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

Catalytic Polymerization of Naphthalene by HF/BF_3 Super Acid:

An Ab Initio Density Functional Theory Study

Po-Yu Yang, [a] ***Hsing-Yin Chen,*** [b] ***Shin-Pon Ju,*** [a,b*] ***Chia-Lin Chang*** [c] ***and Gao-Shee Le*** [c]

[a] *Department of Mechanical and Electro-Mechanical Engineering, National Sun Yat-sen University, Kaohsiung, Taiwan*

[b] *Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan*

[c] *Refining & Manufacturing Research Institute, CPC Corporation, Chiayi City, Taiwan*

**Corresponding Author: jushin-pon@mail.nsysu.edu.tw*

Supporting Information

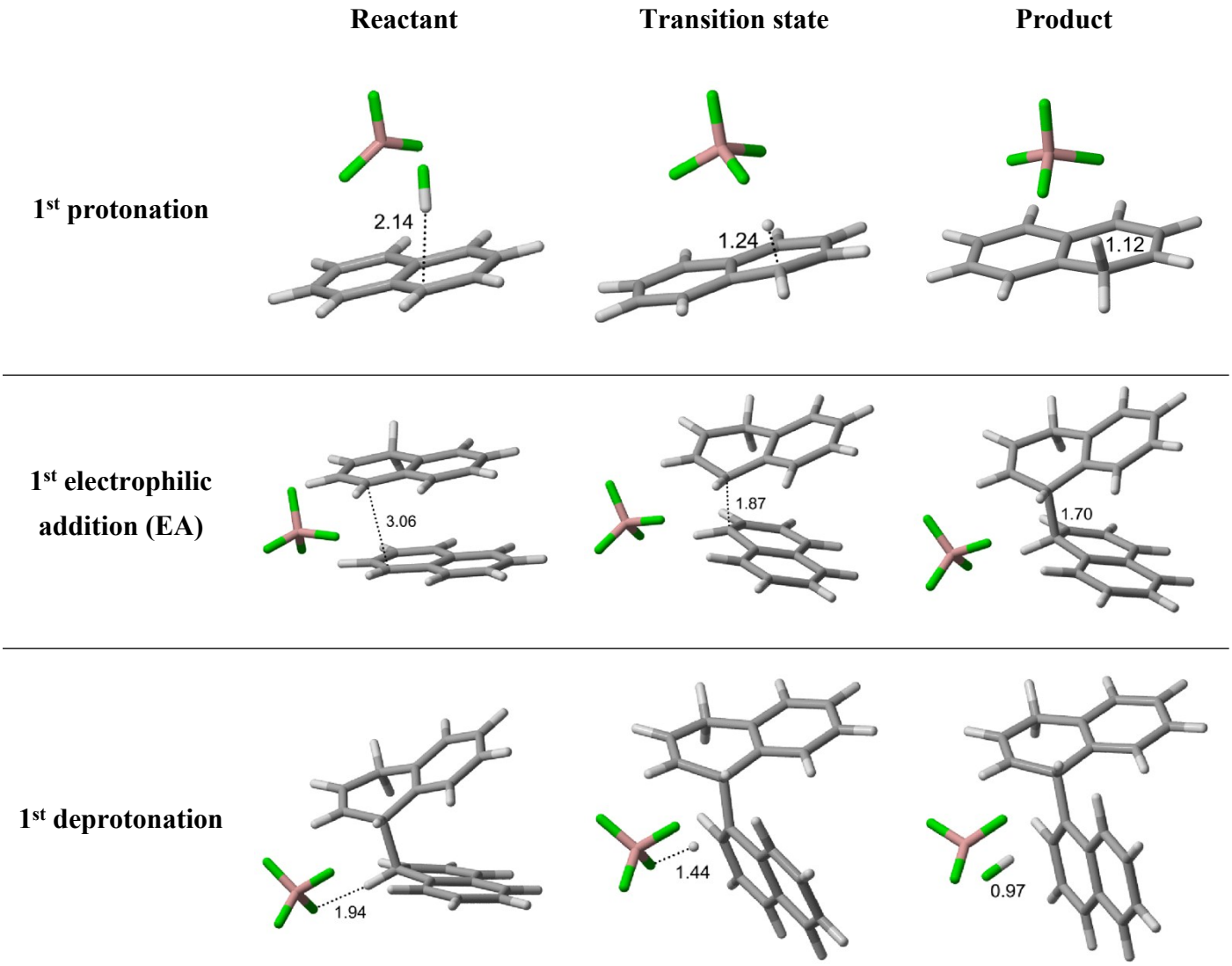
Obtaining Transition State Structure

For verifying the TS structures by the simple scanning approach are identical to those by the synchronous transit-guided quasi-Newton (STQN) method [1], the benchmark test has been conducted for the TS structure of naphthalene protonation. The TS structures obtained by these two methods are identical, revealing the simple scanning approach is both efficient and reliable for the TS search in this study. Intrinsic reaction coordinate (IRC) calculations [2] were performed for each TS to confirm that they connect to the corresponding intermediates. However, the IRC calculations for the transition state could sometimes be difficult to reach the convergence criterion and show relatively lower efficient. In this case, we used the visualization program GaussView [3] to change the TS structure a little bit along the imaginary vibrational vector and reoptimized the geometry to obtain reactant and product. The connectivity between each TS's reactant and product have been further confirmed by using GaussView. The reactant and product of protonation, electrophilic addition and deprotonation in activation stage have been both calculated by IRC and our method. The results show that the structures of intermediates from IRC are identical with that from the method used in the current study.

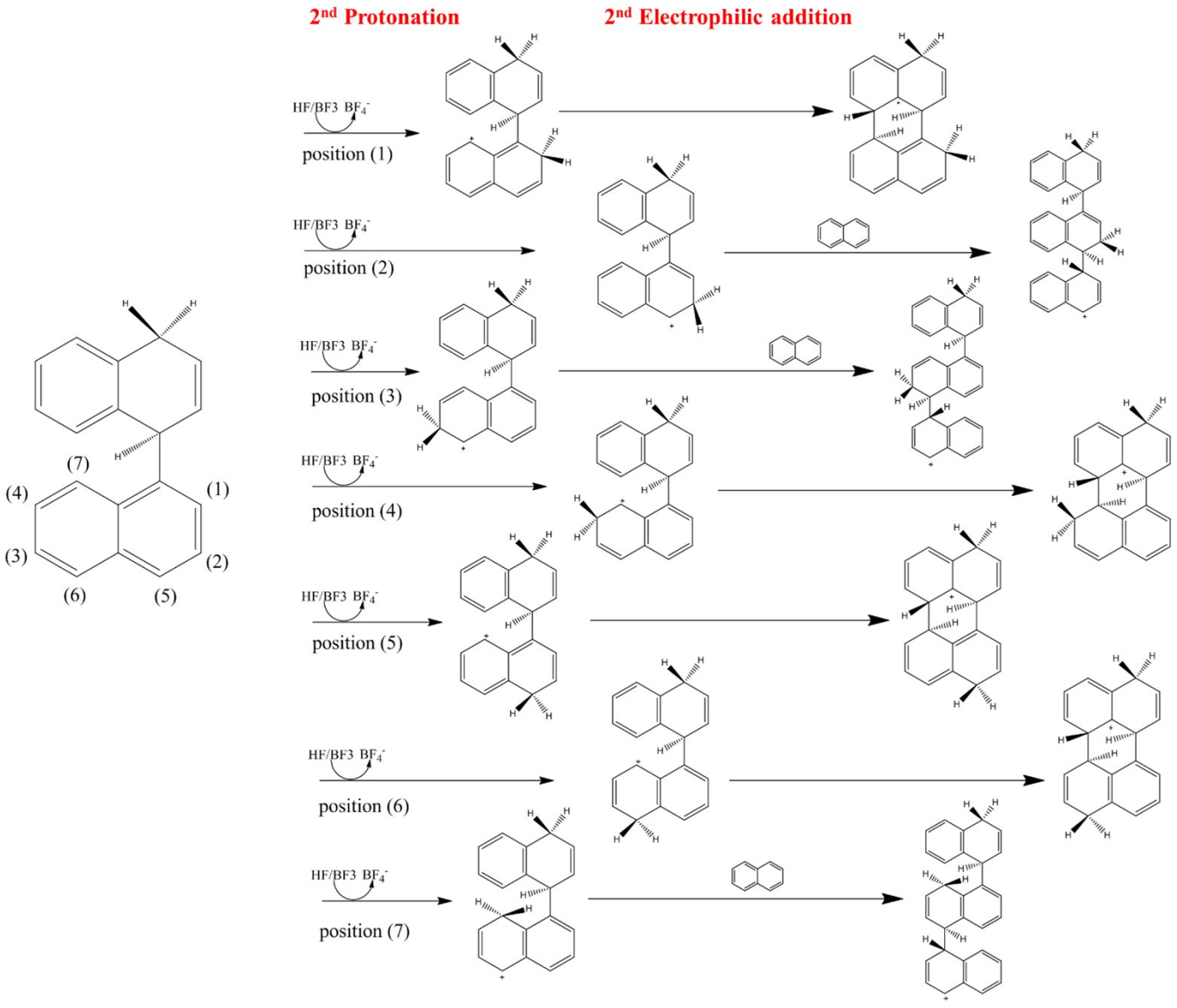
[1] P. Chunyang and B. S. H., "Combining Synchronous Transit and Quasi-Newton Methods to Find Transition States," *Israel Journal of Chemistry,* vol. 33, pp. 449-454, 1993.

[2] K. Fukui, "Formulation of the reaction coordinate," *The Journal of Physical Chemistry,* vol. 74, pp. 4161-4163, 1970.

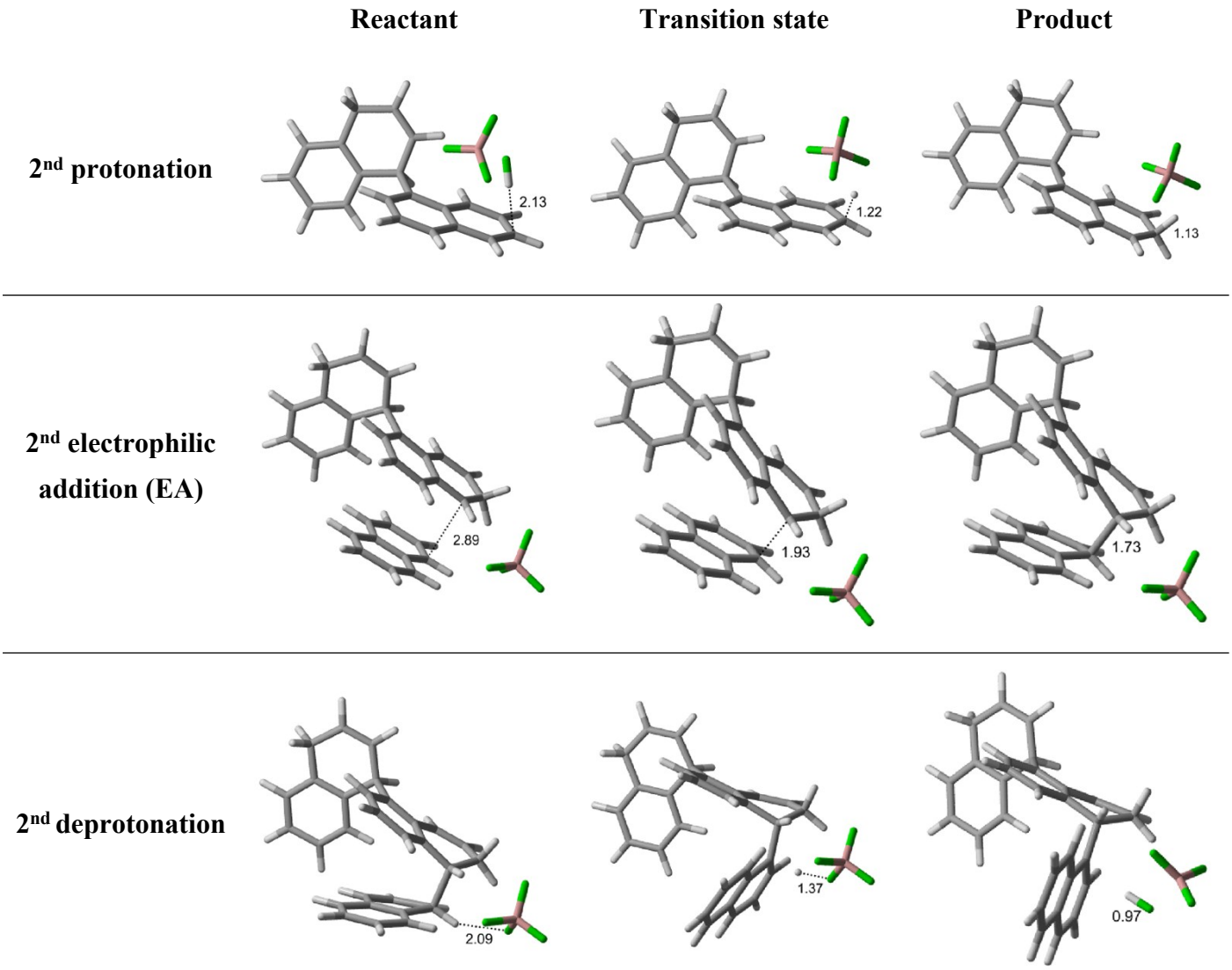
[3] T. A. K. Roy Dennington, John M. Millam, "GaussView, Version 5," ed: Semichem Inc., Shawnee Mission, KS, 2009.



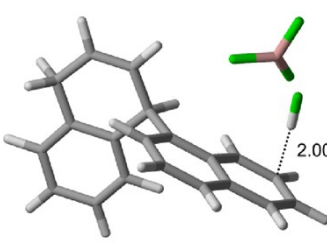
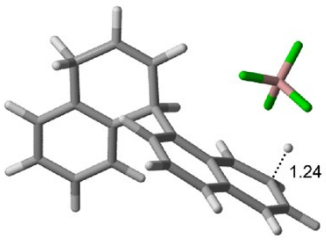
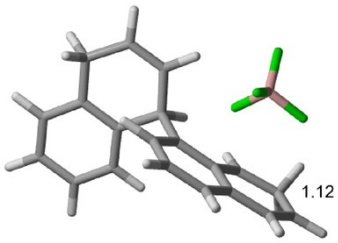
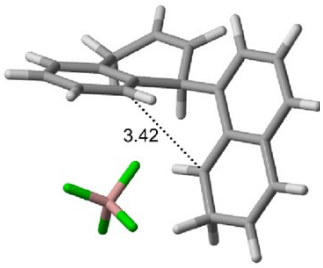
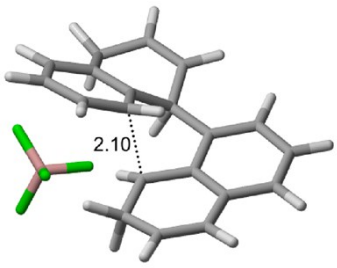
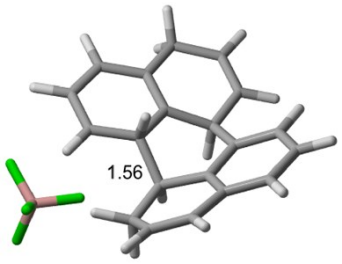
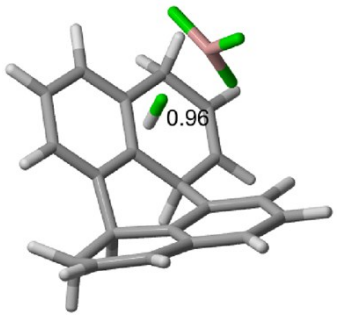
Supplementary Figure S1: All molecular structures of reactants, transition states and products in activation stage.



Supplementary Figure S2: Second protonation products at seven different additional sites on $C_{10}H_9(C_{10}H_7)$ and which follow the second electrophilic addition pathways.



Supplementary Figure S3: All molecular structures of reactants, transition states and products in chain elongation pathway A.

	Reactant	Transition state	Product
2nd protonation			
2nd electrophilic addition (EA)			
2nd deprotonation (no energy barrier)	–	–	

Supplementary Figure S4: All molecular structures of reactants, transition states and products in intramolecular cyclization pathway B.

Supplementary Table S1: Unscaled imaginary vibrational frequency of all transition state structure of naphthalene polymerization. Geometric optimization and vibrational frequency were calculated in M06-2X/6-31G(d) level.

Transition State	Unscaled Imaginary Frequency (cm^{-1})
TS-AB	-490.8984
TS-BC	-212.7717
TS-CD	-320.7164
TS-DE	-293.0561
TS-EF	-222.9397
TS-FG	-597.7080
TS-DH	-448.3683
TS-HI	-265.1043

Supplementary Appendix: The geometries of intermediates and transition states are shown in XYZ file format, the unit is Å

24			
1st protonation reactant			
B	2.17826	-0.54092	-0.02635
F	1.27027	-1.27233	-0.65784
F	1.96750	-0.19808	1.23767
F	3.41002	-0.48537	-0.51053
F	1.62157	1.22387	-0.84562
H	0.68557	1.35726	-0.93864
C	-0.74399	2.46777	0.89859
C	-0.74420	1.24345	1.51659
C	-1.09986	0.06525	0.80717
C	-1.45808	0.16586	-0.56653
C	-1.44263	1.44705	-1.18741
C	-1.09590	2.57225	-0.47190
H	-0.79341	-1.28496	2.46741
H	-0.46186	3.35938	1.44833
H	-0.45420	1.15321	2.55974
C	-1.08306	-1.21389	1.42253
C	-1.79939	-1.01248	-1.28096
H	-1.71189	1.52322	-2.23773
H	-1.08547	3.54272	-0.95816
C	-1.78091	-2.23241	-0.65744
C	-1.41595	-2.33468	0.70814
H	-2.07175	-0.92883	-2.32974
H	-2.04127	-3.12953	-1.21022
H	-1.39743	-3.30976	1.18492

24			
1st protonation TS			
B	-1.89301	-0.87652	-0.26503
F	-0.78607	-1.69330	-0.38110
F	-1.73515	0.28952	-1.00514
F	-3.06988	-1.52102	-0.54248
F	-1.95460	-0.43257	1.14576
H	-0.96620	0.56614	1.28063
C	-0.04113	2.66210	-0.52425
C	0.77098	1.75273	-1.18856
C	1.30798	0.60411	-0.56662
C	1.01338	0.36347	0.80140
C	0.05871	1.23878	1.46617
C	-0.36707	2.42511	0.80116
H	2.35053	-0.10927	-2.32372
H	-0.42658	3.53266	-1.04128
H	1.00778	1.92101	-2.23685
C	2.14286	-0.29725	-1.27440
C	1.56017	-0.76361	1.43590
H	0.07010	1.25221	2.55764
H	-1.01920	3.11144	1.33387
C	2.37652	-1.61822	0.72928
C	2.66634	-1.39135	-0.63500
H	1.32719	-0.95488	2.47905
H	2.80036	-2.48661	1.22391
H	3.29992	-2.08891	-1.17202

24			
1st protonation product			
B	-1.95174	-0.46237	-0.25368
F	-1.03785	-1.40955	-0.72112
F	-1.54063	0.82151	-0.67494
F	-3.22970	-0.73000	-0.71188
F	-1.93801	-0.46633	1.16561
H	-0.76009	1.06326	1.51970
C	0.79415	2.67910	-0.57906
C	1.29922	1.51616	-1.18525
C	1.40305	0.27952	-0.53032
C	0.95937	0.17754	0.81531
C	0.31749	1.34907	1.45591
C	0.33494	2.60457	0.70572
H	2.26492	-0.75505	-2.22632
H	0.75704	3.60661	-1.13737
H	1.63397	1.57122	-2.21940
C	1.93985	-0.85222	-1.19467
C	1.05269	-1.04915	1.46715
H	0.62037	1.49048	2.50125
H	-0.07944	3.48530	1.18899
C	1.58230	-2.14162	0.80132
C	2.02981	-2.04951	-0.53088
H	0.68554	-1.14809	2.48346
H	1.64535	-3.09641	1.31442
H	2.42956	-2.92693	-1.02677

42

1st EA reactant

H	-4.12631	1.22020	-1.85453
C	-0.53295	3.23303	0.33053
H	-0.70823	4.21799	-0.13227
C	0.92146	3.08957	0.57828
H	1.39675	3.86455	1.17408
C	1.65210	2.05254	0.09668
H	2.71194	1.93306	0.28560
C	1.00236	1.05600	-0.67663
H	1.59538	0.22668	-1.05735
C	-0.36451	1.11623	-1.01229
C	-1.16694	2.16805	-0.50378
H	-3.15682	2.98308	-0.42833
C	-2.52492	2.18829	-0.81450
C	-3.06618	1.19395	-1.62043
H	-2.72280	-0.60893	-2.76344
C	-2.27320	0.15822	-2.14304
H	-0.29319	-0.68628	-2.19965
C	-0.93371	0.11135	-1.83402
H	-1.04574	3.30266	1.30267
H	1.60025	0.01236	2.34120
C	-1.17477	-2.69936	-0.13129
H	-0.32773	-3.28378	-0.48200
C	-2.45209	-2.99176	-0.54550
H	-2.62775	-3.81799	-1.22763
C	-3.54594	-2.22209	-0.08390
H	-4.55135	-2.46699	-0.41315
C	-3.33921	-1.16944	0.77548
H	-4.17622	-0.57188	1.12938
C	-2.03225	-0.84411	1.21752
C	-0.93128	-1.62607	0.76509
H	1.23217	-1.83884	0.79487
C	0.38222	-1.28775	1.18676
C	0.58632	-0.23565	2.04862
H	-0.32919	1.36357	3.19256
C	-0.50653	0.53770	2.50843
H	-2.62713	0.84641	2.43197
C	-1.78309	0.24961	2.09217
B	3.70029	-0.77235	-0.37537
F	2.65956	-1.53392	-0.96207
F	3.32166	-0.45255	0.94195
F	4.88673	-1.47695	-0.39323
F	3.81572	0.42964	-1.10021

42

1st EA TS

H	5.01599	-1.55587	-1.40729
C	1.08085	-3.18061	0.51592
H	1.47699	-4.18266	0.31865
C	-0.39241	-3.12942	0.24024
H	-0.97452	-4.02404	0.44299
C	-0.99559	-2.02327	-0.20896
H	-2.06587	-1.98209	-0.38859
C	-0.20751	-0.80582	-0.49190
H	-0.70341	-0.14077	-1.19708
C	1.23864	-1.00068	-0.73832
C	1.87466	-2.15162	-0.24837
H	3.72487	-3.23370	-0.12622
C	3.23507	-2.33582	-0.49451
C	3.95918	-1.39446	-1.21813
H	3.88510	0.47611	-2.29051
C	3.32623	-0.25463	-1.71499
H	1.46964	0.82383	-1.85780
C	1.97258	-0.06201	-1.47490
H	1.23427	-3.01826	1.59871
H	-0.33593	-1.22662	2.39955
C	-0.52881	2.46137	-0.40019
H	-1.52943	2.19919	-0.73129
C	0.11141	3.59581	-0.85915
H	-0.40116	4.25408	-1.55381
C	1.42251	3.91730	-0.44274
H	1.90348	4.81160	-0.82456
C	2.08116	3.09982	0.44278
H	3.08986	3.33042	0.77387
C	1.44107	1.93538	0.93747
C	0.12837	1.61299	0.50759
H	-1.56079	0.29738	0.90717
C	-0.47053	0.36007	0.94574
C	0.17222	-0.35389	1.99713
H	1.96450	-0.63464	3.15865
C	1.45380	-0.03060	2.41704
H	3.10640	1.31075	2.15285
C	2.08587	1.07450	1.85879
B	-3.86591	-0.13501	-0.26371
F	-2.80423	0.49685	-0.97573
F	-3.43148	-0.30580	1.06712
F	-4.99382	0.65939	-0.30930
F	-4.09302	-1.38781	-0.83541

42

1st EA product

H	5.13403	-1.47429	-1.32650
C	1.20850	-3.19348	0.52774
H	1.62165	-4.18226	0.29861
C	-0.26651	-3.16519	0.24322
H	-0.83162	-4.07318	0.43591
C	-0.88883	-2.07664	-0.21212
H	-1.95907	-2.06657	-0.40019
C	-0.14117	-0.81069	-0.47921
H	-0.61973	-0.25625	-1.28815
C	1.33022	-0.99668	-0.71610
C	1.98144	-2.13453	-0.22257
H	3.84895	-3.18267	-0.07838
C	3.34976	-2.29115	-0.45056
C	4.07121	-1.33397	-1.15484
H	3.97348	0.53954	-2.21923
C	3.42237	-0.20602	-1.65488
H	1.54684	0.83079	-1.83092
C	2.05939	-0.04484	-1.43702
H	1.36698	-3.06203	1.61261
H	-0.20314	-1.26511	2.32251
C	-0.61556	2.35299	-0.56313
H	-1.55557	1.98072	-0.95992
C	-0.07895	3.55786	-0.98350
H	-0.61353	4.14817	-1.72136
C	1.14763	4.03726	-0.47573
H	1.54680	4.98042	-0.83242
C	1.82394	3.30949	0.47282
H	2.76481	3.66246	0.88524
C	1.28439	2.08006	0.93154
C	0.06279	1.59265	0.39746
H	-1.52132	0.19763	0.84876
C	-0.42483	0.26382	0.80175
C	0.22192	-0.33747	1.94664
H	1.90140	-0.35225	3.28604
C	1.39233	0.15774	2.47661
H	2.87961	1.70024	2.32025
C	1.93153	1.32916	1.93617
B	-3.84829	-0.26209	-0.23585
F	-2.80269	0.27810	-1.03990
F	-3.39015	-0.26063	1.09951
F	-4.97997	0.51847	-0.36011
F	-4.07926	-1.57562	-0.64166

42

1st deproton reactant

H	5.13403	-1.47429	-1.32648
C	1.20850	-3.19348	0.52775
H	1.62164	-4.18227	0.29862
C	-0.26651	-3.16519	0.24321
H	-0.83163	-4.07318	0.43590
C	-0.88883	-2.07664	-0.21213
H	-1.95907	-2.06658	-0.40020
C	-0.14116	-0.81069	-0.47921
H	-0.61972	-0.25625	-1.28817
C	1.33023	-0.99668	-0.71610
C	1.98144	-2.13454	-0.22256
H	3.84895	-3.18268	-0.07837
C	3.34976	-2.29115	-0.45055
C	4.07121	-1.33398	-1.15482
H	3.97350	0.53953	-2.21922
C	3.42238	-0.20603	-1.65487
H	1.54685	0.83078	-1.83092
C	2.05940	-0.04485	-1.43702
H	1.36698	-3.06203	1.61261
H	-0.20314	-1.26511	2.32250
C	-0.61555	2.35299	-0.56314
H	-1.55555	1.98072	-0.95994
C	-0.07894	3.55786	-0.98352
H	-0.61352	4.14816	-1.72138
C	1.14763	4.03727	-0.47573
H	1.54680	4.98043	-0.83242
C	1.82393	3.30950	0.47282
H	2.76480	3.66247	0.88526
C	1.28439	2.08006	0.93154
C	0.06279	1.59265	0.39745
H	-1.52132	0.19763	0.84875
C	-0.42483	0.26382	0.80174
C	0.22192	-0.33747	1.94663
H	1.90138	-0.35224	3.28606
C	1.39232	0.15775	2.47662
H	2.87959	1.70026	2.32027
C	1.93152	1.32917	1.93618
B	-3.84829	-0.26209	-0.23585
F	-2.80269	0.27810	-1.03990
F	-3.39013	-0.26067	1.09950
F	-4.97996	0.51849	-0.36006
F	-4.07929	-1.57561	-0.64169

42

1st deproton TS

H	5.60222	1.49095	-0.71181
C	3.02406	-2.10594	0.74862
H	3.87083	-2.75132	0.48373
C	1.73576	-2.81154	0.43820
H	1.67111	-3.86159	0.71322
C	0.69600	-2.22171	-0.14812
H	-0.21327	-2.78149	-0.35210
C	0.69296	-0.76597	-0.53674
H	0.21542	-0.68401	-1.51499
C	2.08710	-0.16411	-0.59731
C	3.17132	-0.78017	0.03643
H	5.26911	-0.65773	0.47213
C	4.42822	-0.16906	-0.01505
C	4.61780	1.03412	-0.68122
H	3.67508	2.57561	-1.85974
C	3.53922	1.64161	-1.32335
H	1.44845	1.51169	-1.78568
C	2.28820	1.04080	-1.28010
H	3.11132	-1.95729	1.83629
H	0.73780	-0.93646	2.13366
C	-1.25809	1.51444	-1.29850
H	-1.08289	0.75980	-2.05395
C	-1.91780	2.67702	-1.63533
H	-2.22367	2.83336	-2.66500
C	-2.21720	3.66037	-0.66817
H	-2.74365	4.56264	-0.95996
C	-1.85823	3.45512	0.63870
H	-2.09700	4.18507	1.40688
C	-1.17418	2.26922	1.01198
C	-0.84568	1.29121	0.03017
H	-1.16200	-0.65127	0.66959
C	-0.17191	0.05986	0.46113
C	0.20476	-0.03707	1.83174
H	0.08370	0.76048	3.82861
C	-0.16221	0.90685	2.78360
H	-1.09352	2.80873	3.09266
C	-0.82098	2.04805	2.36431
B	-2.75380	-2.03862	-0.42652
F	-2.05905	-1.29519	-1.38659
F	-2.27182	-1.53905	0.87010
F	-4.10506	-1.82210	-0.48842
F	-2.41460	-3.37396	-0.50251

42

1st deproton product

H	5.82120	1.73848	-0.31408
C	3.30553	-2.08311	0.52812
H	4.10926	-2.68281	0.08102
C	1.98134	-2.71826	0.22934
H	1.89585	-3.78679	0.41350
C	0.93125	-2.05072	-0.24149
H	0.00095	-2.57818	-0.43793
C	0.92861	-0.56929	-0.52234
H	0.53583	-0.43988	-1.53526
C	2.32200	0.04706	-0.46128
C	3.41941	-0.65733	0.04149
H	5.52066	-0.58836	0.47280
C	4.67018	-0.03128	0.08526
C	4.84159	1.27232	-0.35755
H	3.86381	2.99344	-1.21704
C	3.74703	1.97421	-0.86198
H	1.64857	1.91327	-1.29372
C	2.50295	1.36143	-0.90929
H	3.49164	-2.11905	1.61184
H	0.72171	-0.95773	2.10430
C	-1.02840	1.62772	-1.33097
H	-0.48161	1.11162	-2.11142
C	-1.87360	2.65015	-1.68079
H	-1.97630	2.92883	-2.72469
C	-2.61978	3.33808	-0.69640
H	-3.28509	4.14427	-0.98837
C	-2.50369	2.97801	0.62002
H	-3.07497	3.49132	1.38873
C	-1.63495	1.92671	1.01456
C	-0.86998	1.23559	0.02698
H	-1.59623	-0.99882	0.99974
C	0.00277	0.17219	0.44783
C	0.06182	-0.15239	1.79198
H	-0.62653	0.24713	3.80847
C	-0.70269	0.53825	2.76612
H	-2.12652	2.09523	3.11426
C	-1.53033	1.55749	2.38240
B	-2.73100	-2.07749	-0.73917
F	-1.89666	-1.27263	-1.42138
F	-2.48051	-1.38019	0.90833
F	-4.04030	-1.86878	-0.85292
F	-2.30407	-3.32569	-0.51273

42

2nd proton reactant (pathway A)

H	-6.46516	-0.56651	1.04446
C	-3.12970	2.22220	-0.62085
H	-3.86058	2.69784	-1.28918
C	-1.78277	2.20611	-1.27758
H	-1.40498	3.15906	-1.64055
C	-1.03861	1.11323	-1.41830
H	-0.05228	1.18266	-1.87362
C	-1.43657	-0.25178	-0.90702
H	-1.40968	-0.96172	-1.74459
C	-2.85024	-0.29299	-0.35810
C	-3.63516	0.85426	-0.22574
H	-5.54343	1.63155	0.37873
C	-4.93538	0.73452	0.28145
C	-5.45460	-0.49647	0.65366
H	-5.06392	-2.61461	0.80196
C	-4.67042	-1.64340	0.51804
H	-2.76102	-2.42108	-0.08537
C	-3.38241	-1.53352	0.01589
H	-3.09156	2.86883	0.26772
H	-1.53339	-0.09035	1.79480
C	1.17610	-1.44405	-1.70929
H	0.42439	-1.25093	-2.46662
C	2.40472	-1.91082	-2.10601
H	2.60549	-2.08683	-3.15764
C	3.42464	-2.14366	-1.14865
H	4.39895	-2.49831	-1.46961
C	3.17093	-1.91915	0.18597
H	3.94515	-2.08627	0.92992
C	1.89857	-1.46033	0.62482
C	0.87971	-1.19795	-0.33804
H	3.39522	-0.02960	-0.92611
C	-0.38144	-0.68561	0.10883
C	-0.58007	-0.48349	1.45356
H	0.22826	-0.58556	3.45744
C	0.42761	-0.76225	2.40507
H	2.44086	-1.42498	2.71824
C	1.64769	-1.23120	2.00177
B	2.95618	1.79292	0.65045
F	1.63929	1.65540	0.70429
F	3.21822	0.89277	-1.08631
F	3.46968	2.96053	0.28811
F	3.72294	0.94355	1.33511

42

2nd proton TS (pathway A)

H	6.71510	-0.74587	-0.58656
C	3.33754	2.41706	-0.08153
H	3.98357	3.05702	0.53558
C	1.91107	2.58602	0.34324
H	1.50187	3.59197	0.28871
C	1.13280	1.59163	0.75848
H	0.08992	1.78198	1.00538
C	1.57675	0.14778	0.82749
H	1.49948	-0.19844	1.86680
C	3.02231	-0.06043	0.41425
C	3.83634	0.99262	-0.00902
H	5.79306	1.54803	-0.69525
C	5.16379	0.72384	-0.36643
C	5.68297	-0.56074	-0.30513
H	5.26516	-2.62094	0.18753
C	4.87113	-1.61123	0.12665
H	2.91441	-2.16923	0.81257
C	3.55541	-1.35457	0.48132
H	3.45781	2.79492	-1.10651
H	1.83608	-0.67890	-1.72880
C	-1.07682	-0.71818	1.86393
H	-0.35545	-0.28418	2.54553
C	-2.33173	-0.97466	2.30846
H	-2.61657	-0.74091	3.32864
C	-3.35016	-1.47456	1.39907
H	-4.21934	-1.97948	1.82240
C	-2.93567	-1.86628	0.09621
H	-3.66731	-2.29209	-0.58450
C	-1.65046	-1.59691	-0.37303
C	-0.69387	-0.99340	0.50774
H	-3.86410	-0.43315	1.02395
C	0.58550	-0.65796	-0.00942
C	0.86140	-0.95002	-1.33198
H	0.20045	-1.76988	-3.22220
C	-0.07176	-1.57098	-2.19146
H	-2.07460	-2.31840	-2.36975
C	-1.31896	-1.88048	-1.72486
B	-3.61275	1.25990	-0.52194
F	-2.30855	1.31236	-0.04158
F	-4.44970	0.84872	0.60888
F	-4.05846	2.47526	-0.96849
F	-3.74344	0.25551	-1.47855

42

2nd proton product (pathway A)

H	6.74494	-0.83531	-0.62101
C	3.45857	2.42046	-0.09607
H	4.12073	3.04300	0.52168
C	2.03758	2.62716	0.33119
H	1.65501	3.64351	0.27783
C	1.23549	1.65434	0.75236
H	0.20008	1.87172	1.01000
C	1.64390	0.20092	0.82637
H	1.56182	-0.13852	1.86704
C	3.08159	-0.04640	0.40681
C	3.92023	0.98347	-0.02504
H	5.88651	1.48231	-0.72811
C	5.23692	0.67703	-0.39215
C	5.72055	-0.62148	-0.33193
H	5.25033	-2.66859	0.16780
C	4.88373	-1.64858	0.10829
H	2.91812	-2.15047	0.81218
C	3.57853	-1.35477	0.47283
H	3.58797	2.79668	-1.12040
H	1.86830	-0.58319	-1.73723
C	-1.00918	-0.66138	1.88656
H	-0.28064	-0.22924	2.56136
C	-2.25425	-0.91710	2.33407
H	-2.53042	-0.69104	3.35875
C	-3.30066	-1.43754	1.43775
H	-3.94811	-2.19986	1.88964
C	-2.86918	-1.80215	0.10023
H	-3.59503	-2.25006	-0.57088
C	-1.59146	-1.54141	-0.36187
C	-0.63454	-0.92664	0.51747
H	-4.01742	-0.59101	1.24162
C	0.63384	-0.58823	-0.00388
C	0.89755	-0.86608	-1.33796
H	0.23479	-1.67134	-3.23335
C	-0.03152	-1.48694	-2.19880
H	-2.02896	-2.25687	-2.35872
C	-1.26950	-1.81645	-1.72018
B	-3.84645	1.15592	-0.49404
F	-2.57656	1.18633	0.10303
F	-4.80475	0.94653	0.53171
F	-4.11061	2.32657	-1.17049
F	-3.90861	0.04717	-1.36474

60

2nd EA reactant (pathway A)

H	-5.77990	2.16854	2.45540
C	-5.78983	-0.66409	-1.24142
H	-6.80461	-1.00597	-0.99681
C	-5.03060	-1.78512	-1.88476
H	-5.49724	-2.25940	-2.74494
C	-3.84618	-2.22043	-1.46291
H	-3.34871	-3.03729	-1.98069
C	-3.09843	-1.63048	-0.29428
H	-2.88485	-2.44676	0.40300
C	-3.89700	-0.57633	0.45601
C	-5.13568	-0.11649	0.00550
H	-6.76294	1.23143	0.38911
C	-5.79785	0.87424	0.74147
C	-5.24917	1.40012	1.90215
H	-3.57420	1.32997	3.26537
C	-4.01390	0.93211	2.35557
H	-2.38170	-0.41272	1.96562
C	-3.35106	-0.04742	1.63096
H	-5.93143	0.14618	-1.97094
H	-2.82564	0.22662	-2.12860
C	-0.31821	-2.39682	0.76347
H	-1.18603	-2.81648	1.25828
C	0.91246	-2.80165	1.13652
H	1.02910	-3.55172	1.91243
C	2.13304	-2.27989	0.49186
H	2.94583	-2.01131	1.18587
C	1.92490	-1.18855	-0.45186
H	2.80974	-0.72035	-0.88277
C	0.65678	-0.80183	-0.86926
C	-0.50925	-1.41902	-0.28934
H	2.64910	-3.06849	-0.09423
C	-1.77410	-1.03791	-0.77796
C	-1.83938	-0.05863	-1.76715
H	-0.82575	1.33686	-3.06988
C	-0.70958	0.56880	-2.31375
H	1.43975	0.65968	-2.25977
C	0.53566	0.19861	-1.87043
B	5.23804	-1.04669	-0.03297
F	4.68684	-2.15668	-0.69921
F	4.80411	-1.07635	1.31309
F	6.61294	-1.05564	-0.10280
F	4.71313	0.12238	-0.63489
C	2.45986	1.02280	1.32588
C	1.99472	2.00462	0.40843
C	0.61874	2.36594	0.41665
C	-0.25814	1.72049	1.33125
C	0.21812	0.78601	2.21809
C	1.58896	0.43609	2.21678
C	0.15417	3.33551	-0.51107
C	1.01381	3.89812	-1.42045
C	2.37896	3.51623	-1.44666

60

2nd EA TS (pathway A)

H	-5.73774	2.20614	2.41831
C	-5.79319	-0.68326	-1.23393
H	-6.81909	-0.98254	-0.98071
C	-5.06767	-1.84698	-1.84066
H	-5.56132	-2.35227	-2.66745
C	-3.87790	-2.27583	-1.42783
H	-3.40045	-3.11884	-1.92201
C	-3.09440	-1.64448	-0.30612
H	-2.84840	-2.44210	0.40242
C	-3.88342	-0.58054	0.44287
C	-5.12365	-0.11904	-0.00259
H	-6.74034	1.24352	0.37306
C	-5.77413	0.88694	0.72321
C	-5.21471	1.42751	1.87194
H	-3.53623	1.35804	3.23022
C	-3.98060	0.95551	2.32413
H	-2.36491	-0.41136	1.94779
C	-3.32903	-0.03824	1.60805
H	-5.90609	0.10931	-1.98792
H	-2.85302	-0.02096	-2.38195
C	-0.32967	-2.17581	0.88769
H	-1.19597	-2.54446	1.42612
C	0.89573	-2.57957	1.26677
H	1.00424	-3.28562	2.08551
C	2.12655	-2.12938	0.55714
H	3.00776	-2.07590	1.20092
C	1.93000	-0.84356	-0.19258
H	2.78186	-0.57529	-0.81737
C	0.61716	-0.64860	-0.80874
C	-0.52658	-1.28059	-0.25156
H	2.40355	-2.87019	-0.21220
C	-1.79105	-1.04126	-0.83655
C	-1.87547	-0.19606	-1.93923
H	-0.84434	1.04758	-3.36678
C	-0.74689	0.40734	-2.49604
H	1.38564	0.64287	-2.34749
C	0.49501	0.17967	-1.93199
B	5.31732	-1.04040	-0.03239
F	4.71121	-2.12830	-0.67008
F	4.90606	-1.01540	1.32219
F	6.69125	-1.10235	-0.11902
F	4.83738	0.14804	-0.64210
C	2.27910	0.60586	1.03163
C	1.92505	1.80219	0.27967
C	0.62251	2.33932	0.42946
C	-0.24792	1.77021	1.40152
C	0.17119	0.78018	2.27076
C	1.44042	0.22434	2.11096
C	0.21553	3.43298	-0.37000
C	1.09030	3.98269	-1.27873
C	2.38986	3.45427	-1.41304

60

2nd EA product (pathway A)

H	-5.68478	2.23124	2.44102
C	-5.79225	-0.67094	-1.20031
H	-6.82162	-0.95065	-0.93921
C	-5.08798	-1.85190	-1.79908
H	-5.59773	-2.36345	-2.61213
C	-3.89709	-2.28651	-1.39575
H	-3.43419	-3.14096	-1.88410
C	-3.09180	-1.64613	-0.29487
H	-2.83422	-2.43783	0.41622
C	-3.86676	-0.57506	0.45849
C	-5.10769	-0.10620	0.02263
H	-6.71147	1.26890	0.40760
C	-5.74463	0.90696	0.75048
C	-5.17164	1.44751	1.89253
H	-3.48388	1.36788	3.23872
C	-3.93755	0.96727	2.33615
H	-2.33648	-0.41557	1.95171
C	-3.29925	-0.03352	1.61771
H	-5.89565	0.11659	-1.96105
H	-2.87435	-0.06503	-2.41371
C	-0.31826	-2.14856	0.88259
H	-1.17804	-2.49906	1.44395
C	0.91003	-2.55851	1.24593
H	1.02290	-3.25083	2.07643
C	2.13601	-2.12706	0.50939
H	3.02301	-2.09873	1.14602
C	1.94252	-0.79448	-0.18841
H	2.76780	-0.59234	-0.87396
C	0.61110	-0.65126	-0.84369
C	-0.52662	-1.27268	-0.27268
H	2.37507	-2.86175	-0.27439
C	-1.79648	-1.04988	-0.85296
C	-1.89381	-0.23024	-1.97437
H	-0.86664	0.96584	-3.44178
C	-0.76745	0.35139	-2.55242
H	1.36733	0.58524	-2.42810
C	0.48104	0.13560	-1.98928
B	5.34371	-0.99538	0.00936
F	4.76415	-2.08795	-0.64194
F	4.89545	-0.96729	1.35281
F	6.72135	-1.05152	-0.03558
F	4.87951	0.19001	-0.61564
C	2.21151	0.49203	0.93544
C	1.88331	1.74599	0.22847
C	0.60201	2.32139	0.41600
C	-0.25197	1.77688	1.41117
C	0.16425	0.78175	2.28811
C	1.39203	0.17585	2.08342
C	0.20225	3.43607	-0.35674
C	1.07422	3.98117	-1.27264
C	2.35561	3.42327	-1.43314

C	2.86097	2.59198	-0.55248	C	2.80435	2.37565	-0.65360	C	2.75686	2.31356	-0.70427
H	-1.31397	1.98363	1.31930	H	-1.25828	2.16686	1.48578	H	-1.24817	2.20199	1.52376
H	-0.45467	0.31110	2.92726	H	-0.48666	0.42182	3.05564	H	-0.47508	0.47106	3.10755
H	1.95718	-0.30471	2.92150	H	1.78628	-0.54393	2.79564	H	1.74221	-0.58767	2.77114
H	-0.89710	3.61312	-0.49458	H	-0.78923	3.82897	-0.25232	H	-0.78926	3.85495	-0.21044
H	0.64994	4.63656	-2.12861	H	0.78500	4.82519	-1.89048	H	0.78044	4.84120	-1.86476
H	3.04536	3.96036	-2.17970	H	3.07658	3.90021	-2.12585	H	3.04469	3.86748	-2.14491
H	3.89800	2.27196	-0.57452	H	3.79511	1.94996	-0.77133	H	3.73613	1.86957	-0.84789
H	3.50457	0.72736	1.30123	H	3.33767	0.35828	1.10984	H	3.28017	0.32690	1.10119

60

2nd deproton reactant (pathway A)

H	-5.68577	2.22977	2.44164
C	-5.79219	-0.67123	-1.20062
H	-6.82149	-0.95132	-0.93961
C	-5.08756	-1.85178	-1.79975
H	-5.59709	-2.36323	-2.61300
C	-3.89657	-2.28617	-1.39650
H	-3.43335	-3.14029	-1.88514
C	-3.09154	-1.64600	-0.29531
H	-2.83402	-2.43791	0.41558
C	-3.86675	-0.57529	0.45827
C	-5.10782	-0.10667	0.02251
H	-6.71203	1.26780	0.40783
C	-5.74510	0.90604	0.75065
C	-5.17235	1.44640	1.89291
H	-3.48474	1.36686	3.23920
C	-3.93813	0.96643	2.33641
H	-2.33653	-0.41572	1.95150
C	-3.29945	-0.03390	1.61766
H	-5.89579	0.11651	-1.96112
H	-2.87392	-0.06406	-2.41341
C	-0.31805	-2.14901	0.88213
H	-1.17788	-2.50000	1.44310
C	0.91027	-2.55880	1.24558
H	1.02311	-3.25153	2.07575
C	2.13637	-2.12679	0.50960
H	3.02308	-2.09838	1.14664
C	1.94275	-0.79438	-0.18831
H	2.76824	-0.59217	-0.87352
C	0.61143	-0.65100	-0.84347
C	-0.52633	-1.27268	-0.27278
H	2.37589	-2.86134	-0.27418
C	-1.79617	-1.04957	-0.85306
C	-1.89340	-0.22948	-1.97411
H	-0.86612	0.96717	-3.44101
C	-0.76698	0.35237	-2.55188
H	1.36780	0.58616	-2.42727
C	0.48144	0.13635	-1.98877
B	5.34411	-0.99557	0.00886
F	4.76469	-2.08739	-0.64386
F	4.89766	-0.97063	1.35292
F	6.72160	-1.04962	-0.03854
F	4.87706	0.19057	-0.61298
C	2.21225	0.49285	0.93574
C	1.88332	1.74660	0.22887
C	0.60138	2.32076	0.41615
C	-0.25221	1.77552	1.41128
C	0.16489	0.78097	2.28838
C	1.39319	0.17603	2.08366
C	0.20062	3.43508	-0.35654
C	1.07222	3.98128	-1.27211
C	2.35431	3.42489	-1.43210

60

2nd deproton TS (pathway A)

H	5.25405	3.38968	-1.72000
C	6.21042	-0.48997	0.66064
H	7.14772	-0.64257	0.10718
C	5.64916	-1.81914	1.06372
H	6.29391	-2.46145	1.65936
C	4.43223	-2.24036	0.73143
H	4.08588	-3.21693	1.06320
C	3.44780	-1.44750	-0.08810
H	3.25118	-2.03521	-0.99158
C	3.99085	-0.09185	-0.52787
C	5.26940	0.34739	-0.17452
H	6.69969	1.94066	-0.32963
C	5.70385	1.60495	-0.61146
C	4.89535	2.41942	-1.39040
H	2.97255	2.60521	-2.35314
C	3.61949	1.97987	-1.74501
H	2.17448	0.40590	-1.56930
C	3.17752	0.73901	-1.31034
H	6.49919	0.07357	1.55902
H	3.17944	-0.74967	2.46312
C	0.71176	-1.95509	-1.30547
H	1.58202	-2.02947	-1.94866
C	-0.46432	-2.41545	-1.74648
H	-0.53328	-2.87263	-2.73098
C	-1.71586	-2.32786	-0.91948
H	-2.60234	-2.20825	-1.54898
C	-1.65420	-1.19961	0.11585
H	-2.44149	-1.37277	0.85275
C	-0.29860	-1.16425	0.81114
C	0.87026	-1.43247	0.06336
H	-1.87074	-3.27723	-0.38888
C	2.13084	-1.26564	0.66747
C	2.20102	-0.87880	2.00799
H	1.12101	-0.42171	3.80950
C	1.05121	-0.68747	2.75931
H	-1.09642	-0.67732	2.74366
C	-0.19659	-0.82912	2.15671
B	-5.04555	-1.19493	-0.23983
F	-4.57936	-2.49302	-0.26167
F	-4.32942	-0.47100	-1.33052
F	-6.38143	-1.09272	-0.50455
F	-4.67185	-0.54889	0.93128
C	-1.92901	0.20564	-0.52442
C	-2.05698	1.37868	0.35059
C	-1.72127	2.66471	-0.15660
C	-1.29749	2.79611	-1.50206
C	-1.22632	1.71661	-2.35656
C	-1.49502	0.44118	-1.85794
C	-1.83394	3.81279	0.66786
C	-2.29259	3.69530	1.95489
C	-2.67324	2.42786	2.44289

60

2nd deproton product (pathway A)

H	6.19562	3.02438	-2.38421
C	6.64914	-0.35296	0.78403
H	7.58919	-0.69743	0.33053
C	5.93819	-1.51917	1.40120
H	6.49132	-2.09072	2.14324
C	4.69654	-1.87961	1.08904
H	4.23842	-2.73592	1.57943
C	3.82687	-1.16310	0.08775
H	3.57946	-1.88942	-0.69333
C	4.52979	0.00877	-0.58224
C	5.83521	0.38319	-0.25519
H	7.43285	1.76116	-0.65345
C	6.41639	1.47353	-0.91422
C	5.72489	2.18293	-1.88505
H	3.86669	2.35240	-2.97023
C	4.42134	1.80659	-2.21315
H	2.81259	0.44620	-1.79845
C	3.83560	0.73217	-1.56041
H	6.95482	0.34889	1.57310
H	3.66518	0.42279	2.19088
C	1.03450	-1.96143	-0.83570
H	1.86630	-2.16401	-1.50162
C	-0.15017	-2.52466	-1.08975
H	-0.26444	-3.19134	-1.94087
C	-1.34321	-2.30148	-0.20523
H	-2.26701	-2.36343	-0.78876
C	-1.29633	-0.97434	0.57658
H	-1.90842	-1.12437	1.46582
C	0.11855	-0.62488	1.04248
C	1.24923	-1.08352	0.32913
H	-1.39878	-3.12933	0.51564
C	2.53325	-0.70319	0.76226
C	2.66601	0.13452	1.87293
H	1.67162	1.23466	3.42900
C	1.55453	0.58643	2.56601
H	-0.59197	0.55467	2.68699
C	0.28263	0.19989	2.14840
B	-4.99243	-1.82622	-0.42905
F	-4.63889	-2.93040	-1.09690
F	-4.34818	-0.58260	-1.57856
F	-6.27331	-1.46689	-0.43396
F	-4.24558	-1.50338	0.64208
C	-1.86804	0.21540	-0.19142
C	-2.68800	1.21133	0.45405
C	-3.10657	2.35141	-0.29695
C	-2.73364	2.48220	-1.66144
C	-1.98205	1.51579	-2.26959
C	-1.55139	0.38520	-1.52949
C	-3.91137	3.34478	0.32033
C	-4.30319	3.22174	1.62691
C	-3.91371	2.08434	2.37000

C	2.75663	2.31548	-0.70334	C	-2.56360	1.29690	1.66273	C	-3.13411	1.10892	1.80114
H	-1.24884	2.19969	1.52367	H	-1.05406	3.79127	-1.86757	H	-3.06836	3.35685	-2.21222
H	-0.47422	0.46965	3.10774	H	-0.94814	1.84737	-3.39580	H	-1.70723	1.60124	-3.31564
H	1.74398	-0.58740	2.77117	H	-1.43528	-0.40296	-2.53464	H	-0.93426	-0.35864	-2.02380
H	-0.79139	3.85286	-0.21041	H	-1.56459	4.78113	0.25576	H	-4.21313	4.20488	-0.27109
H	0.77769	4.84106	-1.86422	H	-2.38398	4.57052	2.58923	H	-4.91946	3.98571	2.09004
H	3.04326	3.87004	-2.14341	H	-3.07194	2.34134	3.44870	H	-4.24261	1.97654	3.39868
H	3.73683	1.87350	-0.84676	H	-2.91311	0.34740	2.04419	H	-2.87489	0.24108	2.39496
H	3.28099	0.32777	1.10036	H	-3.11232	0.00837	-0.92752	H	-3.44306	-0.33104	-1.34748

42			
2nd proton reactant (pathway B)			
H	-5.61250	-1.37190	-2.01375
C	-3.77944	1.74152	0.91626
H	-4.37858	2.54805	0.47070
C	-2.48037	2.30212	1.40976
H	-2.54166	3.13620	2.10535
C	-1.28694	1.84593	1.04064
H	-0.38008	2.29778	1.43304
C	-1.07220	0.70039	0.08616
H	-0.47506	1.09737	-0.74133
C	-2.37161	0.14516	-0.48571
C	-3.62318	0.62561	-0.09101
H	-5.74733	0.44460	-0.33866
C	-4.77708	0.06497	-0.65234
C	-4.70416	-0.95269	-1.59190
H	-3.37715	-2.22511	-2.72381
C	-3.45449	-1.42979	-1.98879
H	-1.33298	-1.26441	-1.73610
C	-2.30621	-0.88311	-1.43484
H	-4.37349	1.38422	1.76963
H	-1.50849	-0.33697	2.49217
C	1.31644	-0.71410	-1.15686
H	0.84273	0.08599	-1.71453
C	2.40051	-1.35325	-1.72069
H	2.74563	-1.05431	-2.70551
C	3.06849	-2.39128	-1.01853
H	3.92332	-2.88439	-1.46904
C	2.62735	-2.75511	0.22761
H	3.13074	-3.54449	0.77915
C	1.51221	-2.11405	0.83333
C	0.83523	-1.06461	0.13770
H	3.25015	-0.09140	-0.42103
C	-0.27402	-0.41322	0.76608
C	-0.66475	-0.83154	2.01777
H	-0.34324	-2.16998	3.68684
C	-0.00024	-1.87413	2.70038
H	1.59587	-3.30208	2.63837
C	1.07139	-2.50227	2.12332
B	2.88018	2.14802	-0.42853
F	2.95532	1.89820	-1.74356
F	3.61970	0.58761	0.15171
F	3.74971	2.99758	0.11009
F	1.67078	2.03123	0.13967

42			
2nd proton TS (pathway B)			
H	-5.63697	0.38587	2.41115
C	-3.66138	-1.29322	-1.45829
H	-4.33473	-2.15901	-1.40803
C	-2.33839	-1.72102	-2.02147
H	-2.36378	-2.31268	-2.93360
C	-1.16498	-1.42586	-1.46891
H	-0.23249	-1.76578	-1.90898
C	-1.01755	-0.60088	-0.21475
H	-0.35391	-1.15806	0.45130
C	-2.33687	-0.35287	0.50019
C	-3.56559	-0.66006	-0.08894
H	-5.69827	-0.62984	0.15632
C	-4.74319	-0.38584	0.61659
C	-4.71109	0.18216	1.88212
H	-3.44076	0.92174	3.46338
C	-3.48249	0.48339	2.47112
H	-1.34930	0.45336	2.23122
C	-2.31056	0.21624	1.77829
H	-4.14897	-0.59408	-2.15414
H	-1.92490	1.19506	-1.94794
C	1.54229	0.48362	0.99648
H	1.15457	-0.45283	1.37821
C	2.83547	0.86328	1.43575
H	3.19289	0.42490	2.36785
C	3.36542	2.14733	1.01308
H	4.32541	2.47285	1.39850
C	2.68159	2.89324	0.11161
H	3.07327	3.84550	-0.23306
C	1.42631	2.44901	-0.42322
C	0.85795	1.19990	0.00346
H	3.33227	0.04354	0.64902
C	-0.37016	0.73587	-0.56963
C	-0.99577	1.53754	-1.50050
H	-0.97887	3.37175	-2.63082
C	-0.45123	2.77239	-1.89509
H	1.17135	4.16642	-1.70178
C	0.74469	3.22248	-1.37737
B	2.91530	-2.12559	0.03738
F	2.64620	-2.15935	1.40456
F	3.86807	-1.02531	-0.15353
F	3.48121	-3.27697	-0.42578
F	1.76117	-1.76734	-0.66063

42			
2nd proton product (pathway B)			
H	-5.51508	0.42655	2.40667
C	-3.53017	-1.01832	-1.55029
H	-4.17056	-1.91044	-1.54548
C	-2.20325	-1.36442	-2.15730
H	-2.22519	-1.87218	-3.11886
C	-1.03055	-1.10782	-1.58486
H	-0.09423	-1.39612	-2.05305
C	-0.88614	-0.41509	-0.25074
H	-0.24547	-1.05553	0.36059
C	-2.20968	-0.20269	0.46688
C	-3.43651	-0.47024	-0.14488
H	-5.56987	-0.45131	0.09532
C	-4.61592	-0.23731	0.57247
C	-4.58735	0.25353	1.87000
H	-3.32218	0.89353	3.49797
C	-3.36052	0.51644	2.48080
H	-1.22653	0.49118	2.24824
C	-2.18681	0.28820	1.77742
H	-4.05388	-0.29569	-2.19347
H	-1.83606	1.63513	-1.67200
C	1.78380	0.40789	0.87097
H	1.33927	-0.51414	1.23130
C	3.15453	0.66073	1.29588
H	3.26894	0.44675	2.36920
C	3.74837	1.95210	0.89460
H	4.76126	2.17250	1.21517
C	3.05249	2.82207	0.14214
H	3.48025	3.77394	-0.15790
C	1.71474	2.51771	-0.31648
C	1.08790	1.26504	0.03200
H	3.69996	-0.20501	0.84991
C	-0.21142	0.93143	-0.48170
C	-0.85531	1.86837	-1.26711
H	-0.79691	3.81161	-2.18216
C	-0.25688	3.10035	-1.56394
H	1.46830	4.37438	-1.37123
C	1.01321	3.42493	-1.10813
B	2.29618	-2.50641	-0.00719
F	1.29081	-2.55047	0.98416
F	3.52153	-2.19602	0.61442
F	2.37119	-3.69658	-0.69100
F	1.97757	-1.44030	-0.88655

42			
2nd EA reactant (pathway B)			
H	3.39059	-1.16896	3.37987
C	2.71453	-1.90252	-1.19881
H	2.86350	-0.95607	-1.74145
C	1.67376	-2.72074	-1.92227
H	1.99561	-3.50113	-2.60581
C	0.38293	-2.46162	-1.73372
H	-0.39600	-3.00085	-2.26551
C	0.00119	-1.30123	-0.83380
H	0.26896	-0.39799	-1.39525
C	0.89832	-1.27985	0.40821
C	2.25402	-1.56316	0.19889
H	4.18891	-1.74103	1.10134
C	3.13756	-1.52455	1.27228
C	2.68968	-1.20415	2.55179
H	0.98109	-0.68984	3.75523
C	1.34330	-0.93261	2.76105
C	0.44948	-0.97427	1.69166
H	3.68059	-2.41383	-1.17243
H	-1.79957	-3.33778	-0.52413
C	-1.33414	1.21392	-0.23277
H	-0.27169	1.21699	-0.47054
C	-1.90961	2.51314	0.09267
H	-1.29006	2.91877	0.91651
C	-3.35335	2.54672	0.39412
H	-3.80956	3.50575	0.61753
C	-4.08281	1.41457	0.40283
H	-5.14319	1.43078	0.63510
C	-3.47715	0.13368	0.12370
C	-2.07994	0.04747	-0.22258
H	-1.61528	3.21972	-0.70371
C	-1.46345	-1.22968	-0.49000
C	-2.24060	-2.35913	-0.36642
H	-4.18995	-3.17527	0.04326
C	-3.60629	-2.26249	-0.03425
H	-5.27792	-1.00105	0.45244
C	-4.22404	-1.04512	0.19796
B	1.99006	2.43137	-0.48680
F	0.80104	3.04461	-0.01041
F	1.59710	1.26141	-1.20097
F	2.63775	3.29670	-1.35182
F	2.79023	2.07053	0.58207
H	-0.60171	-0.77462	1.87849

42			
2nd EA TS (pathway B)			
H	-2.60715	-1.28226	3.12618
C	-2.33268	2.30121	0.09224
H	-2.59406	1.85692	-0.88011
C	-1.32780	3.41461	-0.09513
H	-1.67209	4.44413	-0.07550
C	-0.04144	3.11804	-0.27554
H	0.71499	3.88493	-0.40481
C	0.32558	1.65141	-0.32971
H	-0.18674	1.24761	-1.22007
C	-0.38605	0.92905	0.81657
C	-1.74735	1.19271	0.93476
H	-3.59614	0.56177	1.80158
C	-2.52535	0.38694	1.76081
C	-1.96886	-0.66783	2.50095
H	-0.14909	-1.64384	3.07599
C	-0.61277	-0.88734	2.44963
C	0.21077	-0.10530	1.59729
H	-3.26242	2.66580	0.53655
H	2.72052	3.15578	-0.63110
C	0.84986	-1.03154	-0.17395
H	-0.06468	-0.80288	-0.70925
C	1.06241	-2.49553	0.01255
H	0.29460	-2.92475	0.66106
C	2.45652	-2.90177	0.35862
H	2.61827	-3.91936	0.70062
C	3.49249	-2.07059	0.17789
H	4.51022	-2.39905	0.36998
C	3.30085	-0.67566	-0.21170
C	1.99747	-0.15735	-0.34293
H	0.81320	-2.91195	-0.98180
C	1.77081	1.23583	-0.43664
C	2.85902	2.08305	-0.55030
H	5.00417	2.23011	-0.65775
C	4.15958	1.55663	-0.54980
H	5.39640	-0.18364	-0.29415
C	4.38326	0.20187	-0.36091
B	-2.57758	-1.14558	-1.23692
F	-1.85706	-1.87435	-0.26610
F	-1.68677	-0.18164	-1.79087
F	-3.02343	-1.99087	-2.23641
F	-3.64066	-0.47087	-0.63363
H	1.26122	-0.06254	1.86209

42			
2nd EA product (pathway B)			
H	2.87593	1.72708	-1.96735
C	-0.84362	3.92337	-0.17241
H	-0.20529	4.54977	0.46538
C	-2.15527	3.68396	0.51617
H	-2.78445	4.55513	0.67690
C	-2.55484	2.49429	0.95484
H	-3.49570	2.40475	1.48956
C	-1.73277	1.24103	0.82386
H	-1.25144	1.05624	1.80517
C	-0.56190	1.41149	-0.11480
C	-0.11373	2.64645	-0.51152
H	1.46064	3.69688	-1.52464
C	1.10863	2.71233	-1.22000
C	1.90510	1.60710	-1.50552
H	2.05278	-0.52335	-1.37749
C	1.46456	0.35560	-1.13446
C	0.13064	0.17830	-0.55953
H	-0.99915	4.50330	-1.09161
H	-4.48548	0.79407	0.46834
C	-0.20414	-1.01839	0.38588
H	0.05033	-0.63766	1.38061
C	0.59928	-2.31866	0.19643
H	1.56787	-2.13074	-0.26895
C	-0.12774	-3.43323	-0.49826
H	0.47554	-4.26553	-0.85141
C	-1.45647	-3.47352	-0.61892
H	-1.95116	-4.32547	-1.07833
C	-2.30338	-2.35529	-0.18932
C	-1.71005	-1.17398	0.27504
H	0.86722	-2.68000	1.19838
C	-2.49154	-0.03272	0.48290
C	-3.87454	-0.08987	0.32029
H	-5.55296	-1.33798	-0.17666
C	-4.47504	-1.28848	-0.05882
H	-4.15762	-3.32570	-0.67454
C	-3.69443	-2.40595	-0.32697
B	3.79558	-0.48834	0.52011
F	3.64905	-1.54710	-0.40461
F	2.50347	-0.19534	1.04301
F	4.64499	-0.84655	1.54519
F	4.25841	0.63962	-0.16368
H	-0.40084	-0.05795	-1.52253

42

2nd EA product (pathway B)

H	-3.66307	0.18460	-1.70918
C	-1.18430	3.65989	0.14428
H	-1.60973	4.41727	-0.52893
C	0.21055	4.05832	0.52036
H	0.32423	5.02154	1.01189
C	1.28709	3.31984	0.26916
H	2.26989	3.69783	0.53904
C	1.25139	1.99732	-0.44197
H	1.75035	2.14627	-1.41750
C	-0.15005	1.51983	-0.75733
C	-1.28013	2.30277	-0.51202
H	-3.42096	2.41516	-0.65609
C	-2.54151	1.81082	-0.86363
C	-2.67994	0.56496	-1.45408
H	-1.67894	-1.21302	-2.10970
C	-1.55155	-0.22608	-1.68097
C	-0.27837	0.23538	-1.32638
H	-1.82671	3.67409	1.03521
H	2.94443	2.05535	1.79071
C	0.97472	-0.61701	-1.50451
H	1.48399	-0.26354	-2.41832
C	0.63145	-2.10482	-1.69420
H	-0.15389	-2.38916	-0.97735
C	1.80315	-3.02258	-1.48045
H	1.79979	-3.98233	-1.98947
C	2.77194	-2.71352	-0.61679
H	3.58369	-3.40643	-0.40941
C	2.78013	-1.42688	0.09057
C	1.93818	-0.39167	-0.34551
H	0.20565	-2.25932	-2.69035
C	2.03815	0.87789	0.22838
C	2.89223	1.08291	1.31287
H	4.34979	0.20741	2.62842
C	3.68671	0.04175	1.78490
H	4.29794	-2.00329	1.49712
C	3.65071	-1.19815	1.15926
B	-2.80999	-1.80123	1.18513
F	-1.45937	-0.58513	1.29334
F	-2.31558	-2.53904	0.17635
F	-2.72627	-2.29327	2.41962
F	-3.82406	-0.98014	0.89755
H	-1.18215	-0.34389	0.40492