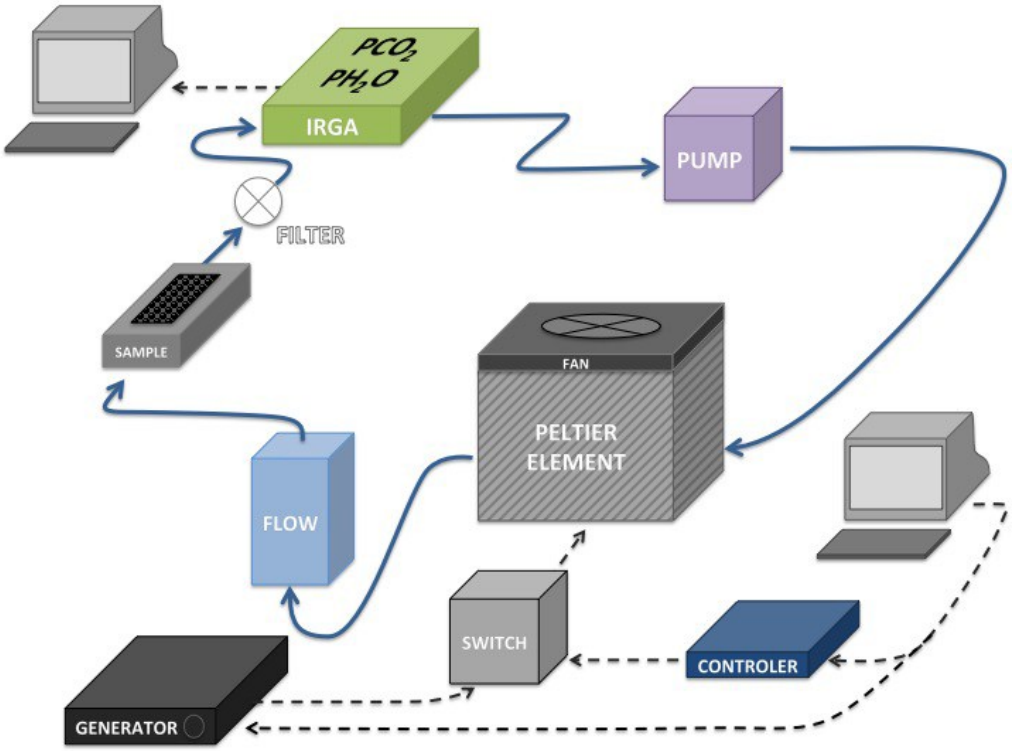
Supporting Information

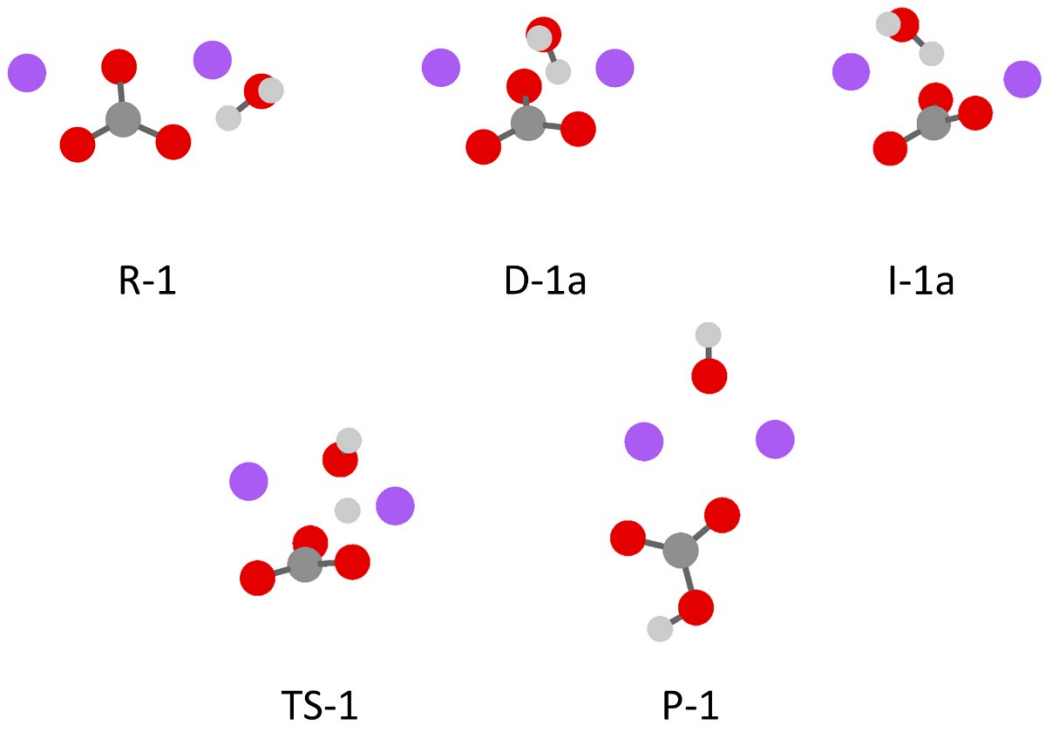
Experimental Device:



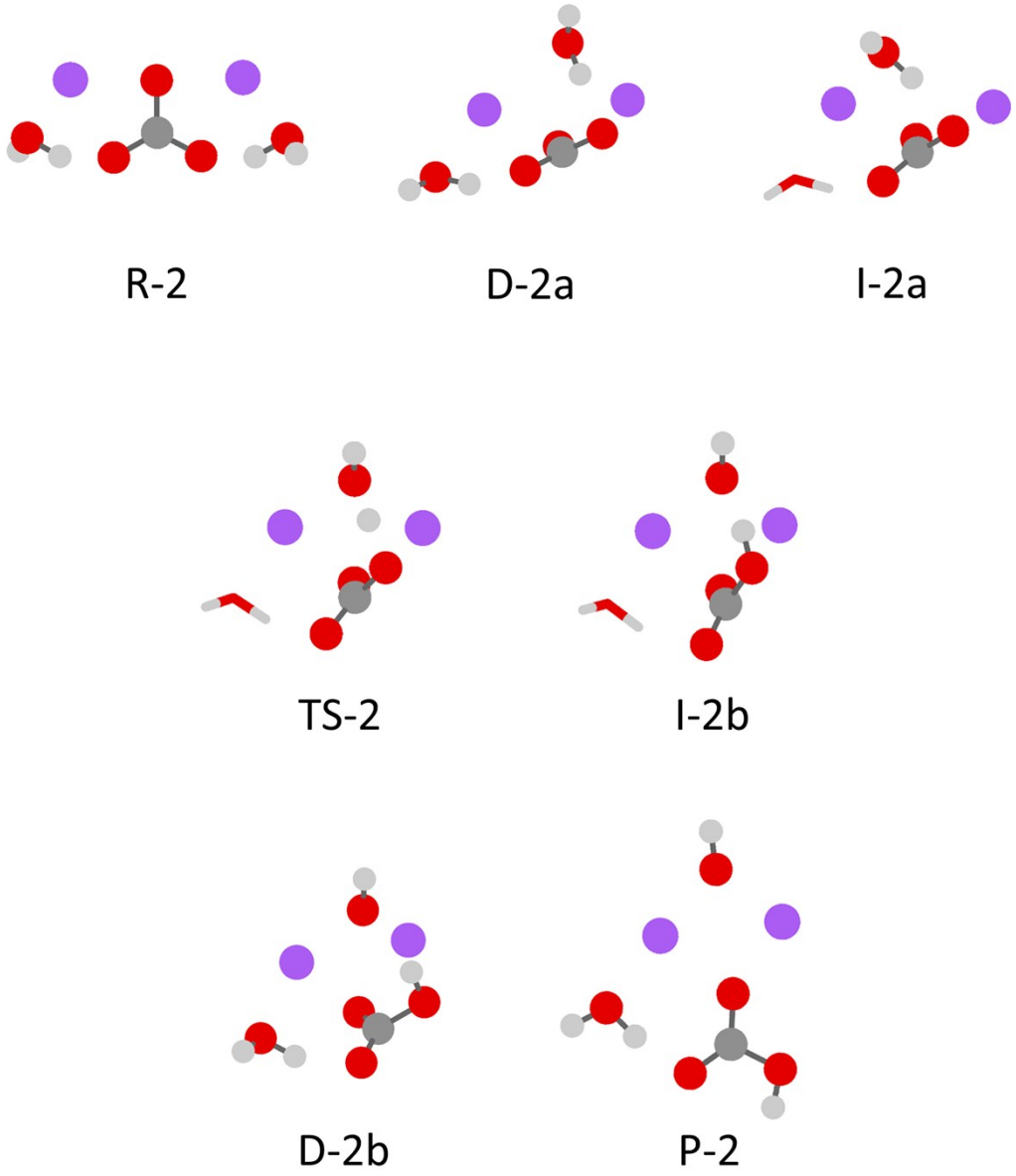
Supporting Figure 1**:** Schematic of Experimental Device. The total amount of carbon dioxide on the sample and in the gas volume is constant. We can track the absorption and desorption of carbon dioxide by measuring the carbon dioxide content of the gas. The device can control the water vapor level in the closed gas circulation system. We can determine and characterize the process of CO_2 absorption/desorption by sorbent in the test sample chamber.

In the sample chamber, ion exchange resin beads were trapped by two metallic meshes with a well-fitted grid, preventing the beads in between the meshes from moving. All beads can be considered as independent when air went through. The partial pressure of H_2O and CO_2 in the device can be continuously measured by an infrared gas analyzer (IRGA, LI-COR, LI-840).

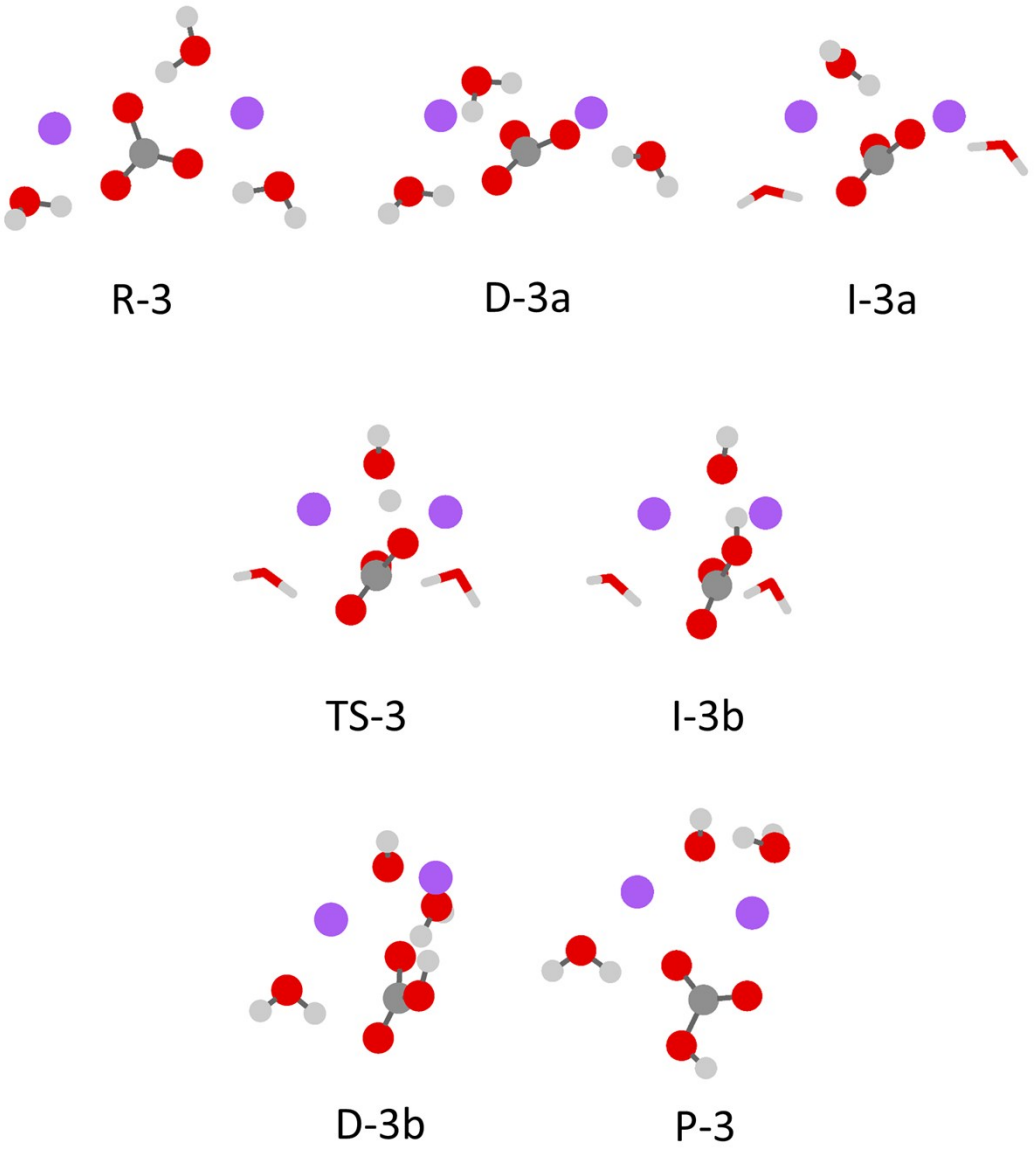
Enlarged structures of reactants, intermediates, products and transition states shown in Fig. 2 and Fig. 4.



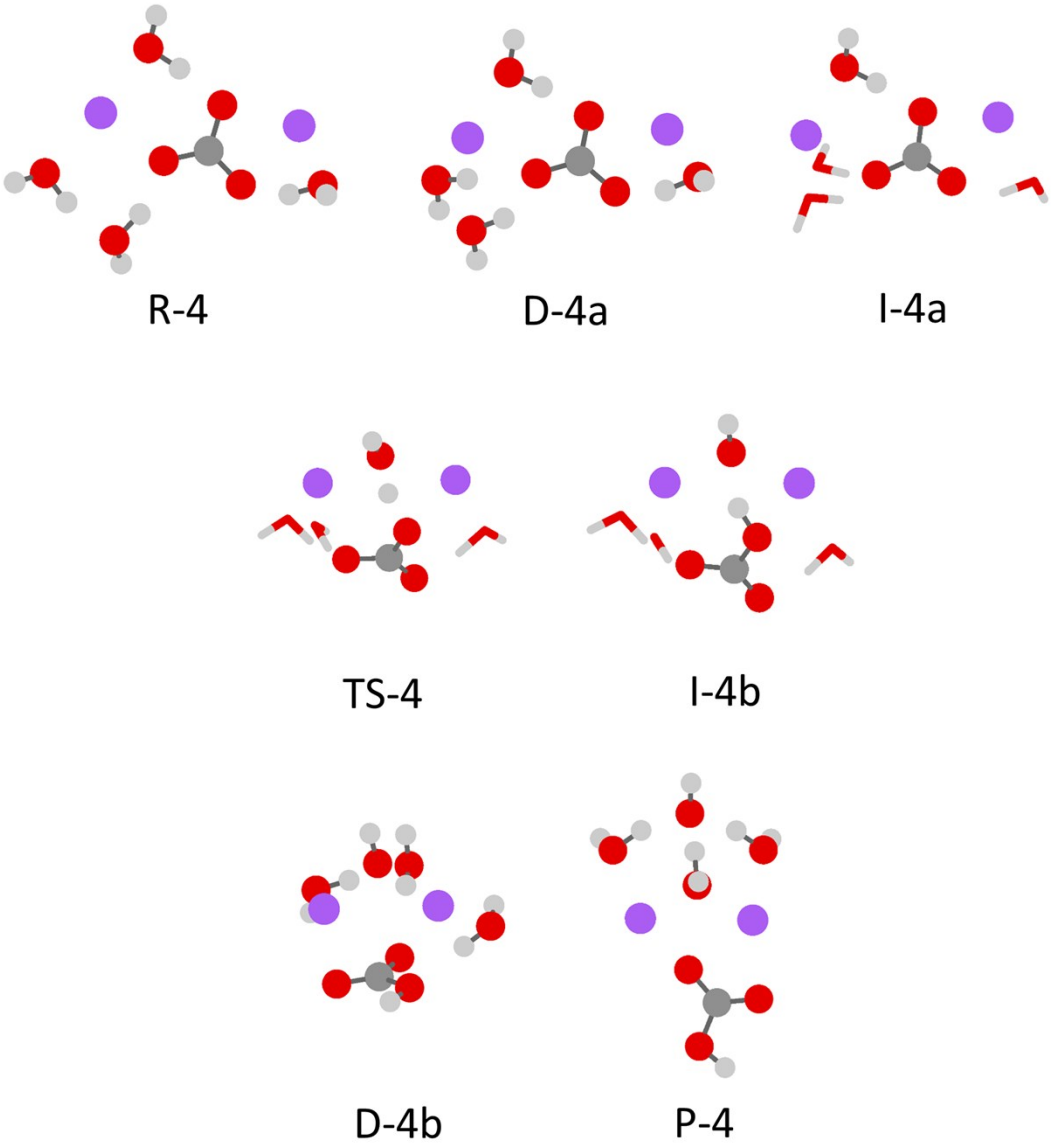
Supporting Figure 2: Enlarged structures of reactants, intermediates, products and transition states for the reaction pathway with n = 1.



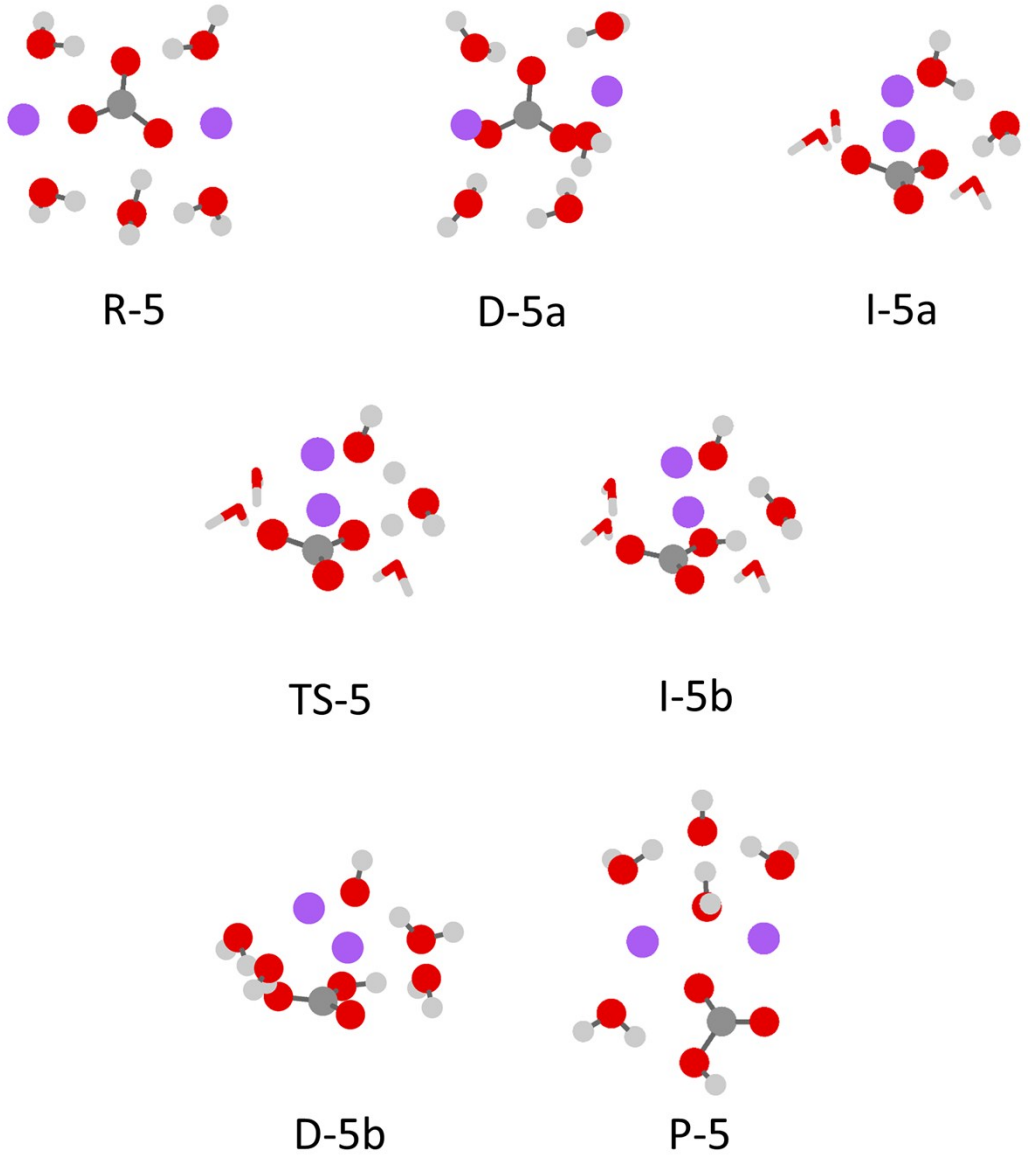
Supporting Figure 3: Enlarged structures of reactants, intermediates, products and transition states for the reaction pathway with $n = 2$.



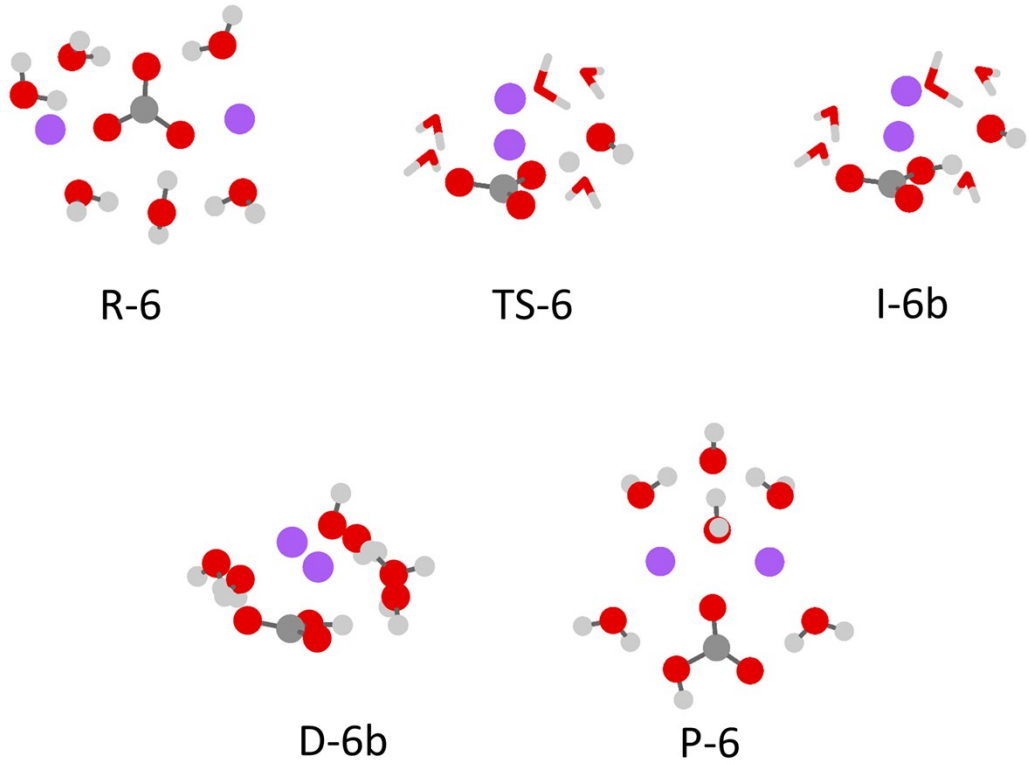
Supporting Figure 4: Enlarged structures of reactants, intermediates, products and transition states for the reaction pathway with $n = 3$.



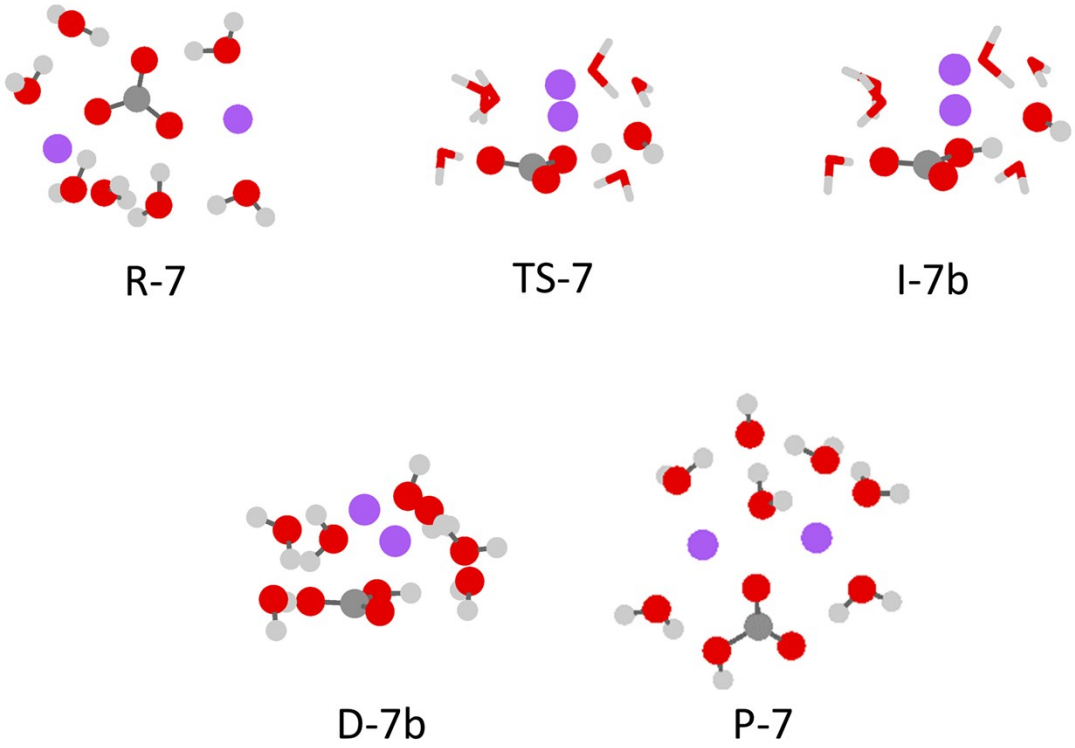
Supporting Figure 5: Enlarged structures of reactants, intermediates, products and transition states for the reaction pathway with $n = 4$.



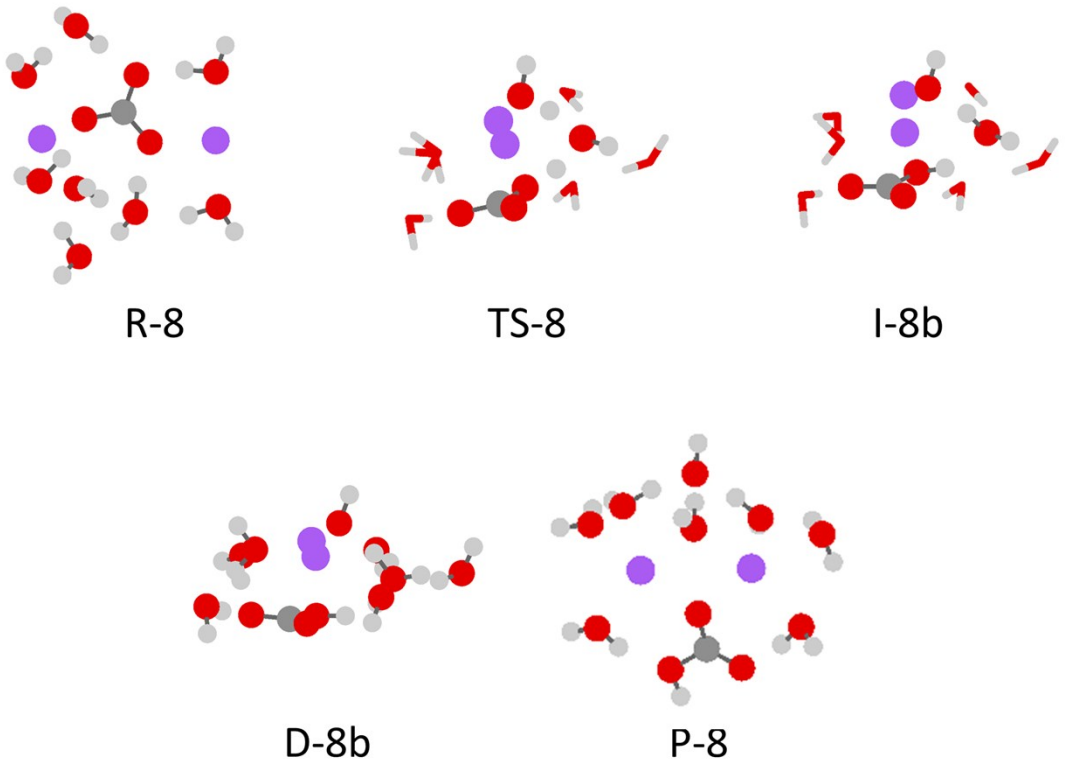
Supporting Figure 6: Enlarged structures of reactants, intermediates, products and transition states for the reaction pathway with $n = 5$.



Supporting Figure 7: Enlarged structures of reactants, intermediates, products and transition states for the reaction pathway with $n = 6$.



Supporting Figure 8: Enlarged structures of reactants, intermediates, products and transition states for the reaction pathway with n = 7.



Supporting Figure 9: Enlarged structures of reactants, intermediates, products and transition states for the reaction pathway with n = 8.

Structure files (xyz format) of reactants, intermediate states, transition states and products of the hydrolysis of CO_3^{2-} with 1-8 water molecules:

R-1:
9

C	0.49611	0.48019	-0.24126
O	0.63545	-0.83591	-0.02575
O	1.50901	1.23402	-0.09146
O	-0.65993	0.91079	-0.59768
H	-2.08209	0.86296	0.29563
O	-2.87794	0.35912	0.62371
H	-3.23155	0.82538	1.38180
Na	-1.50077	-1.16786	-0.36293
Na	2.72662	-0.46065	0.40834

D-1a:
9

C	-0.09966	-0.51745	0.62755
O	-0.00734	-1.02996	-0.60160
O	-1.23256	-0.45212	1.18874
O	0.97290	-0.00074	1.14113
H	0.47659	1.57003	0.40011
O	0.16686	2.21574	-0.27878
H	-0.05476	3.01125	0.21135
Na	2.09631	-0.51168	-0.63560
Na	-2.00747	-0.15559	-0.81646

I-1a:
9

C	0.19734	-0.55714	0.54584
O	0.47880	-0.88614	-0.71189
O	-0.80996	-1.06205	1.11328
O	0.90537	0.40058	1.08213
H	-0.43676	1.48553	0.42401
O	-1.20849	1.79028	-0.11657
H	-1.76226	2.27224	0.50233
Na	2.30185	0.27188	-0.56259
Na	-1.74829	-0.48609	-0.81350

TS-1:
9

C	-0.53592	-0.88007	0.16239
O	-0.14998	-0.79919	-1.07506
O	-1.73341	-0.78544	0.50347
O	0.44685	-0.82783	1.09174
H	0.61618	0.40036	1.05015
O	0.77368	1.50162	0.58758
H	0.98994	2.11793	1.28906
Na	1.91877	-0.29439	-0.53709
Na	-1.29038	1.20792	-0.56976

P-1:
9

C	-1.48275	-0.05403	0.00002
O	-1.52645	1.19707	0.00014
O	-0.44464	-0.76435	0.00000
O	-2.66462	-0.73980	-0.00011
H	-3.35761	-0.06925	-0.00008

O	2.58018	0.36206	-0.00000
H	3.49472	0.63786	0.00018
Na	0.72344	1.42268	-0.00003
Na	1.56780	-1.48489	-0.00001

R-2:
12

C	0.00001	-0.36849	-0.00006
O	-1.04601	-0.98162	0.41149
O	0.00004	0.96007	-0.00002
O	1.04600	-0.98162	-0.41158
H	2.59733	-0.97578	0.29285
O	3.46433	-0.50989	0.43255
H	3.86624	-0.86779	1.22504
Na	-2.10707	1.00372	0.60569
Na	2.10717	1.00368	-0.60570
O	-3.46445	-0.50988	-0.43239
H	-2.59732	-0.97562	-0.29302
H	-3.86658	-0.86766	-1.22482

D-2a:
12

C	0.11485	-0.89683	0.19306
O	-1.00604	-1.03664	0.77513
O	0.16691	-0.45008	-1.04580
O	1.23883	-1.05056	0.82928
H	1.39941	0.58911	1.10455
O	1.49153	1.54667	0.81247
H	1.80431	2.03790	1.57562
Na	-1.19151	1.15876	-0.37269
Na	2.32636	-0.17654	-0.88401
O	-3.14069	0.06306	-0.18665
H	-2.44826	-0.57760	0.16931
H	-3.93231	-0.05242	0.34034

I-2a:
12

C	0.36139	-0.64490	0.49571
O	-0.70016	-0.90097	1.13185
O	0.40629	-0.76028	-0.81887
O	1.41587	-0.14737	1.08621
H	0.79748	1.45526	0.73504
O	0.29021	2.19417	0.30046

H	0.07697	2.80744	1.00737
Na	-1.24214	0.78011	-0.84873
Na	2.56176	-0.49891	-0.72176
O	-2.88536	-0.62281	-0.21643
H	-2.10924	-0.93703	0.35186
H	-3.66416	-0.65136	0.34108

TS-2:
12

C	-0.08812	-1.07345	0.05834
O	-1.16887	-1.61893	0.35483
O	0.11985	-0.46942	-1.08160
O	0.91118	-0.98365	0.95002
H	1.10342	0.27942	1.04022
O	1.28284	1.40492	0.81573
H	1.56905	1.83860	1.62172
Na	-0.76205	1.45287	-0.32203
Na	2.26335	-0.15199	-0.69478
O	-2.75244	0.42605	-0.08355
H	-2.30608	-0.47038	0.00393
H	-3.49249	0.41165	0.52551

I-2b:
12

C	-0.43295	-1.12110	0.01172
O	-1.56829	-1.58615	0.11417
O	0.06481	-0.53596	-1.01465
O	0.38932	-1.16644	1.12985
H	0.91012	-0.31502	1.16089
O	1.66285	1.18267	0.70583
H	2.12086	1.65580	1.40039
Na	-0.31927	1.58911	-0.19101
Na	2.23499	-0.37089	-0.67762
O	-2.52784	0.96591	-0.11257
H	-2.40238	-0.01420	-0.13250
H	-3.27056	1.11937	0.47474

D-2b:
12

C	0.13711	-1.17254	0.05470
O	1.21900	-1.57209	-0.37592
O	-0.09736	-0.53382	1.11961
O	-1.01311	-1.38991	-0.76425

H	-1.07298	-0.57680	-1.30675
O	-1.28668	1.44433	-0.78853
H	-1.62875	2.04455	-1.45047
Na	0.68651	1.47784	0.14850
Na	-2.20642	0.09808	0.62979
O	2.76161	0.55326	0.09856
H	2.38666	-0.36091	0.00745
H	3.54377	0.57902	-0.45536

P-2:
12

C	1.47944	-0.60070	0.00006
O	2.26190	0.36558	0.00012
O	0.22037	-0.57659	0.00002
O	2.02098	-1.86469	0.00002
H	2.97782	-1.74445	0.00006
O	-2.83749	0.03873	-0.00001
H	-3.77481	0.22261	-0.00001
Na	-1.10623	1.31646	-0.00022
Na	-1.64083	-1.68693	0.00011
O	0.76559	2.54230	-0.00008
H	1.42919	1.79506	0.00017
H	1.25789	3.36348	-0.00002

R-3:
15

Na	-2.65829	0.80534	-0.54016
Na	2.70976	0.34712	0.26151
C	-0.33152	-0.26671	-0.13027
O	-1.32273	-1.02618	-0.41905
O	0.82047	-0.72645	0.16612
O	-0.51757	1.03955	-0.14412
O	3.08082	-1.86458	-0.24852
H	2.09394	-1.83525	-0.18195
H	3.36098	-2.76805	-0.09995
O	1.67151	2.28168	0.24979
H	0.74901	1.84130	0.09741
H	1.60251	3.20206	-0.00233
O	-3.69206	-0.84864	0.65441
H	-2.78489	-1.19237	0.43635
H	-3.92217	-1.16755	1.52816

D-3a:
15

C	0.15851	-0.18146	0.34410
O	-0.75685	-0.48127	1.17536
O	0.07010	-0.55894	-0.91190
O	1.15441	0.58291	0.67739
H	-0.34417	2.11064	0.23080
O	-1.30935	2.23217	0.22224
H	-1.54233	1.85990	1.08305
Na	-2.02173	0.22301	-0.94271
Na	2.21304	-0.14828	-1.20618
O	-3.00607	-1.39436	0.27210
H	-2.12894	-1.24516	0.74538
H	-3.66061	-1.60558	0.93873
O	3.58607	-0.36342	0.60710
H	3.98191	-0.95691	1.24709
H	2.73215	-0.03285	0.98984

I-3a:
15

C	-0.05764	-0.59462	-0.23211
O	0.74483	-1.36236	-0.82218
O	0.07654	-0.29487	1.03926
O	-1.02014	0.03006	-0.88162
H	-0.06022	1.47277	-0.97014
O	0.65732	2.14304	-0.80187
H	0.86177	2.52331	-1.65887
Na	1.97687	0.79629	0.59896
Na	-2.01766	0.37541	1.15197
O	3.12576	-1.07719	0.14710
H	2.23083	-1.38877	-0.20966
H	3.78987	-1.40524	-0.46087
O	-3.50774	-0.52725	-0.32341
H	-3.98520	-1.31268	-0.59493
H	-2.65515	-0.50174	-0.83139

TS-3:
15

C	-0.28748	-0.71010	0.78466
O	-1.20544	-1.46779	1.13517
O	0.17788	-0.67632	-0.44610
O	0.23344	0.19860	1.61206
H	0.18410	1.27727	0.98923
O	0.24478	2.15759	0.19842
H	0.12762	2.99418	0.65204

Na	-1.20016	0.94428	-1.13827
Na	2.03390	0.61417	0.14286
O	-2.91085	-0.46885	-0.66218
H	-2.38226	-1.03059	-0.02943
H	-3.79607	-0.42687	-0.29616
O	2.66672	-1.26554	-0.99441
H	3.07874	-2.12805	-0.92231
H	1.68942	-1.38973	-0.89537

I-3b:

15

C	-0.55484	-0.86534	0.70257
O	-1.39803	-1.75746	0.78424
O	0.23981	-0.66180	-0.29690
O	-0.49199	0.06509	1.70035
H	-0.01077	0.87656	1.36634
O	0.62186	2.12864	0.37809
H	0.65503	2.99569	0.78236
Na	-0.93490	1.25091	-0.91917
Na	2.12308	0.59706	0.08737
O	-2.78220	-0.14107	-1.01497
H	-2.46005	-0.89735	-0.47315
H	-3.70261	-0.02539	-0.76941
O	2.68106	-1.41529	-0.84288
H	3.10243	-2.27491	-0.88221
H	1.71100	-1.55508	-0.75292

D-3b:

15

C	-0.91321	-0.88725	0.73248
O	-1.92925	-1.50002	0.41347
O	0.13860	-0.70324	0.02681
O	-0.92110	-0.23616	1.94696
H	-0.12648	0.31496	1.98478
O	1.23517	2.07686	0.42333
H	1.53200	2.94213	0.70212
Na	-0.52119	1.49472	-0.66790
Na	2.23394	0.20854	0.21069
O	-2.43290	0.46792	-1.42245
H	-2.40954	-0.37196	-0.90655
H	-3.35998	0.69786	-1.51009
O	2.29968	-1.70062	-1.04592
H	2.54299	-2.49837	-1.51676
H	1.33833	-1.73470	-0.85670

P-3:
15

C	1.43509	-1.12762	-0.01192
O	0.95574	0.01198	0.25107
O	0.79519	-2.14566	-0.33117
O	2.79851	-1.20809	0.07532
H	3.02661	-2.11934	-0.14324
O	-2.08872	0.91810	-0.79647
H	-2.68744	1.16532	-1.50152
Na	-0.22723	1.85698	-0.29270
Na	-1.24399	-1.14028	-0.22356
O	-3.16976	-0.63163	0.92485
H	-2.95302	0.15795	0.32909
H	-3.52088	-0.30250	1.75292
O	1.84137	2.49714	0.40891
H	1.96197	1.52666	0.48950
H	2.68708	2.91910	0.56355

R-4:
18

C	0.64875	-0.05159	-0.23552
O	-0.58830	-0.32445	-0.04887
O	1.04469	1.19816	-0.17764
O	1.51143	-0.96567	-0.48568
H	-0.10717	2.19773	0.07838
O	-0.94925	2.75800	0.24173
H	-0.71976	3.67782	0.11295
Na	3.14395	0.62020	-0.42875
Na	-2.28909	1.00474	0.18261
O	-3.85719	-0.61763	0.07133
H	-4.68192	-0.91253	0.45979
H	-3.27557	-1.42158	-0.01665
O	3.79493	-1.21646	0.76236
H	2.86523	-1.40682	0.47156
H	3.91620	-1.60853	1.62824
O	-1.98090	-2.49258	-0.07284
H	-1.82747	-3.02445	-0.85675
H	-1.26872	-1.78147	-0.08000

D-4a:
18

C	0.65800	-0.12987	-0.13154

O	-0.55354	-0.49618	0.07377
O	1.57139	-0.96530	-0.46240
O	0.97293	1.13798	-0.00782
H	-0.27365	2.05902	0.06210
O	-1.16756	2.55651	0.05833
H	-0.98457	3.49436	0.10302
Na	-2.39546	0.72755	-0.00841
Na	3.09892	0.72020	-0.33792
O	-3.26319	-1.01421	1.34548
H	-2.39907	-1.19913	1.73325
H	-3.26439	-1.56135	0.54230
O	3.91918	-1.15661	0.66871
H	4.11170	-1.61735	1.48646
H	2.99190	-1.38717	0.40064
O	-2.46952	-1.50142	-1.27276
H	-1.54864	-1.35652	-0.90995
H	-2.39689	-2.06407	-2.04537

I-4a:

18

C	-0.59438	-0.25694	-0.14949
O	0.55344	-0.77211	0.12669
O	-1.60775	-0.98318	-0.42707
O	-0.72546	1.04759	-0.15122
H	0.62357	1.83149	-0.24412
O	1.55111	2.24521	-0.32916
H	1.46955	2.99129	-0.92408
Na	2.59903	0.27775	-0.14077
Na	-2.88883	0.89582	-0.50400
O	2.49592	-1.70833	-1.34167
H	1.60281	-1.68563	-0.91880
H	2.80031	-2.61663	-1.30746
O	-3.98567	-0.74308	0.63789
H	-4.29308	-1.12969	1.45878
H	-3.10112	-1.13626	0.42683
O	2.24813	-0.27303	2.12081
H	1.41985	-0.52258	1.64729
H	1.99436	0.39575	2.76086

TS-4:

18

C	-0.34449	-0.69564	-0.92923
O	0.92053	-0.92995	-0.84689
O	-1.21402	-1.59351	-0.80963

O	-0.72065	0.57234	-1.08167
H	-0.10135	1.33821	-0.28995
O	0.15735	1.94631	0.66312
H	0.52007	2.79252	0.39003
Na	1.84165	0.38582	0.98094
Na	-2.16595	1.32504	0.45231
O	2.89324	0.79829	-1.02805
H	2.16542	0.16818	-1.27429
H	3.66870	0.53764	-1.52779
O	-3.26623	-0.55943	0.32155
H	-3.89237	-1.21970	0.61798
H	-2.52933	-1.04526	-0.19830
O	1.64405	-1.83786	1.47911
H	1.28675	-1.84774	0.55153
H	1.20215	-2.53898	1.96005

I-4b:
18

C	-0.41265	-1.01700	-0.79293
O	0.83324	-1.11898	-0.58151
O	-1.29291	-1.84338	-0.51906
O	-0.84434	0.17375	-1.34464
H	-0.19983	0.89279	-1.11200
O	0.09806	2.10976	0.16538
H	0.35037	3.00042	-0.08305
Na	1.76830	0.79414	0.74697
Na	-1.98391	1.42921	0.28940
O	3.09180	0.23456	-1.09095
H	2.33925	-0.37879	-1.23140
H	3.89069	-0.27011	-1.25522
O	-3.24949	-0.39787	0.48766
H	-3.87531	-0.91289	0.99796
H	-2.62760	-1.04732	0.04559
O	1.66059	-1.20186	1.91866
H	1.27521	-1.54396	1.07924
H	1.31928	-1.74280	2.63217

D-4b:
18

C	-0.98030	1.27447	-0.55796
O	-0.45592	2.37145	-0.33008
O	-0.45426	0.21816	-0.98493
O	-2.33278	1.11845	-0.20971
H	-2.62233	1.97935	0.11495

O	0.40998	-0.40120	1.80813
H	0.70705	-0.59077	2.69868
Na	1.34348	1.18130	0.56975
Na	-1.52518	-0.89718	0.98710
O	3.17747	0.34670	-0.58433
H	2.80433	-0.55725	-0.65587
H	3.41854	0.60629	-1.47667
O	-1.60138	-2.26274	-0.90357
H	-0.89672	-2.90215	-1.04609
H	-1.26747	-1.43293	-1.29999
O	1.62903	-1.93446	-0.35552
H	0.91431	-1.30306	-0.17129
H	1.84568	-2.22244	0.53871

P-4:
18

C	2.48004	-0.13461	-0.15076
O	1.37710	-0.70129	-0.37339
O	2.64726	1.06108	0.17006
O	3.58452	-0.93211	-0.27832
H	-1.96993	0.29963	1.05490
O	-2.99945	0.42801	0.05750
H	-3.86106	0.67345	0.39880
Na	0.40338	1.44071	0.19667
Na	-0.43057	-1.68291	0.22936
O	-2.46626	-1.98060	-0.63800
H	-2.83491	-1.05470	-0.43664
H	-2.82567	-2.25388	-1.48302
O	-1.40464	2.22113	-0.90352
H	-1.59258	2.50169	-1.80010
H	-2.14659	1.59694	-0.62169
O	-1.04910	0.13704	1.55287
H	-1.20599	0.20689	2.49595
H	4.34016	-0.36423	-0.08751

R-5:
21

C	0.33190	-0.57711	0.96489
O	-0.85969	-0.03226	1.03800
O	0.43221	-1.76311	0.44200
O	1.34441	0.06883	1.34682
Na	2.77643	0.49563	-0.20693
Na	-2.53852	-0.64643	-0.21747
O	-3.02343	1.52307	-0.70581

H	-3.47784	2.13364	-1.28773
H	-2.25689	2.00857	-0.31159
O	-0.73593	2.35715	0.46423
H	-0.70819	2.91844	1.24348
H	-0.72337	1.34687	0.82812
O	2.71060	-1.65860	-0.83808
H	2.69903	-2.25724	-1.58576
H	1.86177	-1.83065	-0.31716
O	-1.73777	-2.68471	-0.56092
H	-0.85072	-2.39923	-0.13505
H	-1.88441	-3.59944	-0.31813
O	1.66572	2.37034	-0.84823
H	0.81056	2.39066	-0.34897
H	1.55275	2.96416	-1.59211

D-5a:

21

C	0.22244	0.20291	-1.07298
O	-0.94460	0.68448	-1.31703
O	1.12776	0.99256	-0.54432
O	0.50631	-1.03044	-1.25015
Na	1.87411	-0.99205	0.56343
Na	-1.75453	1.39600	0.63412
O	0.07244	-1.39161	1.94498
H	-0.06767	-1.78354	2.80909
H	-0.54582	-1.85932	1.30984
O	-1.35330	-2.44380	0.00574
H	-2.18198	-1.95494	-0.09977
H	-0.73659	-2.01969	-0.65132
O	3.64508	0.17168	-0.36127
H	2.82099	0.63777	-0.65483
H	4.14300	-0.03072	-1.15594
O	0.00916	2.69819	1.03991
H	0.53258	2.15357	0.36334
H	0.25625	3.61541	0.91488
O	-3.13916	-0.20339	-0.45652
H	-2.33921	-0.01693	-1.04893
H	-3.92112	-0.22382	-1.01216

I-5a:

21

C	0.29500	0.03135	-1.14019
O	-0.81927	0.58207	-1.45171
O	1.28026	0.79290	-0.72969

O	0.45268	-1.24321	-1.11150
Na	1.66921	-0.99574	0.78811
Na	-1.41383	1.27037	0.65456
O	-0.46245	-0.64039	1.88098
H	-0.66774	-0.80944	2.80387
H	-0.94990	-1.34988	1.33492
O	-1.53182	-2.29015	0.22281
H	-2.34523	-1.84236	-0.05408
H	-0.85414	-2.01548	-0.46479
O	3.63834	-0.26274	-0.14353
H	2.91257	0.22810	-0.60942
H	4.17853	-0.66723	-0.82530
O	0.30475	2.74604	0.68158
H	0.76916	2.12195	0.04000
H	0.39403	3.62752	0.31524
O	-3.09443	-0.02315	-0.52247
H	-2.28593	0.07847	-1.12115
H	-3.87505	0.12830	-1.05924

TS-5:

21

C	0.30760	0.08874	-1.18240
O	-0.84788	0.54616	-1.42002
O	1.29316	0.86270	-0.88354
O	0.52546	-1.21136	-1.12193
Na	1.63833	-0.82444	0.90576
Na	-1.47473	1.09706	0.77157
O	-0.46823	-0.71818	1.81530
H	-0.68486	-0.97851	2.71251
H	-0.93038	-1.53443	1.05379
O	-1.24378	-2.24794	0.11824
H	-2.12542	-1.96912	-0.15762
H	-0.43993	-1.78295	-0.65209
O	3.60638	-0.18632	-0.08553
H	2.91780	0.26670	-0.63295
H	4.17656	-0.65854	-0.69552
O	0.16855	2.69682	0.66561
H	0.66455	2.17392	-0.02322
H	0.18551	3.61028	0.37471
O	-3.16524	-0.08705	-0.49194
H	-2.39269	0.02363	-1.10848
H	-3.96380	0.07909	-0.99680

I-5b:

21

C	0.35120	0.29438	-1.24330
O	-0.82888	0.67644	-1.38687
O	1.34133	1.03271	-0.97903
O	0.62444	-1.04556	-1.29069
Na	1.60854	-1.09960	0.89036
Na	-1.38348	0.92406	0.97756
O	-0.38004	-0.89679	1.76954
H	-0.58138	-1.19694	2.65703
H	-1.10016	-1.87443	0.66514
O	-1.40899	-2.33737	-0.17468
H	-2.29299	-1.98836	-0.33173
H	-0.22541	-1.54595	-1.15803
O	3.49764	-0.15576	0.03977
H	2.86520	0.36014	-0.51976
H	4.20682	-0.44722	-0.53589
O	0.13639	2.67857	0.82668
H	0.65467	2.27388	0.09142
H	0.03045	3.60356	0.59615
O	-3.19200	0.09280	-0.39228
H	-2.46353	0.20795	-1.04287
H	-3.99563	0.41168	-0.80828

D-5b:

21

C	-0.41496	0.25342	1.25157
O	0.77127	0.56915	1.42527
O	-1.37519	1.01081	0.92795
O	-0.75453	-1.08460	1.32770
Na	-1.54384	-1.10719	-0.93608
Na	1.40842	1.02059	-0.82488
O	0.46721	-0.79609	-1.73261
H	0.70447	-1.03509	-2.62972
H	1.11599	-1.79977	-0.67520
O	1.34868	-2.31948	0.16456
H	2.18914	-2.75747	0.02140
H	0.08200	-1.59242	1.32690
O	-3.48413	-0.15322	-0.20985
H	-2.88058	0.35975	0.38359
H	-4.22147	-0.44564	0.32883
O	-0.10958	2.77349	-0.69535
H	-0.65914	2.30404	-0.02210
H	-0.02658	3.67729	-0.38544
O	3.29880	0.06091	0.26931
H	2.58846	-0.35407	0.78927

H	3.78686	0.58773	0.90790

P-5:
21

C	-1.96881	-0.98381	-0.31565
O	-1.09526	-0.29177	-0.88574
O	-1.84167	-2.09691	0.22062
O	-3.23128	-0.38519	-0.26109
Na	0.46481	-1.75157	0.12444
Na	-0.14668	1.57489	-0.05925
O	3.12740	0.41548	0.31187
H	1.93339	0.28083	1.13245
H	3.93103	0.61170	0.79643
O	1.83243	2.30986	-0.85519
H	2.47044	1.62761	-0.46078
H	2.15607	2.52184	-1.73177
O	-2.31356	2.21233	0.41714
H	-2.82031	1.42477	0.14783
H	-2.94114	2.92975	0.51822
O	2.61985	-1.97950	-0.47021
H	3.09310	-2.25563	-1.25604
H	2.97236	-1.06299	-0.21356
O	0.94689	0.13867	1.47118
H	0.95421	0.18281	2.42881
H	-3.79421	-0.99799	0.22658

R-6:
24

C	0.13427	-0.59025	-0.83358
O	1.14015	0.11642	-1.15005
O	0.27075	-1.76643	-0.30909
O	-1.06663	-0.10476	-0.98764
Na	-2.87426	-0.78953	0.03182
Na	2.42811	0.78316	0.59242
O	1.04840	2.53013	1.07305
H	0.83996	3.15891	1.76572
H	0.25395	2.49126	0.48750
O	-1.17306	2.32544	-0.52696
H	-1.06851	2.85495	-1.32199
H	-1.04114	1.32016	-0.82895
O	-1.95133	-2.73866	0.53411
H	-1.04229	-2.43309	0.17792
H	-2.00229	-3.68628	0.40621
O	2.12996	-1.31676	1.50535

H	1.45492	-1.60995	0.82353
H	1.85372	-1.70924	2.33518
O	3.77403	-0.28935	-1.03816
H	2.83582	-0.37571	-1.33076
H	4.01787	-1.16538	-0.72745
O	-3.55645	1.35894	0.33832
H	-4.14804	1.95705	0.79700
H	-2.77845	1.88905	0.03945

TS-6:
24

C	-0.42608	0.58834	-1.21267
O	-1.49551	-0.09203	-1.25248
O	-0.42670	1.83072	-0.89373
O	0.73779	0.00501	-1.42728
Na	1.98738	0.51082	0.44020
Na	-2.05156	-0.24987	0.96342
O	0.15474	-0.81524	1.59134
H	0.41720	-1.22196	2.42080
H	0.35945	-1.49590	0.86296
O	0.85626	-2.17928	-0.46624
H	0.27738	-2.87973	-0.77269
H	0.71268	-1.16773	-1.09892
O	1.81105	2.73311	0.10474
H	0.95973	2.52383	-0.38338
H	2.28515	3.37517	-0.42574
O	-2.26329	2.01612	1.00153
H	-1.64228	2.09570	0.22143
H	-2.99179	2.61407	0.82636
O	-2.38441	-2.30452	-0.21408
H	-1.99959	-1.66626	-0.86689
H	-3.14273	-2.70929	-0.64022
O	3.20081	-1.46309	0.49891
H	4.02170	-1.72740	0.07953
H	2.47971	-1.98737	0.07132

I-6b:
24

C	0.50914	0.67407	1.24331
O	1.49204	-0.10067	1.26877
O	0.54933	1.90114	0.93916
O	-0.72901	0.16874	1.49197
Na	-1.97327	0.50844	-0.51862
Na	1.95090	-0.39571	-0.99718

O	-0.24167	-0.84516	-1.51210
H	-0.51512	-1.26199	-2.33245
H	-0.51144	-1.53927	-0.70591
O	-0.99022	-2.15041	0.41941
H	-0.57479	-2.99735	0.58698
H	-0.70477	-0.82943	1.35846
O	-1.66969	2.73411	-0.23548
H	-0.84721	2.57330	0.30167
H	-2.14798	3.44459	0.19466
O	2.36276	1.86256	-1.05310
H	1.79144	2.04352	-0.26351
H	3.14702	2.40346	-0.94548
O	2.41638	-2.36851	0.21125
H	2.00709	-1.79763	0.89503
H	3.19018	-2.76414	0.61759
O	-3.31629	-1.34192	-0.36219
H	-4.08609	-1.56551	0.16323
H	-2.54620	-1.87293	0.00229

D-6b:

24

C	-0.39097	-0.76072	1.25821
O	-1.38889	-0.03193	1.37233
O	-0.34199	-1.95788	0.86769
O	0.84741	-0.19326	1.51792
Na	1.85416	-0.38827	-0.70058
Na	-1.95696	0.23919	-0.88666
O	0.11483	0.80849	-1.52299
H	0.24053	1.16825	-2.40303
H	0.37981	1.81597	-0.55032
O	0.64984	2.40499	0.29949
H	0.40765	3.31635	0.11896
H	0.68779	0.75798	1.63178
O	1.93387	-2.63865	-0.33177
H	1.11192	-2.55845	0.21612
H	2.52653	-3.22277	0.14411
O	-2.36978	-2.03646	-0.92368
H	-1.69822	-2.19043	-0.21493
H	-3.13647	-2.55801	-0.67895
O	-2.41228	2.35832	0.15784
H	-1.60639	2.13150	0.65098
H	-3.10763	2.32193	0.82094
O	3.15334	1.48480	-0.22655
H	3.81469	1.62021	0.45504
H	2.36569	2.01428	0.03749

P-6:
24

C	-2.32381	-0.04067	-0.36550
O	-2.96338	1.19220	-0.55563
O	-1.08032	0.04491	-0.26621
O	-3.06035	-1.03564	-0.31361
Na	0.46426	1.60806	0.29535
Na	0.32804	-1.71171	0.24642
O	1.51772	-0.10750	1.51380
H	-3.90863	1.00323	-0.57766
H	1.71637	-0.13351	2.45123
O	3.45247	-0.09196	-0.03470
H	4.35617	-0.14621	0.27972
H	2.43518	-0.11229	0.98805
O	2.37432	2.10665	-0.80179
H	2.93762	1.29335	-0.57942
H	2.60068	2.37184	-1.69403
O	-1.49418	-3.02648	0.50450
H	-1.85391	-3.90794	0.39985
H	-2.18405	-2.38543	0.19033
O	2.18783	-2.12976	-0.97173
H	2.81454	-1.38546	-0.69717
H	2.36567	-2.32650	-1.89220
O	-1.26267	3.10942	0.53658
H	-1.99202	2.58925	0.15082
H	-1.43160	4.02911	0.32432

R-7:
27

C	-0.00316	0.76593	-0.75498
O	-1.02296	0.08854	-1.13399
O	-0.13049	1.99307	-0.39757
O	1.16734	0.20535	-0.70894
Na	3.03619	0.92586	0.14210
Na	-2.20100	-1.22298	0.25881
O	-0.72872	-2.13083	1.76757
H	-0.46707	-1.74811	2.60731
H	0.09460	-2.20869	1.22780
O	1.32110	-2.20811	-0.01428
H	0.88099	-2.76206	-0.67278
H	1.18119	-1.24936	-0.36901
O	2.13884	2.91813	0.42755
H	1.21427	2.64005	0.10620

H	2.08265	3.83075	0.71020
O	-3.66707	0.31861	0.97215
H	-3.32026	1.18994	0.62718
H	-4.23293	0.52784	1.71650
O	-1.08741	-2.43422	-1.60671
H	-0.91258	-1.44323	-1.63970
H	-1.37911	-2.69645	-2.48229
O	3.79273	-1.20307	0.46050
H	4.48297	-1.76756	0.81152
H	3.01608	-1.77935	0.27163
O	-2.66734	2.58342	0.01219
H	-1.69966	2.37656	-0.15797
H	-3.03748	2.71533	-0.86448

TS-7:

27

C	-0.35873	0.48187	-1.25713
O	-1.05564	-0.58363	-1.27930
O	-0.88637	1.63477	-1.12205
O	0.95761	0.41096	-1.31382
Na	1.93414	1.25862	0.58995
Na	-1.26384	-1.41950	0.84434
O	0.86707	-0.79973	1.64275
H	1.28191	-1.11728	2.44849
H	1.35073	-1.25679	0.86182
O	1.98384	-1.58974	-0.49372
H	1.65611	-2.43593	-0.81100
H	1.41323	-0.68079	-1.04226
O	0.71838	3.11058	0.32958
H	0.07090	2.67442	-0.30140
H	0.25777	3.84413	0.73822
O	-3.08381	-0.37678	1.61809
H	-3.25344	0.34016	0.94219
H	-3.48333	-0.08083	2.43715
O	-0.57649	-3.08266	-0.77280
H	-0.66974	-2.21145	-1.24469
H	-1.06045	-3.73240	-1.28695
O	3.86938	-0.01293	0.46538
H	4.68772	0.14316	-0.01000
H	3.42183	-0.77074	0.01773
O	-3.36318	1.47354	-0.24691
H	-2.43884	1.54475	-0.63080
H	-3.90157	1.14293	-0.97055

I-7b:

27

C	0.42113	-0.55595	-1.28536
O	1.05213	0.53043	-1.28390
O	0.92911	-1.70153	-1.14589
O	-0.93175	-0.52726	-1.38823
Na	-1.94322	-1.17280	0.67525
Na	1.18625	1.44950	0.84951
O	-0.91452	0.83768	1.55271
H	-1.33460	1.17964	2.34515
H	-1.42939	1.29735	0.69337
O	-2.04851	1.58110	-0.47576
H	-1.91771	2.49230	-0.74352
H	-1.27838	0.41695	-1.26181
O	-0.72038	-3.05087	0.44782
H	-0.07183	-2.69830	-0.21852
H	-0.27061	-3.74783	0.92742
O	3.04444	0.43643	1.61130
H	3.23951	-0.29731	0.96784
H	3.42118	0.16757	2.45059
O	0.72104	3.12928	-0.76868
H	0.70078	2.29435	-1.28507
H	1.28930	3.73277	-1.25218
O	-3.90443	-0.01629	0.37901
H	-4.66994	-0.18393	-0.17332
H	-3.41051	0.74907	-0.03292
O	3.40363	-1.50553	-0.17721
H	2.50424	-1.59464	-0.59571
H	3.98163	-1.22352	-0.89073

D-7b:
27

C	0.41618	-0.61387	-1.27710
O	0.96154	0.50163	-1.34911
O	0.95178	-1.73126	-1.06086
O	-0.96318	-0.66058	-1.38703
Na	-1.77540	-1.16508	0.85707
Na	1.13697	1.43227	0.77753
O	-0.90917	0.83663	1.50755
H	-1.21620	1.18030	2.34863
H	-1.61134	1.44840	0.46186
O	-2.11379	1.71431	-0.45615
H	-2.34984	2.64420	-0.42186
H	-1.27773	0.25921	-1.45463
O	-0.63622	-3.10736	0.58856

H	-0.00707	-2.75798	-0.09360
H	-0.15007	-3.75506	1.10123
O	3.15422	0.63154	1.42354
H	3.34720	-0.13129	0.81806
H	3.58329	0.42943	2.25662
O	0.46054	3.28125	-0.59886
H	-0.09466	2.60241	-1.01404
H	1.13169	3.47334	-1.26032
O	-3.83732	-0.28187	0.23961
H	-4.41579	-0.60789	-0.45329
H	-3.42863	0.54365	-0.10506
O	3.48707	-1.41729	-0.26453
H	2.56618	-1.55706	-0.61048
H	4.00491	-1.16346	-1.03276

P-7:

27

C	2.22115	1.14976	-0.29345
O	3.43869	0.45520	-0.24988
O	1.22149	0.43351	-0.06826
O	2.29473	2.36134	-0.54078
H	4.12857	1.10975	-0.40764
O	-1.23521	-1.02681	1.27673
H	-1.76415	-0.77193	2.03623
Na	0.79193	-1.73010	0.45897
Na	-0.97846	1.14214	0.16304
O	-2.55380	-1.98406	-0.65647
H	-3.31101	-2.55612	-0.52139
H	-1.87367	-1.47662	0.60665
O	-0.23288	-3.01140	-1.11131
H	-1.19406	-2.70386	-1.04238
H	-0.04571	-3.12699	-2.04402
O	-0.21325	3.22349	-0.34719
H	-0.32004	4.17498	-0.34408
H	0.75489	3.03505	-0.45675
O	-2.88509	0.45920	-1.09743
H	-2.84786	-0.57541	-1.01691
H	-3.18034	0.67915	-1.98221
O	3.02434	-2.02489	0.94462
H	3.36338	-1.19658	0.55708
H	3.66737	-2.70789	0.74511
O	-3.07261	1.40826	1.42448
H	-3.56371	2.19937	1.65589
H	-3.38008	1.13534	0.53698

R-8:
30

C	-0.02836	0.92601	-0.77738
O	-1.06426	0.19231	-0.98593
O	-0.17596	2.18838	-0.58409
O	1.14913	0.39669	-0.73889
O	-2.68264	2.83515	-0.12509
H	-1.72618	2.59256	-0.31936
H	-3.08862	2.92286	-0.99113
Na	2.97329	1.35211	0.01902
Na	-2.24799	-0.89889	0.55391
O	-3.69617	0.72012	1.10878
H	-4.24037	1.02612	1.83560
H	-3.34584	1.53902	0.65441
O	-0.75181	-1.84762	1.99528
H	-0.57232	-1.65094	2.91656
H	0.12664	-1.85050	1.53522
O	1.50164	-1.79928	0.52099
H	1.37657	-2.59460	-0.03608
H	1.27437	-1.00117	-0.06680
O	0.64254	-3.89999	-1.05860
H	-0.16187	-3.37402	-1.26593
H	0.33374	-4.65347	-0.54943
O	3.82652	-0.52692	0.94561
H	3.07960	-1.16904	0.84795
H	4.60450	-1.02746	1.19434
O	-1.49756	-2.23639	-1.46212
H	-1.95121	-2.33555	-2.30271
H	-1.14766	-1.27765	-1.43728
O	2.06546	3.35958	-0.06390
H	1.14523	2.98751	-0.28205
H	1.95024	4.26869	0.21234

TS-8:
30

C	-0.67671	0.28636	-1.28174
O	-0.70907	-0.97358	-1.10423
O	-1.73628	0.98641	-1.36054
O	0.48030	0.92125	-1.32835
O	-3.85228	-0.29101	-0.45858
H	-3.05942	0.17881	-0.85445
H	-4.13969	-0.90639	-1.13763
Na	0.69207	2.36417	0.48628
Na	-0.67276	-1.51244	1.12021

O	-2.84446	-1.51922	1.65344
H	-3.41714	-1.37767	2.40864
H	-3.28782	-1.07729	0.87456
O	0.79980	0.14607	1.79685
H	1.25405	0.23018	2.63844
H	1.53316	-0.02217	1.07492
O	2.34938	0.00373	-0.15415
H	2.81851	-0.80512	-0.40728
H	1.39731	0.33182	-0.89854
O	3.34158	-2.64097	-0.69369
H	2.41828	-2.92320	-0.54887
H	3.85807	-3.05022	0.00427
O	2.98290	2.41054	0.62237
H	3.01322	1.48144	0.26094
H	3.63874	2.91972	0.14272
O	0.60399	-3.03484	-0.34431
H	0.23139	-3.81725	-0.75929
H	0.25866	-2.25424	-0.86786
O	-1.29239	3.22776	-0.06343
H	-1.55403	2.46464	-0.65598
H	-2.10310	3.65076	0.22137

I-8b:

30

C	-0.78775	0.39096	-1.29543
O	-0.79608	-0.86040	-1.18450
O	-1.79476	1.14041	-1.27218
O	0.41045	1.03186	-1.39794
O	-3.93982	-0.25075	-0.44833
H	-3.17576	0.27517	-0.80095
H	-4.19302	-0.83268	-1.16936
Na	0.77412	2.17974	0.76622
Na	-0.61538	-1.39770	1.13771
O	-2.82669	-1.59911	1.57629
H	-3.35380	-1.44763	2.36298
H	-3.29470	-1.12673	0.83832
O	0.88705	0.11560	1.69863
H	1.28975	0.09648	2.56871
H	1.95202	-0.16212	0.61171
O	2.52153	-0.13955	-0.24213
H	2.94123	-1.01055	-0.34877
H	1.15028	0.39753	-1.23944
O	3.22631	-2.84822	-0.52075
H	2.27300	-3.05457	-0.48009
H	3.62775	-3.29019	0.23114

O	3.04067	2.44452	0.30840
H	3.13738	1.50367	0.03735
H	3.46158	2.96721	-0.37723
O	0.44023	-3.02827	-0.42057
H	-0.01181	-3.79568	-0.78091
H	0.12698	-2.25350	-0.95076
O	-1.15613	3.25488	0.24212
H	-1.49849	2.59810	-0.41424
H	-1.55426	4.09956	0.02860

D-8b:
30

C	-1.03034	-0.30851	1.26474
O	-0.67214	0.88286	1.31977
O	-2.18373	-0.76191	1.04996
O	-0.05316	-1.27721	1.39404
O	-3.84327	1.23194	0.36100
H	-3.26315	0.48135	0.65356
H	-3.97311	1.76495	1.14958
Na	0.15859	-2.22524	-0.85761
Na	-0.27392	1.62347	-0.85112
O	-2.28784	2.48624	-1.41231
H	-2.76588	2.58888	-2.23713
H	-2.92288	2.06546	-0.77462
O	0.81961	-0.18185	-1.58054
H	1.23790	-0.17130	-2.44327
H	1.83319	-0.18962	-0.50234
O	2.37155	-0.29387	0.38944
H	3.19238	0.21755	0.30660
H	0.80549	-0.81829	1.43845
O	4.27548	1.84583	0.18939
H	3.46549	2.37754	0.26542
H	4.69677	2.11392	-0.63069
O	2.28489	-2.94739	-0.23963
H	2.54341	-2.05355	0.08054
H	2.53631	-3.56516	0.45015
O	1.55986	2.50199	0.55689
H	1.12725	2.98782	1.26626
H	1.53210	1.57334	0.85485
O	-2.00120	-2.87160	-0.57733
H	-2.21449	-2.18428	0.10346
H	-2.54041	-3.63828	-0.37867

P-8:
30

C	0.87935	2.29319	0.30756
O	-0.01970	3.29420	0.69363
O	0.33353	1.23354	-0.06544
O	2.08309	2.58603	0.38506
H	0.51315	4.06252	0.92815
O	-0.53191	-1.54375	-1.23201
H	-0.96903	-1.91654	-2.00040
Na	-1.74663	0.33584	-0.37761
Na	1.52712	-0.69097	-0.58652
O	-0.90565	-2.79437	0.93244
H	-1.06516	-3.73919	0.96056
H	-0.70822	-2.18630	-0.44707
O	-2.78661	-1.15735	1.18518
H	-2.07255	-1.91026	1.18290
H	-3.11207	-1.06749	2.08202
O	3.49459	0.63743	-0.72262
H	4.00118	0.99166	-1.45628
H	3.06622	1.42047	-0.28157
O	1.42502	-1.88287	1.49545
H	0.51577	-2.32238	1.38821
H	1.44643	-1.49471	2.37212
O	-2.56077	2.50295	-0.12597
H	-1.75746	2.95167	0.19442
H	-3.30185	2.90550	0.33021
O	3.35616	-2.29664	-0.49969
H	3.91925	-1.52280	-0.37520
H	2.96561	-2.46429	0.37252
O	-3.64816	-0.81735	-1.35510
H	-4.53150	-0.52355	-1.58681
H	-3.68802	-1.13163	-0.43103