Supplementary Material (ESI) for PCCP

Supporting Information for

The association reaction between C_2H and 1-butyne: A computational chemical kinetics study

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Table S1 Optimized Cartesian coordinates at M06-2X/6-311++G(d,p) for all the species involved in the title reaction

C_2H

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.000000	0.000000	-0.471867
1	0.000000	0.000000	-1.537428
6	0.000000	0.000000	0.728105

CH_3

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-0.000002	0.000037	-0.000008
1	0.956513	-0.498942	0.000017
1	-0.910286	-0.578995	0.000017
1	-0.046216	1.077712	0.000017

C_2H_5

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.694220	0.000020	-0.000538
6	-0.793661	0.000000	-0.023691
1	-1.348125	-0.925395	0.051377
1	-1.348221	0.925331	0.051396
1	1.103872	-0.884448	-0.493407
1	1.085303	-0.001461	1.026956
1	1.103821	0.885852	-0.490947

1-Butyne

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.949490	-0.262969	0.000021
1	2.945320	-0.636332	0.000352
6	0.827778	0.164671	-0.000198
6	-0.551374	0.653711	0.000064
6	-1.571400	-0.490826	0.000003
1	-0.699008	1.289235	0.877515
1	-0.699195	1.289501	-0.877160
1	-2.587832	-0.094017	0.000152
1	-1.443206	-1.117832	-0.883187
1	-1.443044	-1.118078	0.882994

R1

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.377297	-0.538201	-0.443815
6	-1.328677	-0.156290	0.608292
6	-0.445711	0.926719	0.146480
6	0.827090	1.079835	-0.170378
6	1.768507	0.000955	-0.087412
6	2.554455	-0.906997	-0.019535
1	-1.892568	-0.883194	-1.358322
1	-3.003719	0.319678	-0.693610
1	-3.019704	-1.336742	-0.069908
1	3.252497	-1.707299	0.040145
1	-1.824956	0.154560	1.533008
1	-0.703486	-1.025170	0.856577
1	1.201735	2.042042	-0.509685

R2

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.295970	-0.695824	-0.451314
6	-1.270010	-0.279986	0.552570
6	-0.562079	0.973582	0.123458
6	0.740521	1.071001	-0.163259
6	1.664080	-0.016871	-0.075649
6	2.461736	-0.914974	-0.011880
1	-2.035204	-0.729623	-1.500884
1	-1.177932	1.862080	0.014756
1	-3.257458	-1.082706	-0.144294
1	3.165226	-1.710654	0.046936
1	-1.749426	-0.108412	1.521572
1	-0.526744	-1.074464	0.702682
1	1.151870	2.022213	-0.484328

M1

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.628992	0.709403	0.000007
6	-1.844945	-0.609421	0.000101
6	-0.401331	-0.393440	-0.000174
6	0.786747	-0.185532	-0.000091
6	2.143565	0.045040	-0.000020
6	3.330077	0.246843	0.000082
1	-2.384136	1.300273	0.883276
1	-3.701520	0.509939	0.000227
1	-2.384448	1.299945	-0.883568
1	4.378735	0.424651	0.000112
1	-2.109863	-1.206232	-0.877424
1	-2.109496	-1.205932	0.877942

M2

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.611771	-0.591713	-0.299453
6	-1.620161	0.193495	0.519025
6	-0.421036	0.503334	0.123184
6	0.785148	0.820573	-0.285225
6	1.929101	-0.009632	-0.066579
6	2.908983	-0.684631	0.100807
1	-2.189859	-0.866206	-1.265319
1	-3.518224	-0.004869	-0.465136
1	-2.899710	-1.503226	0.229246
1	3.771371	-1.287653	0.254084
1	-1.927737	0.517101	1.511535
1	0.942575	1.756299	-0.814965

IM

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.029325	0.725872	-0.349145
6	-1.399908	-0.419655	0.450519
6	0.033717	-0.570903	0.120733
6	1.066379	-1.271001	-0.282396
6	1.314107	0.127321	0.002474
6	2.090755	1.164963	0.078252
1	-1.979812	0.522824	-1.420003
1	-1.500278	1.660779	-0.157330
1	-3.075825	0.855340	-0.070849
1	2.019589	2.204019	0.345535
1	-1.475481	-0.205528	1.521376
1	-1.918731	-1.362839	0.265178
1	1.476191	-2.214180	-0.606526

IM1

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.861604	0.344355	0.000027
6	-1.573101	-0.394245	0.000057
6	-0.343159	0.172108	-0.000073
6	0.791410	-0.698283	-0.000065
6	2.032371	-0.095030	-0.000049
6	3.172752	0.335358	0.000075
1	-2.714736	1.423939	-0.000087
1	-3.453702	0.061317	0.875927
1	-3.453783	0.061143	-0.875765
1	4.176705	0.687729	0.000177
1	-1.606622	-1.481530	0.000132
1	-0.259867	1.261824	-0.000207

M3

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.560606	-0.574439	-0.000001
6	-1.233920	-0.429708	0.000001
6	-0.581820	0.871027	0.000000
6	0.747956	1.062543	0.000001
6	1.705810	0.005832	-0.000002
6	2.531358	-0.869253	0.000001
1	-3.220242	0.287460	-0.000004
1	-1.227414	1.744659	0.000000
1	-3.023917	-1.553024	0.000003
1	3.260275	-1.643910	-0.000003
1	-0.587350	-1.302437	0.000004
1	1.145985	2.071239	0.000001

M4

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.258961	-0.445992	0.000007
6	-1.107426	0.153821	0.000000
6	0.049791	0.770113	-0.000021
6	1.301828	0.080790	-0.000016
6	2.368663	-0.471449	-0.000017
1	3.309069	-0.968130	0.000142
1	-2.752338	-0.705923	0.930382
1	-2.752340	-0.705902	-0.930374
1	0.072239	1.856254	0.000127

M5

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.515698	-0.000455	0.000101
6	-1.059578	0.000578	-0.000135
6	0.145586	0.000778	-0.000274
6	1.521905	0.000142	0.000011
6	2.725279	-0.000413	0.000109
1	3.788839	-0.001164	0.000254
1	-2.897568	-0.659730	-0.781547
1	-2.899020	1.005711	-0.179325
1	-2.897218	-0.348593	0.961745

IM2

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.301166	-0.030721	0.000462
6	-1.024410	0.394101	-0.000466
6	0.012585	-0.607832	-0.000504
6	1.309419	-0.146980	-0.000234
6	2.491120	0.155682	0.000418
1	3.529430	0.389659	0.001006
1	-2.504686	-1.096169	0.000890
1	-3.140871	0.657341	0.000920
1	-0.809156	1.463673	-0.000867

R3

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.767306	-0.941749	-0.392904
6	-1.225698	0.136026	0.547338
6	0.124909	0.654591	0.094452
6	0.329777	1.906365	-0.265965
6	1.211522	-0.288267	0.050104
6	2.104441	-1.093390	0.024813
1	2.901151	-1.797828	-0.000615
1	1.171802	2.484392	-0.616277
1	-1.914439	0.981255	0.603429
1	-1.115446	-0.271426	1.556825
1	-1.901895	-0.539642	-1.399081
1	-2.730304	-1.312864	-0.037917
1	-1.076745	-1.785343	-0.453384

R4

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.319153	-0.475918	-0.000099
6	-0.854810	-0.764400	0.000155
6	0.118783	0.240250	0.000287
6	-0.177167	1.590555	0.000089
6	1.503282	-0.164652	-0.000305
6	2.654952	-0.506706	-0.000159
1	3.674634	-0.809443	0.001052
1	0.611566	2.329162	-0.000462
1	-1.202378	1.935914	-0.000011
1	-0.519502	-1.793858	-0.000014
1	-2.608695	0.109007	0.880188
1	-2.902458	-1.395466	-0.000748
1	-2.608491	0.109904	-0.879804

R5

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.325365	-1.264919	-0.281318
6	-0.609607	-0.162394	0.483334
6	0.845705	0.109024	0.044578
6	1.956798	-0.608932	0.001942
6	0.381312	1.453241	-0.313608
6	-0.892179	1.284138	0.040629
1	-1.789563	1.885273	0.037034
1	2.879474	-0.190821	-0.381853
1	1.967442	-1.635547	0.349545
1	-0.684844	-0.291572	1.567451
1	-1.200030	-1.118756	-1.356570
1	-2.393568	-1.265736	-0.052235
1	-0.918893	-2.243796	-0.016717

R6

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.919162	-0.713140	0.000070
6	-0.677413	0.094120	0.000012
6	0.774598	-0.258332	-0.000029
6	1.477257	-1.386431	-0.000069
6	1.046744	1.203704	0.000161
6	-0.338519	1.452562	-0.000169
1	-0.930252	2.359257	-0.000296
1	2.560186	-1.375712	0.000003
1	0.979494	-2.349233	-0.000138
1	1.938481	1.810747	0.000319
1	-1.962937	-1.363038	-0.880248
1	-2.803073	-0.073996	0.000036
1	-1.962927	-1.362935	0.880465

R7

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.638890	-1.204860	-0.418212
6	-1.257629	-0.089475	0.496671
6	0.027423	0.594900	0.080814
6	0.093588	1.886403	-0.248144
6	1.199312	-0.235240	0.051548
6	2.153969	-0.966233	0.041667
1	3.007083	-1.601883	0.030654
1	1.029461	2.344971	-0.541295
1	-2.056517	0.655313	0.551637
1	-1.120087	-0.472147	1.520816
1	-0.794699	2.507204	-0.228794
1	-2.658437	-1.563793	-0.440344
1	-0.873448	-1.782637	-0.918736

R8

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.511179	0.588855	-0.000174
6	0.058848	1.141676	0.000166
6	-0.858194	-0.083268	0.000036
6	-2.189941	-0.094828	-0.000110
6	0.049470	-1.218305	0.000107
6	1.338234	-0.921491	0.000024
1	2.167497	-1.616504	0.000032
1	-2.739565	-1.027671	-0.000159
1	-0.136554	1.755616	0.880768
1	-0.136856	1.756131	-0.880006
1	-2.759643	0.826981	-0.000179
1	2.073519	0.914699	-0.879171
1	2.074027	0.914919	0.878413

R9

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.478116	-0.689950	0.000034
6	0.049734	-1.138249	-0.000015
6	-0.800554	-0.027787	-0.000031
6	-2.180080	-0.020593	-0.000015
6	0.066282	1.172435	0.000067
6	1.353705	0.812407	-0.000086
1	2.204151	1.480758	-0.000144
1	-2.735280	0.908155	0.000033
1	-0.270392	-2.170793	-0.000015
1	-0.317174	2.184780	0.000123
1	-2.742247	-0.945325	-0.000023
1	2.028751	-1.053488	0.877447
1	2.028974	-1.053663	-0.877148

M6

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.688519	-0.000314	-0.000118
6	1.890909	0.000375	-0.000038
6	-0.688519	-0.000367	0.000013
6	-1.890909	0.000020	0.000078
1	-2.954870	0.001575	-0.000120
1	2.954871	0.000139	0.000510

M7

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.621479	-1.278365	-0.000002
6	1.356296	0.025648	0.000026
6	0.003032	0.608065	-0.000004
6	-0.189476	1.934353	0.000023
6	-1.120222	-0.288934	-0.000081
6	-2.043688	-1.057355	-0.000124
1	-2.870215	-1.727131	0.000860
1	-1.184401	2.359144	-0.000004
1	2.166727	0.748954	0.000075
1	0.656626	2.611553	0.000068
1	2.642095	-1.639291	0.000023
1	0.824644	-2.013702	-0.000050

IM3

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.149326	1.430811	0.121158
6	-0.482961	0.156245	-0.322381
6	0.891059	-0.170777	-0.038486
6	2.158674	0.254105	-0.107167
6	0.007868	-1.009253	0.700972
6	-1.139576	-1.164865	-0.272100
1	-2.144960	-1.187148	0.140846
1	2.911867	-0.177621	0.538012
1	2.446676	1.026530	-0.807299
1	-0.966688	-1.901121	-1.052224
1	-2.025583	1.210609	0.737931
1	-1.483360	2.007155	-0.744464
1	-0.452385	2.044000	0.695224

M8

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.700648	-1.068291	0.000067
6	0.753971	-0.138887	0.000019
6	-0.753980	-0.138877	-0.000019
6	-1.700652	-1.068286	-0.000067
6	-0.676348	1.340994	0.000145
6	0.676359	1.340984	-0.000145
1	1.425981	2.120823	-0.000270
1	-2.750980	-0.802807	-0.000012
1	-1.443620	-2.120936	-0.000122
1	-1.425961	2.120842	0.000270
1	1.443630	-2.120944	0.000122
1	2.750972	-0.802796	0.000012

M9

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.399073	0.738188	0.000135
6	-0.126322	1.178225	-0.000180
6	0.759236	-0.000048	-0.000326
6	2.095799	-0.000004	0.000262
6	-0.126352	-1.178206	-0.000224
6	-1.399091	-0.738161	0.000151
1	-2.290659	-1.350220	0.000470
1	2.658293	-0.927066	0.000430
1	0.219848	2.201783	-0.000447
1	0.219774	-2.201778	-0.000318
1	2.658218	0.927105	0.000525
1	-2.290660	1.350211	0.000439

TS1

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.648881	0.722369	0.145601
6	-1.859621	-0.541901	-0.219154
6	-0.419608	-0.340575	-0.142316
6	0.778188	-0.284313	0.086622
6	2.116201	0.067663	-0.005075
6	3.278921	0.365306	-0.075968
1	-2.405051	1.537667	-0.536141
1	-2.410867	1.042292	1.160433
1	-3.720073	0.526047	0.084345
1	4.306480	0.631721	-0.142754
1	-2.125125	-1.362767	0.457405
1	-2.117753	-0.871737	-1.229621
1	1.001196	-1.434518	1.468066

TS2

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.585537	-0.420028	-0.472655
6	-1.557788	0.042929	0.537181
6	-0.389411	0.546955	0.196932
6	0.823944	0.922023	-0.124927
6	1.941641	0.027880	-0.084233
6	2.893135	-0.705376	-0.058167
1	-2.109194	-0.667650	-1.420390
1	-3.318104	0.371932	-0.645134
1	-3.113915	-1.299463	-0.103593
1	3.730610	-1.360626	-0.031947
1	-1.893186	0.202735	1.559973
1	1.013924	1.946367	-0.436740
1	-1.066039	-1.679589	1.113041

TS3

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	2.340188	-0.130562	0.450830
6	1.216555	-0.789276	-0.348847
6	0.587379	0.558591	-0.413984
6	-0.617733	1.020606	-0.055560
6	-1.736732	0.141927	0.064654
6	-2.671581	-0.610412	0.164044
1	2.267604	-0.172129	1.532087
1	1.777874	1.058193	0.053980
1	3.341319	-0.123597	0.029558
1	-3.501207	-1.270332	0.249396
1	1.553416	-1.164290	-1.315182
1	0.635630	-1.551785	0.170378
1	-0.783095	2.078698	0.112962

TS4

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-3.119933	-0.499228	-0.001383
6	-1.395409	0.932250	0.000445
6	-0.250200	0.262116	0.002051
6	0.753539	-0.579777	0.001616
6	2.128013	-0.179356	0.000145
6	3.290873	0.124246	-0.001579
1	-2.970708	-1.000059	0.946114
1	-2.906450	-1.073673	-0.893152
1	-3.946445	0.198722	-0.058343
1	4.317393	0.402697	-0.003141
1	-1.743307	1.379987	-0.924731
1	-1.745855	1.382434	0.923461
1	0.554074	-1.651610	0.002019

TS5

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	2.544189	-0.539426	-0.109000
1	3.197415	0.320934	-0.014405
1	1.198793	1.770865	0.055225
1	3.009564	-1.509016	-0.230042
6	1.200544	-0.409304	-0.024621
1	0.776544	-0.819870	1.742859
1	0.561792	-1.265327	-0.221898
6	0.548910	0.902084	0.011818
6	-0.778953	1.089973	-0.012890
1	-1.184347	2.095241	0.002146
1	-3.224327	-1.676546	-0.050662
6	-2.517577	-0.881527	-0.043395
6	-1.719685	0.018820	-0.035782

TS6

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.840522	0.449066	-0.069136
6	-1.692898	-0.454088	0.263758
6	-0.373736	-0.197245	-0.080015
6	0.846430	-0.422300	-0.442296
6	2.099020	-0.000718	-0.078125
6	3.245598	0.298851	0.181678
1	-2.510139	1.328493	-0.622563
1	-3.396026	0.765352	0.817661
1	-3.541275	-0.104859	-0.703538
1	4.249847	0.563499	0.409821
1	-1.907883	-1.332466	0.872080
1	-0.597876	0.738582	0.571351

TS7

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	2.734592	0.529901	-0.115636
6	1.626220	-0.320609	0.436235
6	0.394220	-0.369067	-0.036827
6	-0.853077	-0.726831	-0.401807
6	-2.000623	-0.007441	-0.057004
6	-3.069545	0.496375	0.198180
1	2.404045	1.095405	-0.988365
1	3.586320	-0.086628	-0.413972
1	3.092708	1.242784	0.631254
1	-4.002038	0.951737	0.432059
1	1.831517	-0.944901	1.299956
1	0.096729	0.127636	-1.099780

TS8

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.474117	-0.279065	-0.407315
6	-1.382779	-0.560458	0.481334
6	-0.579845	0.509717	0.258410
6	0.668986	0.960873	0.069633
6	1.781408	0.081700	-0.063042
6	2.730722	-0.651044	-0.172700
1	-3.148823	0.520705	-0.122842
1	-1.578666	0.865722	-0.663778
1	-2.935751	-1.055190	-1.018896
1	3.567277	-1.300692	-0.266430
1	-1.222986	-1.423710	1.118370
1	0.852698	2.022825	-0.044334

TS9

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	2.325466	-0.348186	-0.015058
6	1.092557	0.124876	0.045859
6	-0.097175	0.686857	-0.218188
6	-1.336230	0.076266	-0.033760
6	-2.465594	-0.347408	0.046830
1	-3.452634	-0.737139	0.123491
1	2.706993	-0.703909	-0.962529
1	2.953394	-0.405162	0.860603
1	0.678106	0.691776	1.024337

TS10

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.453498	0.015858	0.151770
6	-1.098505	0.014203	-0.148305
6	0.118443	-0.371061	-0.262381
6	1.423143	-0.061756	-0.035453
6	2.607349	0.133262	0.144290
1	3.644349	0.307764	0.303088
1	-2.834635	-0.499521	1.027800
1	-3.126990	0.653599	-0.404442
1	-1.264311	1.155122	-0.025966

TS11

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.821731	-1.080197	-0.316219
6	-1.160125	-0.032316	0.537408
6	0.169483	0.520570	0.087494
6	-0.223860	1.748304	-0.226971
6	1.421925	-0.149251	0.021054
6	2.462163	-0.751390	-0.023867
1	3.387772	-1.274117	-0.066019
1	0.238167	2.652582	-0.615554
1	-1.490239	1.274676	0.205437
1	-1.277912	-0.124997	1.617675
1	-1.831840	-0.770038	-1.363939
1	-2.846636	-1.268722	0.005835
1	-1.266439	-2.023701	-0.256822

TS12

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.231498	-0.232109	0.000003
6	-0.876174	-0.928883	-0.000003
6	0.134155	0.211873	-0.000001
6	-0.428159	1.416581	-0.000001
6	1.539677	-0.039253	-0.000001
6	2.717144	-0.284986	0.000002
1	3.760957	-0.490090	0.000004
1	-0.017919	2.418016	-0.000002
1	-0.727593	-1.560908	0.879021
1	-0.727597	-1.560902	-0.879031
1	-1.768139	0.990133	-0.000002
1	-2.825283	-0.327791	0.905495
1	-2.825297	-0.327800	-0.905479

TS13

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.797920	-0.891312	-0.451518
6	-1.358934	-0.009126	0.671783
6	0.547781	0.863570	-0.015009
6	0.450838	2.071655	-0.224090
6	1.284290	-0.319593	0.005017
6	1.889439	-1.358819	0.029891
1	2.444559	-2.266150	0.045355
1	0.108856	3.076015	-0.320926
1	-1.909677	0.909527	0.838621
1	-0.976791	-0.478713	1.572369
1	-1.949155	-0.318278	-1.369104
1	-2.748194	-1.386539	-0.214029
1	-1.062568	-1.674112	-0.648726

TS14

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.931963	-0.331416	-0.267437
6	0.647772	-0.341548	0.497508
6	-0.461453	0.599621	0.112625
6	-0.447633	1.918713	-0.047255
6	-1.498565	-0.389955	-0.159068
6	-1.086514	-1.576568	-0.097485
1	-1.103778	-2.646974	-0.151760
1	-1.329433	2.450852	-0.380516
1	0.450764	2.491234	0.153139
1	0.663895	-0.620594	1.547285
1	1.740682	-0.350300	-1.343218
1	2.562553	-1.181258	-0.003024
1	2.501899	0.583966	-0.055232

TS15

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.754289	-0.986175	0.129350
6	0.636794	-0.065805	-0.195402
6	-0.831924	-0.113274	-0.069738
6	-1.739202	-1.086574	-0.022785
6	-0.923087	1.360738	0.252389
6	0.485258	1.452598	-0.037727
1	1.227925	2.221713	0.143451
1	-2.769318	-0.844066	0.214051
1	-1.481291	-2.125670	-0.200628
1	0.582904	1.050288	-1.156408
1	1.856293	-1.100009	1.217095
1	2.701513	-0.596515	-0.250202
1	1.589202	-1.974789	-0.303881

TS16

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.885857	-0.821229	0.002056
6	-0.664684	0.017692	-0.018212
6	0.770200	-0.227064	0.012006
6	1.587753	-1.282891	0.008535
6	1.107338	1.266851	-0.102291
6	-0.343030	1.461074	-0.030928
1	-0.933802	2.349789	-0.236987
1	2.660144	-1.126356	0.001581
1	1.215777	-2.301982	-0.006288
1	0.259238	1.723969	0.988396
1	-2.563368	-0.562518	-0.817630
1	-2.446321	-0.693694	0.935691
1	-1.621990	-1.875802	-0.091762

TS17

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.795769	-0.749096	-0.178207
6	-0.705519	0.018604	-0.105424
6	0.775368	-0.233471	-0.013375
6	1.552954	-1.307982	-0.003815
6	0.938651	1.238211	0.067237
6	-0.395010	1.459345	-0.015909
1	-1.009138	2.349695	-0.014846
1	2.629767	-1.223851	0.078639
1	1.125996	-2.301017	-0.078435
1	1.801585	1.883988	0.157675
1	-1.708234	-1.825894	-0.259897
1	-2.784904	-0.315403	-0.260211
1	-2.279129	-1.121180	1.874028

TS18

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.426929	-0.963318	0.220454
6	-0.006406	-1.190801	-0.219375
6	0.812225	0.096957	-0.048920
6	2.129848	0.160267	0.128328
6	-0.109243	1.207347	-0.093256
6	-1.343101	1.285357	-0.038925
1	-2.305397	1.750035	-0.011611
1	2.636698	1.112620	0.215104
1	0.469089	-2.004227	0.336755
1	0.010674	-1.460554	-1.279134
1	2.726037	-0.742898	0.189472
1	-2.238504	-1.275629	-0.423967
1	-1.636966	-0.954199	1.283548

TS19

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.565776	-1.308138	-0.170839
6	-1.323858	0.002579	0.034809
6	0.027754	0.608912	-0.021803
6	0.196504	1.933467	-0.109552
6	1.158270	-0.275360	0.014547
6	2.088352	-1.035213	0.047902
1	2.920395	-1.697568	0.079543
1	1.183948	2.371991	-0.164812
1	-2.145294	0.712555	0.007556
1	-1.452592	0.163542	1.895358
1	-0.660511	2.596957	-0.124003
1	-2.579594	-1.683048	-0.221020
1	-0.753821	-2.021911	-0.243010

TS20

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.373001	-0.609447	-0.465088
6	0.201824	-0.888313	0.487297
6	-0.901013	0.028067	0.141863
6	-2.106123	0.000049	-0.391883
6	0.117160	0.953928	0.696869
6	1.194686	0.874318	-0.318903
1	1.780150	1.690653	-0.711428
1	-2.673652	0.913678	-0.521829
1	0.047316	-1.775371	1.096066
1	0.548764	-0.046354	1.473257
1	-2.552589	-0.932973	-0.714050
1	2.329224	-0.957225	-0.060514
1	1.243577	-1.044022	-1.462426

TS21

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.373001	-0.609447	-0.465088
6	0.201824	-0.888313	0.487297
6	-0.901013	0.028067	0.141863
6	-2.106123	0.000049	-0.391883
6	0.117160	0.953928	0.696869
6	1.194686	0.874318	-0.318903
1	1.780150	1.690653	-0.711428
1	-2.673652	0.913678	-0.521829
1	0.047316	-1.775371	1.096066
1	0.548764	-0.046354	1.473257
1	-2.552589	-0.932973	-0.714050
1	2.329224	-0.957225	-0.060514
1	1.243577	-1.044022	-1.462426

TS22

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	0.475478	1.678227	0.000002
6	-0.783130	1.214890	-0.000007
6	-0.704780	-0.242738	0.000008
6	-1.582462	-1.248077	-0.000002
6	0.755604	-0.453446	0.000036
6	1.914255	-0.926766	-0.000053
1	2.670314	-1.684353	0.000089
1	-1.258039	-2.280817	0.000023
1	-1.726406	1.752688	-0.000015
1	-2.645934	-1.046500	-0.000043
1	0.707747	2.745749	-0.000002
1	1.802520	0.380694	0.000044

TS23

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	2.149960	-0.795256	-0.324159
6	1.522000	0.377834	0.437153
6	0.089261	0.526781	0.128531
6	-0.943255	1.209716	-0.278824
6	-1.588736	-0.040087	-0.039784
6	-2.333069	-1.022512	0.100372
1	2.073668	-0.639983	-1.401266
1	1.636734	-1.725731	-0.078168
1	3.204283	-0.896596	-0.063152
1	-2.708652	-1.995669	0.311934
1	1.622534	0.214404	1.514624
1	2.044271	1.313950	0.201073
1	-1.249810	2.190766	-0.624774

TS24

Standard orientation:

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.967677	-0.794123	-0.350121
6	1.376893	0.361026	0.460593
6	-0.056603	0.585001	0.110931
6	-0.936797	1.453566	-0.298702
6	-1.208491	-0.266593	0.061986
6	-2.068379	-1.157950	0.085571
1	1.944285	-0.568834	-1.417781
1	1.393741	-1.707927	-0.184856
1	3.002527	-0.979371	-0.059060
1	-2.972657	-1.715486	0.020748
1	1.432706	0.132570	1.529178
1	1.925404	1.289567	0.289916
1	-1.171800	2.463914	-0.599691

Table S2 Harmonic vibartional frequencies for the transition states

TS1	TS2	TS3	TS4	TS5	TS6	TS7	TS8
-948.716	-847.963	-1803.22	-609.677	-955.9673	-1072.61	-636.975	-1748.97
53.0518	81.2782	72.5634	67.3681	98.1615	95.9579	103.7277	108.7606
98.9411	128.0379	127.606	89.3034	133.3278	119.0338	174.1906	175.1613
122.1888	165.3571	207.5971	101.1085	263.6634	189.8283	190.1882	288.7041
232.7806	221.9716	346.2072	167.8057	310.9121	244.3284	274.3884	329.3853
266.2083	287.4922	404.7056	350.3492	402.2354	384.8788	358.1118	475.4046
321.7525	430.1604	504.1378	351.897	438.7522	451.4844	456.9741	557.0386
461.7462	450.5018	569.6724	394.3442	465.6492	494.2771	541.4022	649.0577
539.227	486.6677	662.4051	502.1214	511.3279	511.7683	547.7211	653.0912
560.7023	566.0666	718.4373	558.9416	673.7093	535.4134	562.4768	722.0129
571.8901	629.6506	726.9614	606.128	686.1948	744.6686	762.9923	745.6097
697.927	696.5603	797.8621	679.8407	711.5684	771.9497	800.4487	827.4106
708.7801	731.3928	836.6502	717.6262	726.3413	785.0415	814.4556	901.9914
715.4387	794.693	909.5331	723.5903	800.1124	908.3137	903.1846	937.4524
777.313	878.4457	967.3852	813.0256	901.1218	980.0548	989.5219	979.3682
970.1405	940.7143	1011.2551	890.5613	929.7975	1040.872	1060.3824	1030.9916
1088.077	991.1875	1050.7661	930.0496	983.4336	1116.718	1134.6618	1097.8582
1095.813	1062.801	1093.0778	946.7375	1003.9307	1244.925	1228.0707	1186.8533
1167.917	1095.763	1188.1524	1038.849	1078.3837	1405.114	1396.0487	1271.6575
1280.293	1143.35	1224.3558	1108.535	1157.2994	1425.051	1427.9232	1332.1342
1349.08	1286.296	1242.4404	1333.718	1255.0292	1477.104	1487.0413	1424.8056
1414.293	1408.023	1328.8101	1425.023	1299.8629	1505.852	1514.0398	1522.059
1467.284	1423.935	1425.5857	1429.483	1380.6734	1859.463	1907.7674	1742.5989
1499.227	1489.794	1485.6439	1452.389	1463.3903	2147.993	2158.5575	1818.5299
1507.162	1502.011	1641.9641	1950.305	1612.2056	2561.79	2376.6121	2221.3409
2163.139	2011.728	1922.3025	2238.837	1697.837	3034.942	3052.5037	3093.7314
2319.011	2243.838	2220.5765	3103.638	2231.8636	3094.64	3114.6395	3176.9535
3034.699	3058.816	3090.0316	3109.577	3154.8355	3135.528	3134.3084	3183.3899
3061.61	3132.099	3117.5032	3131.611	3168.0164	3148.525	3177.0155	3198.1556
3083.874	3136.04	3148.3738	3216.228	3176.5445	3475.791	3482.1765	3486.1276
3142.417	3138.457	3188.1097	3263.083	3193.222			
3148.029	3154.781	3236.1835	3276.183	3259.1256			
3482.708	3487.352	3484.9267	3471.994	3484.3954			

TS9	TS10	TS11	TS12	TS13	TS14	TS15	TS16
-651.04	-1141.61	-1986.696	-1654.26	-652.565	-787.236	-1655.81	-843.884
131.2635	98.4965	119.9126	96.119	34.286	104.341	142.901	-88.305
257.0691	177.067	164.053	165.834	137.846	189.090	164.350	128.919
430.9738	314.442	214.9216	248.973	147.505	226.839	184.147	200.845
463.7892	449.777	231.0852	445.434	207.772	251.611	241.224	219.246
549.762	493.217	344.0346	513.872	264.840	403.713	376.012	396.153
568.4372	518.638	527.463	525.770	276.134	561.736	543.663	632.464
672.0256	594.173	561.4578	549.137	470.460	602.053	633.951	643.844
793.4419	755.901	603.2232	641.984	512.335	664.356	706.711	693.645
816.8426	784.310	706.6652	704.260	541.801	692.831	743.997	754.191
819.9302	789.092	721.3341	724.313	607.012	735.314	768.066	870.831
846.8311	950.37	738.6703	775.652	699.209	793.719	832.671	884.846
1092.521	1043.101	779.3878	834.937	717.507	832.825	897.246	932.202
1252.175	1294.936	830.2208	865.167	726.177	939.738	1000.81	963.42
1457.141	1477.328	948.385	949.580	818.366	952.924	1005.882	988.499
1887.255	1909.792	1019.3306	1007.720	830.051	1006.145	1056.891	1013.59
2162.011	2146.557	1065.4115	1075.502	900.122	1071.848	1114.119	1141.488
2404.986	2583.624	1090.1956	1100.806	1031.909	1124.011	1151.418	1164.324
3187.861	3134.027	1157.0134	1190.201	1080.269	1240.203	1161.540	1258.528
3286.104	3247.618	1223.8789	1220.282	1213.317	1346.86	1323.899	1305.976
3481.218	3485.968	1334.0285	1269.357	1399.233	1407.834	1339.972	1383.679
		1405.9912	1308.441	1471.679	1433.868	1407.23	1415.780
		1486.058	1450.994	1483.971	1482.558	1438.243	1449.643
		1488.8292	1488.406	1493.332	1486.27	1478.583	1467.566
		1674.6648	1648.914	1961.627	1737.140	1481.906	1484.814
		1882.2675	1708.027	2263.94	1769.686	1747.275	1708.701
		2239.015	2235.719	3013.099	3008.852	2323.473	2221.509
		3029.740	3055.916	3083.632	3086.432	3015.492	3017.593
		3100.990	3095.34	3127.481	3140.476	3100.582	3073.483
		3120.935	3113.114	3132.862	3155.236	3141.538	3124.425
		3138.577	3197.392	3229.817	3185.444	3152.528	3147.785
		3172.135	3226.301	3451.198	3250.651	3203.750	3170.649
		3483.166	3487.5748	3487.613	3370.345	3252.758	3246.314

TS17	TS18	TS19	TS20	TS21	TS22	TS23	TS24
-487.826	-646.528	-935.214	-1273.16	-706.876	-1899.54	-752.2753	-787.0664
163.807	106.8924	93.4274	178.557	182.865	178.9863	47.8614	51.7173
178.074	247.2837	166.036	271.612	269.963	244.6523	115.1527	152.7107
242.014	361.7404	251.715	325.068	308.796	266.33	166.9357	195.4556
256.908	455.6298	316.578	392.678	340.835	310.4325	258.5355	270.2304
335.692	509.1513	379.956	599.134	518.101	480.6958	368.0508	356.4888
409.048	553.7765	453.6504	639.402	631.713	485.9297	423.2086	436.9748
694.420	605.1555	487.294	693.019	678.171	550.188	442.1654	466.4115
716.992	687.7975	529.722	783.618	693.893	659.6533	495.5809	541.6204
735.921	696.038	624.660	847.990	793.826	680.5091	566.0592	605.3662
780.544	749.9197	705.091	897.301	810.233	696.1482	773.4298	692.7134
786.832	794.2807	722.748	921.964	813.434	731.998	807.9277	721.8873
838.262	818.5569	736.243	947.760	915.9452	769.1038	820.8221	750.2099
915.125	858.5215	756.198	960.762	957.9286	783.3278	955.6906	794.1358
923.777	943.4935	764.28	993.0678	965.6996	915.8572	1018.3759	971.8121
925.066	946.8632	938.788	1007.882	969.3995	925.5192	1086.7324	1062.1758
934.317	1053.042	948.027	1041.350	980.8435	978.9403	1092.3092	1091.5301
968.417	1080.113	960.667	1109.186	1003.895	1006.678	1162.0215	1193.7994
1073.052	1215.41	1043.696	1163.919	1091.383	1227.818	1273.0382	1291.2814
1156.394	1253.699	1057.299	1203.158	1106.295	1294.429	1326.8256	1338.7019
1217.871	1309.651	1304.181	1278.467	1254.076	1437.962	1409.5003	1411.7069
1297.207	1436.925	1322.976	1283.973	1352.94	1576.846	1467.6955	1477.4285
1433.149	1458.826	1415.571	1339.111	1368.058	1709.706	1499.7388	1501.2952
1452.223	1479.183	1455.247	1449.764	1454.178	1963.804	1508.4332	1507.2245
1571.056	1727.264	1619.911	1469.840	1533.659	2167.023	1817.7509	1765.0681
1718.727	1939.39	1705.255	1811.998	1628.478	3115.522	1916.9777	1940.5921
1794.358	3063.492	2246.056	2059.916	1714.203	3169.544	3016.7147	3054.1936
3157.031	3109.271	3157.922	3049.054	3151.672	3169.748	3058.0338	3059.744
3157.825	3150.636	3163.551	3090.040	3211.644	3264.614	3078.4406	3106.5012
3216.31	3158.531	3164.929	3143.651	3231.288	3371.945	3138.307	3134.0523
3247.666	3253.4	3259.633	3145.729	3243.265		3142.1456	3138.9741
3250.907	3254.771	3261.276	3238.253	3245.221		3176.3527	3253.5878
3256.053	3392.622	3485.186	3242.536	3255.196		3447.6091	3447.8858

Table S3 Structure dependent rate constants for barrier less terminal association

T (K)	2.02	2.12	2.22	2.32	2.42	2.52
70	1.149E39	3.514E20	4.789E10	103500	234.1	27.45
80	3.192E32	2.143E16	4.332E7	496.8	2.566	0.4
90	2.561E27	1.144E13	186700	7.872	0.07765	0.01513
100	2.165E23	2.792E10	2404	0.288	0.00478	0.00111
110	1.015E20	2.056E8	68.61	0.01937	4.939E-4	1.334E-4
120	1.719E17	3.468E6	3.559	0.00206	7.509E-5	2.294E-5
130	7.826E14	110600	0.2924	3.1E-4	1.537E-5	5.212E-6
140	7.743E12	5820	0.03448	6.159E-5	3.971E-6	1.474E-6
150	1.426E11	456.8	0.00543	1.525E-5	1.236E-6	4.961E-7
160	4.348E9	49.61	0.00108	4.518E-6	4.476E-7	1.924E-7
170	2.009E8	7.04	2.609E-4	1.551E-6	1.835E-7	8.381E-8
180	1.312E7	1.248	7.404E-5	6.017E-7	8.342E-8	4.022E-8
190	1.147E6	0.2668	2.406E-5	2.588E-7	4.136E-8	2.094E-8
200	128500	0.06687	8.771E-6	1.215E-7	2.208E-8	1.168E-8
210	17790	0.01921	3.53E-6	6.153E-8	1.256E-8	6.909E-9
220	2958	0.00621	1.547E-6	3.323E-8	7.54E-9	4.302E-9
230	577	0.00222	7.303E-7	1.899E-8	4.747E-9	2.8E-9
240	129.4	8.69E-4	3.678E-7	1.14E-8	3.114E-9	1.894E-9
250	32.78	3.678E-4	1.961E-7	7.145E-9	2.119E-9	1.325E-9
260	9.259	1.669E-4	1.1E-7	4.654E-9	1.489E-9	9.555E-10
270	2.88	8.052E-5	6.45E-8	3.135E-9	1.076E-9	7.075E-10
280	0.9761	4.105E-5	3.937E-8	2.178E-9	7.978E-10	5.365E-10
290	0.3574	2.199E-5	2.491E-8	1.554E-9	6.051E-10	4.156E-10
300	0.1402	1.231E-5	1.628E-8	1.136E-9	4.684E-10	3.281E-10

Table S4 Structure dependent rate constants for barrier less central association

T(K)	2.03	2.13	2.23	2.33	2.43	2.53
70	6.733E32	8.403E14	145700	31.13	3.732	3.581
80	1.031E27	2.35E11	702.8	0.4499	0.07397	0.07502
90	3.11E22	4.092E8	11.26	0.01697	0.00358	0.0038
100	7.573E18	2.565E6	0.4185	0.00125	3.225E-4	3.575E-4
110	8.425E15	40830	0.02867	1.509E-4	4.575E-5	5.259E-5
120	2.931E13	1308	0.00311	2.618E-5	9.111E-6	1.081E-5
130	2.451E11	71.75	4.788E-4	6.018E-6	2.354E-6	2.873E-6
140	4.083E9	6.007	9.735E-5	1.724E-6	7.46E-7	9.334E-7
150	1.181E8	0.7052	2.469E-5	5.89E-7	2.782E-7	3.559E-7
160	5.348E6	0.109	7.493E-6	2.321E-7	1.184E-7	1.545E-7
170	350300	0.02111	2.636E-6	1.028E-7	5.614E-8	7.458E-8
180	31210	0.00494	1.048E-6	5.021E-8	2.913E-8	3.933E-8
190	3604	0.00135	4.623E-7	2.661E-8	1.63E-8	2.233E-8
200	518.5	4.243E-4	2.225E-7	1.512E-8	9.726E-9	1.35E-8
210	90.11	1.493E-4	1.155E-7	9.114E-9	6.129E-9	8.612E-9
220	18.43	5.805E-5	6.391E-8	5.782E-9	4.049E-9	5.753E-9
230	4.344	2.461E-5	3.742E-8	3.835E-9	2.786E-9	3.999E-9
240	1.159	1.125E-5	2.301E-8	2.643E-9	1.986E-9	2.878E-9
250	0.3448	5.498E-6	1.477E-8	1.885E-9	1.461E-9	2.136E-9
260	0.113	2.849E-6	9.848E-9	1.385E-9	1.105E-9	1.628E-9
270	0.04034	1.556E-6	6.792E-9	1.045E-9	8.562E-10	1.271E-9
280	0.01554	8.9E-7	4.826E-9	8.072E-10	6.78E-10	1.013E-9
290	0.00641	5.307E-7	3.523E-9	6.368E-10	5.473E-10	8.233E-10
300	0.00282	3.286E-7	2.634E-9	5.12E-10	4.496E-10	6.803E-10

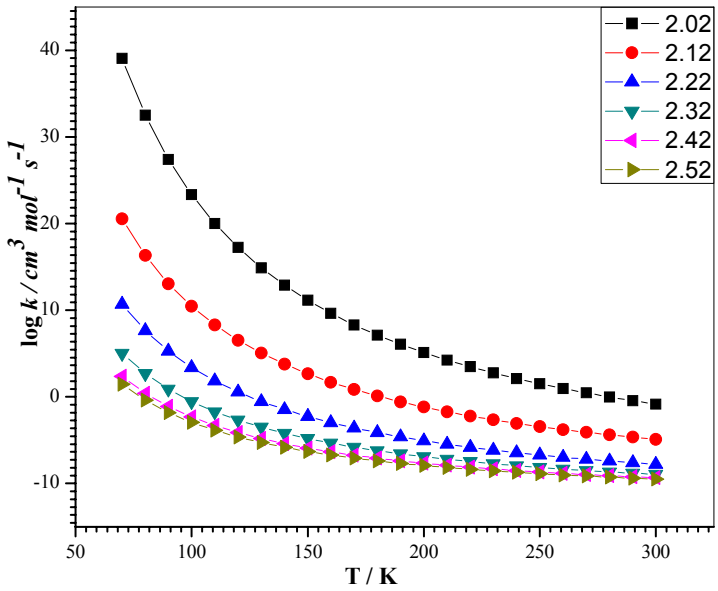

Figure S1 Variation of rate constant as a function of temperature and position for terminal barrier-less C_2H + 1-butyne addition

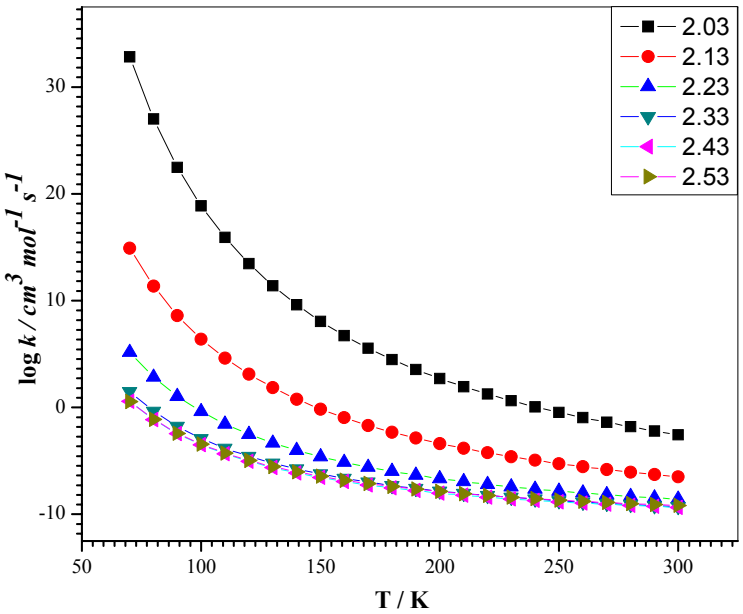

Figure S2 Variation of rate constant as a function of temperature and position for central barrier-less C_2H + 1-butyne addition

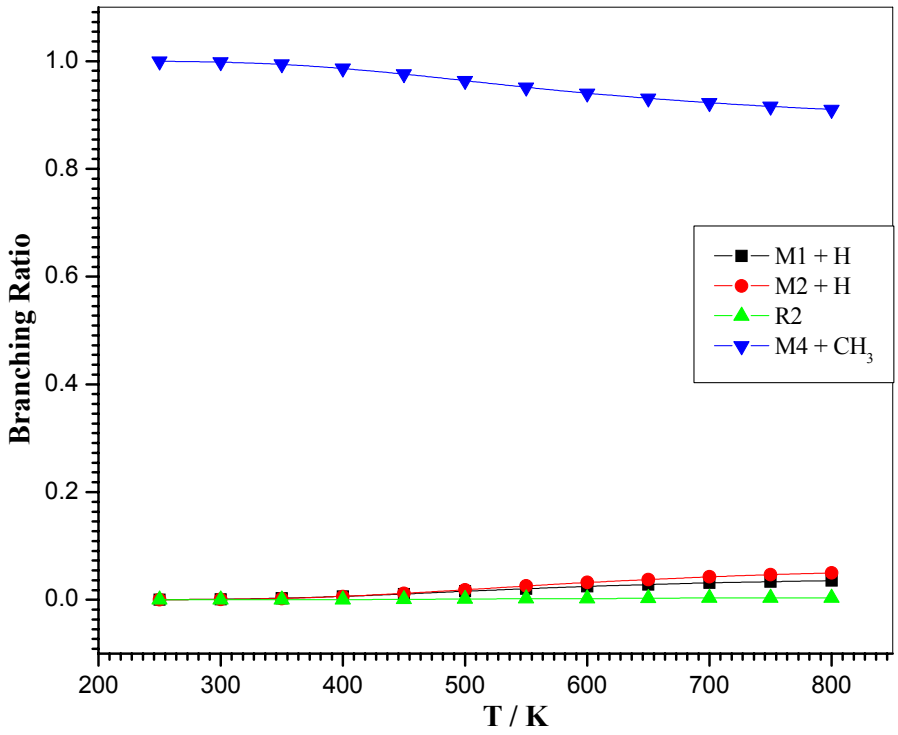

Figure S3 Branching ratio for the initial reactions of R1