
O	4.06542	-3.37646	-0.32601
Si	5.3793	-2.40311	-0.11162

H	5.61814	-2.20553	1.33908
H	6.52634	-3.0652	-0.76917
O	5.17277	-0.94128	-0.84047
Zn	-0.65771	0.7241	0.04274
C	-3.60493	1.75986	-0.51272
H	-3.19512	2.7451	-0.29728
H	-4.02736	1.28954	0.37875
C	-4.5546	1.70306	-1.71792
H	-4.35395	2.51734	-2.42282
C	-6.02586	1.61236	-1.37001
H	-6.33474	2.52732	-0.85108
H	-6.62808	1.51435	-2.27781
H	-6.2069	0.75223	-0.71842
O	-4.13192	0.47643	-2.40082
K	-1.97914	-2.9391	-0.41602
I	-4.66981	-1.65505	0.97892
C	-2.96068	0.06124	-1.94987
O	-2.31826	-0.88208	-2.33614
O	-2.50161	0.91031	-0.96096