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

Abstraction and addition kinetics of C_2H Radical with CH_4, C_2H_6, C_3H_8, C_2H_4, and C_3H_6: CVT/SCT/ISPE and hybrid meta-DFT methods

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Table S-I: The variation of the bond length between forming bond and breaking bond for all the transition states at M06-2X/6-31G(d), M06-2X/6-311++G(d,p), and M06-2X/6-311++G(d,p) level of theories.

Transition State	Bond	M06-2X/ 6-31G(d)	M06-2X/6-31+G(d,p)	M06-2X/6-311++G(d,p)
TS1	C-H(GS)[a]	1.091	1.091	1.09
	C-H(GS)[b]	1.067	1.067	1.064
	C-H(TS)[c]	1.145(5%)	1.135(4%)	1.140(4%)
	C-H(TS)[d]	1.643(35%)	1.689(37%)	1.666(36%)
TS1	C-H(GS)[a]	1.094	1.094	1.092
	C-H(GS)[b]	1.067	1.067	1.064
	C-H(TS)[c]	1.132(3%)	1.125(3%)	1.13(3%)
	C-H(TS)[d]	1.739(38%)	1.795(41%)	1.755(39%)
TS1	C-H(GS)[a]	1.094	1.094	1.092
	C-H(GS)[b]	1.067	1.067	1.064
	C-H(TS)[c]	1.132(3%)	1.124(3%)	1.13(3%)
	C-H(TS)[d]	1.739(39%)	1.798(41%)	1.755(%)
TS2	C-H(GS)[a]	1.095	1.095	1.093
	C-H(GS)[b]	1.067	1.067	1.064
	C-H(TS)[c]	1.133(3%)	1.127(3%)	1.131(3%)
	C-H(TS)[d]	1.747(39%)	1.794(39%)	1.762(40%)
TS3	C-H(GS)[a]	1.096	1.096	1.094
	C-H(GS)[b]	1.067	1.067	1.064
	C-H(TS)[c]	1.13(3%)	1.122(2%)	1.126(3%)
	C-H(TS)[d]	1.789(40%)	1.862(43%)	1.824(42%)
TS1	C-H(GS)[a]	1.086	1.086	1.085
	C-H(GS)[b]	1.067	1.067	1.065
	C-H(TS)[c]	1.143(5%)	1.136(4%)	1.142(5%)
	C-H(TS)[d]	1.617(34%)	1.653(35%)	1.625(34%)
TS1	C-H(GS)[a]	1.094	1.093	1.091
	C-H(GS)[b]	1.067	1.067	1.064
	C-H(TS)[c]	1.138(4%)	1.131(3%)	1.136(4%)
	C-H(TS)[d]	1.698(36%)	1.737(39%)	1.709(37%)
TS2	C-H(GS)[a]	1.096	1.095	1.093
	C-H(GS)[b]	1.067	1.067	1.064
	C-H(TS)[c]	1.131(3%)	1.125(3%)	1.127(3%)
	C-H(TS)[d]	1.794(40%)	1.838(42%)	1.816(41%)
TS3	C-H(GS)[a]	1.085	1.09	1.088
	C-H(GS)[b]	1.062	1.067	1.064
	C-H(TS)[c]	1.126(4%)	1.127(3%)	1.132(4%)
	C-H(TS)[d]	1.716(38%)	1.738(39%)	1.705(38%)
TS4	C-H(GS)[a]	1.081	1.085	1.083
	C-H(GS)[b]	1.062	1.067	1.064

	C-H(TS)[c]	1.135(5%)	1.134(4%)	1.139(5%)
	C-H(TS)[d]	1.634(35%)	1.656(36%)	1.63(35%)
TS5	**C-H(GS)[a]**	1.083	1.088	1.086
	C-H(GS)[b]	1.062	1.067	1.064
	C-H(TS)[c]	1.135(5%)	1.135(4%)	1.14(5%)
	C-H(TS)[d]	1.65(36%)	1.669(36%)	1.644(35%)

[a]C-H bond length (the leaving hydrogen) in the reactants in its ground state
[b]The actual C-H bond length in C_2H_2 at the corresponding theories.
[c]C-H bond length (the leaving hydrogen) in the transition state
[d]C-H bond length (the forming hydrogen) in the transition state.
The numbers are given in the parenthesis corresponds to the % change in the bond length in transition state when compared the same bond length in the reactant.

Table S-II. Summary of C=C bond distances (Å) in ethylene and propylene and their corresponding adducts.

$C_2H_4+C_2H$			
C_1=C_2 bond	**M06-2X/6-31G(d)**	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
C_2H_4	1.327	1.330	1.326
Adduct1	1.500	1.500	1.499
Adduct2	1.516	1.518	1.517
$C_3H_6+C_2H$			
C_5=C_7 bond	**M06-2X/6-31G(d)**	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
C_3H_6	1.329	1.332	1.328
Adduct1	1.503	1.503	1.502
Adduct1a	1.502	1.502	1.501
Adduct2	1.516	1.518	1.517

Table S-III: Optimized geometries in Cartesian Coordinates of reactants, pre-reaction complexes (PRCs), transition states (TSs), and products (Ps) at M06-2X level of theory using 6-31G(d), 6-31+G(d,p), and 6-311++G(d,p) basis sets.

$CH_4 + C_2H$

CH_4 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0	0	0
2	1	0	0.62993	0.62993	0.62993
3	1	0	-0.62993	-0.62993	0.62993
4	1	0	-0.62993	0.62993	-0.62993
5	1	0	0.62993	-0.62993	-0.62993

CH_4 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	0	0	0
2	1	0	0.629705	0.629705	0.629705
3	1	0	-0.62971	-0.62971	0.629705
4	1	0	-0.62971	0.629705	-0.62971
5	1	0	0.629705	-0.62971	-0.62971

CH_4 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0	0	0
2	1	0	0.629118	0.629118	0.629118
3	1	0	-0.62912	-0.62912	0.629118
4	1	0	-0.62912	0.629118	-0.62912
5	1	0	0.629118	-0.62912	-0.62912

C_2H (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0	0	0.73122
2	6	0	0	0	-0.4742
3	1	0	0	0	-1.54213

C_2H (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	15.87532	15.87532	16.60772
2	6	0	15.87532	15.87532	15.40017
3	1	0	15.87532	15.87532	14.33182

C_2H (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0	0	0.728131
2	6	0	0	0	-0.47197
3	1	0	0	0	-1.53695

TS1 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0	0	-1.99718
2	1	0	0	0	-0.85247
3	1	0	0	1.040798	-2.32008
4	1	0	0.901357	-0.5204	-2.32008
5	1	0	-0.90136	-0.5204	-2.32008
6	6	0	0	0	0.790684
7	6	0	0	0	1.997685
8	1	0	0	0	3.065584

TS1 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	2.134604	0.000405	0.000298
2	1	0	0.99923	-0.00119	-0.00212
3	1	0	2.462036	-0.76924	-0.69788
4	1	0	2.458893	0.991116	-0.31643
5	1	0	2.457893	-0.21945	1.017245
6	6	0	-0.68989	-0.00131	-0.00096
7	6	0	-1.89915	0.000637	0.000473
8	1	0	-2.96723	0.001923	0.001395

TS1 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0	0	-2.00605
2	1	0	0	0	-0.86608
3	1	0	0	1.039317	-2.32697
4	1	0	0.900075	-0.51966	-2.32697
5	1	0	-0.90008	-0.51966	-2.32697
6	6	0	0	0	0.800175
7	6	0	0	0	2.002463
8	1	0	0	0	3.067448

CH_3 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0	0	0.000603
2	1	0	0	1.079331	-0.00121
3	1	0	0.934728	-0.53967	-0.00121
4	1	0	-0.93473	-0.53967	-0.00121

CH_3 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	0	0	0
2	1	0	0	1.079969	0
3	1	0	0.935281	-0.53999	0
4	1	0	-0.93528	-0.53999	0

CH_3 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0	0	0.000101
2	1	0	0	1.078954	-0.0002
3	1	0	-0.9344	-0.53948	-0.0002
4	1	0	0.934402	-0.53948	-0.0002

C_2H_2 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0	0	-0.60102
2	6	0	0	0	0.601015

3	1	0	0	0	1.66778
4	1	0	0	0	-1.66778

C_2H_2 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	15.87532	15.87532	16.47762
2	6	0	15.87532	15.87532	15.27301
3	1	0	15.87532	15.87532	14.20582
4	1	0	15.87532	15.87532	17.54481

C_2H_2 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0	0	-0.59845
2	6	0	0	0	0.598448
3	1	0	0	0	1.6627
4	1	0	0	0	-1.6627

C_2H_6 + C_2H

C_2H_6 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0	0	0.763309
2	6	0	0	0	-0.76331
3	1	0	0	-1.01956	-1.15977
4	1	0	0.882969	0.509782	-1.15977
5	1	0	-0.88297	0.509782	-1.15977
6	1	0	0	1.019564	1.159772
7	1	0	-0.88297	-0.50978	1.159772
8	1	0	0.882969	-0.50978	1.159772

C_2H_6 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	0	0	0.763781
2	6	0	0	0	-0.76378
3	1	0	0	-1.01932	-1.15994
4	1	0	0.882761	0.509662	-1.15994

5	1	0	-0.88276	0.509662	-1.15994
6	1	0	0	1.019324	1.159939
7	1	0	-0.88276	-0.50966	1.159939
8	1	0	0.882761	-0.50966	1.159939

C_2H_6 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0	0	0.763526
2	6	0	0	0	-0.76353
3	1	0	0	-1.01753	-1.15936
4	1	0	0.881208	0.508766	-1.15936
5	1	0	-0.88121	0.508766	-1.15936
6	1	0	0	1.017532	1.15936
7	1	0	-0.88121	-0.50877	1.15936
8	1	0	0.881208	-0.50877	1.15936

PRC (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	1.712826	-0.74686	0
2	6	0	1.489807	0.763621	0.000003
3	1	0	0.928207	1.082775	0.884627
4	1	0	0.928216	1.082779	-0.884625
5	1	0	2.439614	1.306679	0.000008
6	1	0	2.274061	-1.06359	-0.883607
7	1	0	2.274053	-1.0636	0.883612
8	1	0	0.762001	-1.29058	-0.000005
9	6	0	-1.49583	0.108965	-0.000013
10	6	0	-2.6848	-0.09067	0.000005
11	1	0	-3.73822	-0.26482	0.000021

PRC (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-1.75347	0.733968	-0.000041
2	6	0	-1.47722	-0.76863	-0.000165
3	1	0	-0.90556	-1.06859	0.884742
4	1	0	-0.90664	-1.06874	-0.885695
5	1	0	-2.40723	-1.34457	0.000519
6	1	0	-2.32659	1.03062	-0.88286

7	1	0	-2.32497	1.030716	0.883791
8	1	0	-0.82344	1.311827	-0.00097
9	6	0	1.5107	-0.07098	0.000751
10	6	0	2.708027	0.085529	-0.000185
11	1	0	3.766161	0.229446	-0.001684

PRC (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-1.75375	-0.73108	0.000048
2	6	0	-1.46231	0.768866	0.00015
3	1	0	-0.8901	1.062764	-0.884065
4	1	0	-0.89028	1.062646	0.884525
5	1	0	-2.38613	1.351414	0.000091
6	1	0	-2.3291	-1.01983	0.881731
7	1	0	-2.32819	-1.01989	-0.882214
8	1	0	-0.83203	-1.31817	0.000521
9	6	0	1.505239	0.069723	-0.000756
10	6	0	2.695101	-0.08828	0.000126
11	1	0	3.750189	-0.23436	0.002002

TS1 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	-1.08219	1.031793	0
2	6	0	-1.98426	-0.19123	0
3	1	0	-1.80783	-0.81001	0.883951
4	1	0	-1.80783	-0.81001	-0.883951
5	1	0	-3.03849	0.10348	0
6	1	0	-1.20465	1.651446	-0.892161
7	1	0	-1.20465	1.651446	0.892161
8	1	0	0	0.698051	0
9	6	0	1.512259	-0.15962	0
10	6	0	2.500985	-0.85247	0
11	1	0	3.382643	-1.45524	0

TS1 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-1.14782	1.099832	0
2	6	0	-2.15641	-0.03862	0

3	1	0	-2.03901	-0.67074	0.884141
4	1	0	-2.03901	-0.67074	-0.884141
5	1	0	-3.17958	0.349816	0
6	1	0	-1.21914	1.728574	-0.891061
7	1	0	-1.21914	1.728574	0.891061
8	1	0	-0.10405	0.680919	0
9	6	0	1.429917	-0.2507	0
10	6	0	2.420379	-0.94431	0
11	1	0	3.297904	-1.5534	0

TS1 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-1.11179	1.050635	0
2	6	0	-1.86714	-0.26776	0
3	1	0	-1.62191	-0.86057	0.882919
4	1	0	-1.62191	-0.86057	-0.882919
5	1	0	-2.94587	-0.09548	0
6	1	0	-1.30281	1.649645	-0.89148
7	1	0	-1.30281	1.649645	0.89148
8	1	0	0	0.848033	0
9	6	0	1.498088	-0.06555	0
10	6	0	2.408809	-0.85048	0
11	1	0	3.22749	-1.53172	0

C_2H_5 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0.015058	0.795177	0
2	6	0	0.015058	-0.69362	0
3	1	0	0.517028	-1.09586	0.885631
4	1	0	0.517028	-1.09586	-0.885631
5	1	0	-1.00563	-1.10815	0
6	1	0	-0.10456	1.345276	-0.925232
7	1	0	-0.10456	1.345276	0.925232

C_2H_5 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	0.012012	0.794771	0
2	6	0	0.012012	-0.69442	0

3	1	0	0.511977	-1.09688	0.885944
4	1	0	0.511977	-1.09688	-0.885944
5	1	0	-1.0098	-1.10464	0
6	1	0	-0.07915	1.348144	-0.926301
7	1	0	-0.07915	1.348144	0.926301

C_2H_5 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0.011642	0.793954	0
2	6	0	0.011642	-0.69402	0
3	1	0	0.509544	-1.09614	0.885064
4	1	0	0.509544	-1.09614	-0.885064
5	1	0	-1.00965	-1.10109	0
6	1	0	-0.07457	1.346869	-0.925331
7	1	0	-0.07457	1.346869	0.925331

C_3H_8 + C_2H

C_3H_8 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0	1.266587	-0.260878
2	6	0	0	0	0.591596
3	6	0	0	-1.26659	-0.260878
4	1	0	0.883595	1.300155	-0.907244
5	1	0	-0.8836	1.300155	-0.907244
6	1	0	0	2.169701	0.356278
7	1	0	0.877498	0	1.24869
8	1	0	-0.8775	0	1.24869
9	1	0	0.883595	-1.30016	-0.907244
10	1	0	-0.8836	-1.30016	-0.907244
11	1	0	0	-2.1697	0.356278

C_3H_8 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	0	1.267457	-0.260927
2	6	0	0	0	0.591709
3	6	0	0	-1.26746	-0.260927
4	1	0	0.883622	1.301511	-0.90711

5	1	0	-0.88362	1.301511	-0.90711
6	1	0	0	2.170548	0.355992
7	1	0	0.877515	0	1.248664
8	1	0	-0.87752	0	1.248664
9	1	0	0.883622	-1.30151	-0.90711
10	1	0	-0.88362	-1.30151	-0.90711
11	1	0	0	-2.17055	0.355992

C_3H_8 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0	1.266192	-0.261178
2	6	0	0	0	0.592603
3	6	0	0	-1.26619	-0.261178
4	1	0	0.882338	1.298132	-0.906126
5	1	0	-0.88234	1.298132	-0.906126
6	1	0	0	2.168485	0.353668
7	1	0	0.876185	0	1.247845
8	1	0	-0.87619	0	1.247845
9	1	0	0.882338	-1.29813	-0.906126
10	1	0	-0.88234	-1.29813	-0.906126
11	1	0	0	-2.16849	0.353668

PRC1 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0.857671	1.282192	-0.000006
2	6	0	0.945163	-0.24239	0.000045
3	6	0	2.388494	-0.74073	-0.000028
4	1	0	1.350844	1.699727	0.884248
5	1	0	1.350692	1.699658	-0.884377
6	1	0	-0.18139	1.628711	0.000068
7	1	0	0.421262	-0.64038	0.879405
8	1	0	0.421161	-0.64044	-0.879231
9	1	0	2.923616	-0.37778	0.884056
10	1	0	2.923447	-0.37804	-0.884319
11	1	0	2.439347	-1.83327	0.000136
12	6	0	-2.09928	-0.23179	0.000014
13	6	0	-3.30481	-0.22358	-0.000011
14	1	0	-4.37238	-0.22044	-0.000071

PRC1 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	0.934446	1.301718	0.000001
2	6	0	0.938534	-0.22605	0.000092
3	6	0	2.353021	-0.80295	-0.000025
4	1	0	1.450249	1.691064	0.884104
5	1	0	1.449793	1.690967	-0.884408
6	1	0	-0.0828	1.706838	0.000246
7	1	0	0.395369	-0.59475	0.880415
8	1	0	0.395199	-0.59485	-0.88009
9	1	0	2.907094	-0.47035	0.884165
10	1	0	2.906942	-0.47037	-0.88432
11	1	0	2.343517	-1.89641	-0.000008
12	6	0	-2.12497	-0.15528	-0.000201
13	6	0	-3.32946	-0.24201	0.000071
14	1	0	-4.39481	-0.31468	0.000272

PRC1 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0.921585	1.299088	0
2	6	0	0.932317	-0.22825	-0.000072
3	6	0	2.34965	-0.79687	0.000021
4	1	0	1.434684	1.689181	0.882922
5	1	0	1.435164	1.689257	-0.882613
6	1	0	-0.09542	1.699567	-0.000265
7	1	0	0.392769	-0.59916	0.878884
8	1	0	0.3929	-0.59908	-0.879135
9	1	0	2.900264	-0.46147	0.882962
10	1	0	2.900364	-0.4615	-0.882868
11	1	0	2.34606	-1.88844	0.000037
12	6	0	-2.11448	-0.15357	0.00014
13	6	0	-3.31128	-0.24476	-0.000033
14	1	0	-4.37354	-0.32215	-0.00026

PRC2 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	-1.03769	1.266945	0.000035
2	6	0	-1.88993	0.000393	-0.00019
3	6	0	-1.03833	-1.2666	0.000056

4	1	0	-0.39174	1.30114	0.885714
5	1	0	-0.39056	1.300721	-0.8848
6	1	0	-1.65168	2.172583	-0.00058
7	1	0	-2.54648	0.000589	0.877637
8	1	0	-2.54601	0.000498	-0.87837
9	1	0	-0.39097	-1.30018	0.884743
10	1	0	-0.39281	-1.30177	-0.88592
11	1	0	-1.65281	-2.17192	0.001448
12	6	0	1.865511	-0.0023	0.000511
13	6	0	3.071168	0.000784	-0.00026
14	1	0	4.138651	0.003035	-0.0008

PRC2 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-1.05193	1.26749	-0.00017
2	6	0	-1.90261	-0.00094	0.000167
3	6	0	-1.04951	-1.26774	-0.00016
4	1	0	-0.40643	1.30335	0.88561
5	1	0	-0.40687	1.303232	-0.88626
6	1	0	-1.66716	2.172044	-6.9E-05
7	1	0	-2.55806	-0.00155	0.878699
8	1	0	-2.55875	-0.00156	-0.87785
9	1	0	-0.40377	-1.30223	0.885477
10	1	0	-0.40465	-1.30247	-0.88645
11	1	0	-1.66305	-2.17346	0.000259
12	6	0	1.890129	0.002227	0.000564
13	6	0	3.097806	-0.00025	-0.00017
14	1	0	4.165445	-0.0021	-0.00082

PRC2 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-1.03473	1.266979	-0.00013
2	6	0	-1.88658	-0.00002	0.000258
3	6	0	-1.03431	-1.26674	-0.00014
4	1	0	-0.39041	1.301532	0.884302
5	1	0	-0.39119	1.301498	-0.88512
6	1	0	-1.64827	2.170492	0.000099
7	1	0	-2.54042	-0.00013	0.877365
8	1	0	-2.5411	-0.00014	-0.87635

9	1	0	-0.39017	-1.30118	0.884435
10	1	0	-0.39067	-1.30098	-0.88508
11	1	0	-1.64754	-2.17047	-6.2E-05
12	6	0	1.862001	-0.00139	-5E-06
13	6	0	3.062363	0.000677	0.000061
14	1	0	4.127279	0.002353	0.000125

TS1 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0.928506	0.25086	0
2	6	0	0.536991	-1.21863	0
3	6	0	1.766534	-2.12744	0
4	1	0	1.496461	0.532366	0.892078
5	1	0	1.496461	0.532366	-0.892078
6	1	0	0	0.898949	0
7	1	0	-0.0818	-1.433	0.878403
8	1	0	-0.0818	-1.433	-0.878403
9	1	0	2.386026	-1.94478	0.884272
10	1	0	2.386026	-1.94478	-0.884272
11	1	0	1.480958	-3.18324	0
12	6	0	-1.5408	1.704351	0
13	6	0	-2.61158	2.261432	0
14	1	0	-3.56024	2.751707	0

TS1 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	0.993809	0.109229	0
2	6	0	0.595651	-1.35981	0
3	6	0	1.821383	-2.275	0
4	1	0	1.566368	0.384247	0.891134
5	1	0	1.566368	0.384247	-0.891134
6	1	0	0.078684	0.762641	0
7	1	0	-0.02348	-1.57222	0.878551
8	1	0	-0.02348	-1.57222	-0.878551
9	1	0	2.441497	-2.09526	0.884306
10	1	0	2.441497	-2.09526	-0.884306
11	1	0	1.531467	-3.32944	0
12	6	0	-1.44965	1.70897	0
13	6	0	-2.48071	2.340484	0

14	1	0	-3.39317	2.895649	0

TS1 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0.966307	0.470058	0
2	6	0	0.669971	-1.02112	0
3	6	0	1.954645	-1.84959	0
4	1	0	1.511814	0.787519	0.891704
5	1	0	1.511814	0.787519	-0.891704
6	1	0	0	1.055667	0
7	1	0	0.066467	-1.27276	0.876534
8	1	0	0.066467	-1.27276	-0.876534
9	1	0	2.559876	-1.62827	0.882863
10	1	0	2.559876	-1.62827	-0.882863
11	1	0	1.737199	-2.9193	0
12	6	0	-1.7083	1.456321	0
13	6	0	-2.89432	1.653267	0
14	1	0	-3.94338	1.837016	0

TS2 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	-0.85318	1.239488	0.230557
2	6	0	-1.5754	0.098292	-0.4676
3	6	0	-1.33993	-1.24018	0.227276
4	1	0	-1.13992	1.333647	1.282717
5	1	0	0.258522	1.018586	0.232056
6	1	0	-0.97316	2.203272	-0.27097
7	1	0	-2.64986	0.320323	-0.49612
8	1	0	-1.24233	0.03988	-1.51009
9	1	0	-1.68809	-1.20722	1.26518
10	1	0	-0.2714	-1.48267	0.240443
11	1	0	-1.86586	-2.05371	-0.28008
12	6	0	1.831535	0.277485	0.062761
13	6	0	2.892219	-0.2787	-0.09207
14	1	0	3.840643	-0.75046	-0.2287

TS2 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-0.93341	1.232086	0.23765
2	6	0	-1.68571	0.109399	-0.46115
3	6	0	-1.47364	-1.23853	0.224265
4	1	0	-1.21442	1.327576	1.291195
5	1	0	0.167855	0.993016	0.231849
6	1	0	-1.04014	2.200258	-0.25813
7	1	0	-2.75543	0.353445	-0.47898
8	1	0	-1.36299	0.049413	-1.50675
9	1	0	-1.8129	-1.2046	1.264943
10	1	0	-0.41081	-1.50516	0.228265
11	1	0	-2.01982	-2.03827	-0.28324
12	6	0	1.773451	0.209942	0.062728
13	6	0	2.873681	-0.26987	-0.08625
14	1	0	3.847762	-0.68801	-0.21828

TS2 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0.84641	1.248911	-0.22992
2	6	0	1.505995	0.09834	0.51204
3	6	0	1.381485	-1.22182	-0.24375
4	1	0	1.235833	1.370217	-1.24356
5	1	0	-0.25628	1.026053	-0.34904
6	1	0	0.904147	2.198695	0.303812
7	1	0	2.563179	0.336992	0.669941
8	1	0	1.057333	0.001308	1.504974
9	1	0	1.841332	-1.14787	-1.23292
10	1	0	0.329664	-1.48742	-0.38256
11	1	0	1.867431	-2.03794	0.293995
12	6	0	-1.80973	0.224183	-0.13041
13	6	0	-2.87678	-0.27472	0.1116
14	1	0	-3.82696	-0.70942	0.317973

Rad1 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	1.334109	-0.08146	0
2	6	0	0	0.585456	0
3	6	0	-1.16246	-0.42351	0

4	1	0	1.760321	-0.45228	0.92525
5	1	0	1.760321	-0.45228	-0.92525
6	1	0	-0.09436	1.233625	0.879602
7	1	0	-0.09436	1.233625	-0.879602
8	1	0	-1.11581	-1.06695	0.883891
9	1	0	-1.11581	-1.06695	-0.883891
10	1	0	-2.13023	0.088242	0

Rad1 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	1.332314	-0.0864	0
2	6	0	0	0.583665	0
3	6	0	-1.16553	-0.4243	0
4	1	0	1.77846	-0.42773	0.926891
5	1	0	1.77846	-0.42773	-0.926891
6	1	0	-0.09331	1.230156	0.880226
7	1	0	-0.09331	1.230156	-0.880226
8	1	0	-1.12013	-1.06704	0.884015
9	1	0	-1.12013	-1.06704	-0.884015
10	1	0	-2.13077	0.091464	0

Rad1 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	1.330297	-0.08791	0
2	6	0	0	0.584016	0
3	6	0	-1.16456	-0.42396	0
4	1	0	1.777684	-0.42576	0.92599
5	1	0	1.777684	-0.42576	-0.92599
6	1	0	-0.09201	1.228992	0.878962
7	1	0	-0.09201	1.228992	-0.878962
8	1	0	-1.11892	-1.06537	0.882734
9	1	0	-1.11892	-1.06537	-0.882734
10	1	0	-2.12792	0.091391	0

Rad2 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	1.29332	-0.29713	-0.04169
2	6	0	0.078055	0.560149	0.058357

3	6	0	-1.21806	-0.24639	-0.04163
4	1	0	1.289062	-1.29507	0.383756
5	1	0	2.251427	0.123152	-0.32285
6	1	0	0.078201	1.115599	1.01197
7	1	0	0.100437	1.328645	-0.72464
8	1	0	-1.26673	-0.99905	0.752403
9	1	0	-1.27444	-0.77	-1.00068
10	1	0	-2.09783	0.396956	0.049775

Rad2 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-1.29539	-0.29573	-0.03566
2	6	0	-0.07823	0.559853	0.055885
3	6	0	1.219341	-0.24596	-0.04074
4	1	0	-1.28155	-1.30586	0.359556
5	1	0	-2.25311	0.121387	-0.32205
6	1	0	-0.10314	1.325457	-0.72925
7	1	0	-0.07952	1.117846	1.00752
8	1	0	1.278001	-0.77105	-0.99857
9	1	0	1.267571	-0.99584	0.755384
10	1	0	2.097442	0.399054	0.05048

Rad2 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	1.294314	-0.29595	-0.03271
2	6	0	0.078516	0.560004	0.052449
3	6	0	-1.21851	-0.24527	-0.03827
4	1	0	1.270289	-1.31489	0.333795
5	1	0	2.254857	0.122512	-0.30177
6	1	0	0.08245	1.124496	0.997913
7	1	0	0.104938	1.318871	-0.73689
8	1	0	-1.27015	-0.98366	0.76579
9	1	0	-1.27368	-0.78099	-0.9884
10	1	0	-2.09464	0.400964	0.040701

Rad3 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0.013517	-0.19955	1.291656

2	6	0	0.013517	0.545175	0
3	6	0	0.013517	-0.19955	-1.29166
4	1	0	-0.95967	-0.67769	1.492673
5	1	0	0.757522	-1.00602	1.281653
6	1	0	0.232119	0.453823	2.141081
7	1	0	-0.30325	1.58332	0
8	1	0	-0.95967	-0.67769	-1.49267
9	1	0	0.757522	-1.00602	-1.28165
10	1	0	0.232119	0.453823	-2.14108

Rad3 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	1.290318	-0.20051	0.00466
2	6	0	0	0.543854	-0.05633
3	6	0	-1.29032	-0.20051	0.00466
4	1	0	1.461126	-0.64176	1.00042
5	1	0	1.297839	-1.0358	-0.707
6	1	0	2.145931	0.44247	-0.21617
7	1	0	0	1.613125	0.127551
8	1	0	-1.46113	-0.64176	1.00042
9	1	0	-1.29784	-1.0358	-0.707
10	1	0	-2.14593	0.44247	-0.21617

Rad3 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0.01187	-0.20006	1.29024
2	6	0	0.01187	0.545089	0
3	6	0	0.01187	-0.20006	-1.29024
4	1	0	-0.952	-0.69989	1.470735
5	1	0	0.772634	-0.98829	1.28941
6	1	0	0.201046	0.456025	2.141257
7	1	0	-0.25701	1.594507	0
8	1	0	-0.952	-0.69989	-1.47074
9	1	0	0.772634	-0.98829	-1.28941
10	1	0	0.201046	0.456025	-2.14126

$C_2H_4 + C_2H$

C_2H_4 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0	0	0.66361
2	6	0	0	0	-0.66361
3	1	0	0	0.924043	-1.234204
4	1	0	0	-0.92404	-1.234204
5	1	0	0	0.924043	1.234204
6	1	0	0	-0.92404	1.234204

C_2H_4 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	0	0	0.665065
2	6	0	0	0	-0.665065
3	1	0	0	0.925118	-1.233675
4	1	0	0	-0.92512	-1.233675
5	1	0	0	0.925118	1.233675
6	1	0	0	-0.92512	1.233675

C_2H_4 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0	0	0.662931
2	6	0	0	0	-0.662931
3	1	0	0	0.923605	-1.230739
4	1	0	0	-0.92361	-1.230739
5	1	0	0	0.923605	1.230739
6	1	0	0	-0.92361	1.230739

TSabs (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	-2.11233	0.284171	0
2	6	0	-1.02795	1.039762	0
3	1	0	0	0.539127	0
4	1	0	-1.00468	2.125255	0
5	1	0	-2.04994	-0.79995	0
6	1	0	-3.10691	0.723261	0
7	6	0	1.331932	-0.37819	0

8	6	0	2.306541	-1.09094	0
9	1	0	3.172375	-1.71649	0

TSabs (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-2.1759	0.400322	0
2	6	0	-1.05201	1.100789	0
3	1	0	-0.05584	0.555241	0
4	1	0	-0.98003	2.184165	0
5	1	0	-2.1688	-0.68544	0
6	1	0	-3.14498	0.892843	0
7	6	0	1.269464	-0.43264	0
8	6	0	2.232612	-1.16413	0
9	1	0	3.085195	-1.80786	0

TSabs (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-2.06049	0.140711	0
2	6	0	-1.07872	1.021826	0
3	1	0	0	0.646513	0
4	1	0	-1.18531	2.100664	0
5	1	0	-1.86297	-0.92539	0
6	1	0	-3.09899	0.456365	0
7	6	0	1.343491	-0.26696	0
8	6	0	2.295854	-1.00148	0
9	1	0	3.146456	-1.64272	0

TSadd1 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	1.340781	-0.66552	0.080546
2	6	0	1.318972	0.678498	0.070267
3	1	0	1.542078	1.240587	-0.83073
4	1	0	1.077929	1.247264	0.962115
5	1	0	1.580932	-1.23384	-0.81209
6	1	0	1.117035	-1.22797	0.980911
7	6	0	-0.97864	-0.02268	-0.42465
8	6	0	-2.05701	0.0024	0.140393
9	1	0	-3.06261	0.017767	0.500447

TSadd1 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	1.345031	-0.67373	0.066454
2	6	0	1.344935	0.673792	0.066399
3	1	0	1.538792	1.236448	-0.84086
4	1	0	1.150612	1.238021	0.972524
5	1	0	1.538978	-1.23643	-0.84075
6	1	0	1.150801	-1.2379	0.972627
7	6	0	-0.97627	-0.00013	-0.37179
8	6	0	-2.09187	0.000012	0.1209
9	1	0	-3.11014	0.000141	0.444661

TSadd1 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	1.372048	-0.6713	0.057855
2	6	0	1.373417	0.670434	0.058444
3	1	0	1.547646	1.233287	-0.85081
4	1	0	1.197602	1.233959	0.966862
5	1	0	1.54514	-1.23371	-0.85189
6	1	0	1.195097	-1.23527	0.965771
7	6	0	-1.00105	0.001601	-0.32452
8	6	0	-2.13281	-0.0002	0.102727
9	1	0	-3.15516	-0.00149	0.402997

TSadd2 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0.845559	-0.71497	0
2	6	0	1.051817	0.763126	-1E-06
3	1	0	1.196044	1.29042	0.932939
4	1	0	1.196034	1.290429	-0.93294
5	1	0	1.144514	-1.24661	0.903941
6	1	0	1.1445	-1.24661	-0.90394
7	6	0	-0.51427	-0.20675	0.000003
8	6	0	-1.7283	0.036849	-3E-06
9	1	0	-2.60998	0.642841	0.000014

TSadd2 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-0.84729	-0.71618	0.000144
2	6	0	-1.04971	0.764061	0.000081
3	1	0	-1.19207	1.289951	-0.93408
4	1	0	-1.19044	1.290053	0.934435
5	1	0	-1.14245	-1.24601	-0.90527
6	1	0	-1.14121	-1.24583	0.906068
7	6	0	0.510409	-0.20398	-0.00065
8	6	0	1.727528	0.037128	0.000324
9	1	0	2.620566	0.625607	-0.00054

TSadd2 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-0.85126	-0.71495	-1.2E-05
2	6	0	-1.03538	0.7676	-6E-06
3	1	0	-1.17158	1.293055	-0.93288
4	1	0	-1.17162	1.29296	0.932912
5	1	0	-1.14675	-1.24034	-0.90494
6	1	0	-1.14699	-1.24044	0.904782
7	6	0	0.505159	-0.20418	0.000052
8	6	0	1.716932	0.034757	-6E-06
9	1	0	2.624187	0.595369	-3.5E-05

C_2H_3 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0.050133	-0.58592	0
2	6	0	0.050133	0.723276	0
3	1	0	-0.70256	1.500635	0
4	1	0	0.976008	-1.15821	0
5	1	0	-0.87505	-1.16659	0

C_2H_3 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	0.049782	-0.58778	0
2	6	0	0.049782	0.723389	0

3	1	0	-0.69439	1.508138	0
4	1	0	0.97582	-1.15888	0
5	1	0	-0.87881	-1.16293	0

C_2H_3 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0.049343	-0.58544	0
2	6	0	0.049343	0.720095	0
3	1	0	-0.68853	1.50853	0
4	1	0	0.974142	-1.15627	0
5	1	0	-0.87773	-1.16016	0

Adduct1 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	-0.63662	0.636119	-0.000285
2	6	0	-1.6131	-0.50289	-0.000026
3	1	0	-1.82716	-1.01877	0.927608
4	1	0	-1.82448	-1.0214	-0.926814
5	1	0	-0.79111	1.272264	0.879196
6	1	0	-0.79066	1.27147	-0.880452
7	6	0	0.756528	0.156113	0.000336
8	6	0	1.884654	-0.26687	0.000072
9	1	0	2.884613	-0.63841	-0.00012

Adduct1 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-0.63535	0.634847	-0.000288
2	6	0	-1.6128	-0.5033	-0.000005
3	1	0	-1.85365	-1.00224	0.930129
4	1	0	-1.85071	-1.00516	-0.929332
5	1	0	-0.78544	1.269728	0.880122
6	1	0	-0.78499	1.268893	-0.881407
7	6	0	0.757134	0.153727	0.000277
8	6	0	1.888569	-0.26767	0.000082
9	1	0	2.889487	-0.63686	0.000091

Adduct1 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-0.6326	0.635254	-0.000297
2	6	0	-1.60767	-0.50367	-0.000002
3	1	0	-1.85151	-0.99944	0.929222
4	1	0	-1.84833	-1.00257	-0.928386
5	1	0	-0.78158	1.2684	0.8791
6	1	0	-0.78114	1.267556	-0.880411
7	6	0	0.757261	0.154718	0.000248
8	6	0	1.880549	-0.26868	0.00011
9	1	0	2.877317	-0.63971	0.000121

Adduct2 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	-0.91136	-0.72454	0.000136
2	6	0	-0.83039	0.789076	0.000111
3	1	0	-1.08312	1.315176	-0.91597
4	1	0	-1.08208	1.315574	0.916254
5	1	0	-1.22777	-1.2176	-0.91496
6	1	0	-1.2268	-1.21806	0.915303
7	6	0	0.400877	-0.04644	-0.00046
8	6	0	1.689105	-0.14032	0.000075
9	1	0	2.530392	0.538295	0.00021

Adduct2 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-0.91157	-0.72618	0.000061
2	6	0	-0.8324	0.78995	0.000055
3	1	0	-1.08209	1.314325	-0.91737
4	1	0	-1.08155	1.314435	0.91756
5	1	0	-1.22279	-1.21812	-0.91687
6	1	0	-1.22227	-1.21829	0.917079
7	6	0	0.39988	-0.04648	-0.00025
8	6	0	1.689274	-0.13785	0.000053
9	1	0	2.537639	0.531024	0.000059

Adduct2 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-0.91101	-0.72531	0.000061
2	6	0	-0.83125	0.789431	0.000054
3	1	0	-1.07755	1.312073	-0.91631
4	1	0	-1.07701	1.312184	0.916489
5	1	0	-1.21895	-1.21574	-0.91578
6	1	0	-1.21844	-1.21591	0.915982
7	6	0	0.400711	-0.047	-0.00024
8	6	0	1.684192	-0.13663	0.00005
9	1	0	2.536059	0.524425	0.00006

C_3H_6 + C_2H

C_3H_6 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	-1.23003	-0.16252	0
2	1	0	-1.80474	0.145816	-0.88054
3	1	0	-1.80474	0.145808	0.880545
4	1	0	-1.16401	-1.25463	-0.000005
5	6	0	0.134527	0.459698	0
6	1	0	0.16908	1.54875	0
7	6	0	1.275619	-0.22248	0
8	1	0	2.239868	0.275894	0
9	1	0	1.283819	-1.30986	0

C_3H_6 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-1.23178	-0.1632	0
2	1	0	-1.80368	0.148501	-0.880366
3	1	0	-1.80367	0.148499	0.880367
4	1	0	-1.16749	-1.25449	-0.000002
5	6	0	0.133494	0.458881	0
6	1	0	0.169157	1.548071	0
7	6	0	1.278102	-0.22255	0
8	1	0	2.239529	0.280633	0
9	1	0	1.28723	-1.31001	0

C_3H_6 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-1.1342	-0.50318	0
2	1	0	-1.76962	-0.36318	-0.878781
3	1	0	-1.76962	-0.36318	0.878781
4	1	0	-0.76716	-1.53072	0
5	6	0	0	0.47685	0
6	1	0	-0.27233	1.530208	0
7	6	0	1.28615	0.146466	0
8	1	0	2.065794	0.898655	0
9	1	0	1.601248	-0.89262	0

PRC1 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0.524623	-0.31412	-0.00003
2	1	0	0.085204	-0.79665	0.881646
3	1	0	0.08532	-0.79623	-0.881996
4	1	0	0.227481	0.739657	0.00019
5	6	0	2.01943	-0.45119	0.000005
6	1	0	2.409289	-1.46853	0.000077
7	6	0	2.869601	0.570272	-0.000002
8	1	0	3.944304	0.418665	0.000069
9	1	0	2.517675	1.599193	0.000004
10	6	0	-2.48535	0.028307	0.000037
11	6	0	-3.68265	0.168684	-0.000003
12	1	0	-4.7432	0.292144	-0.000035

PRC1 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-0.53182	-0.31583	-0.000274
2	1	0	-0.09698	-0.79945	-0.882916
3	1	0	-0.09636	-0.80016	0.881664
4	1	0	-0.23363	0.737401	0.000017
5	6	0	-2.02727	-0.45082	0.000151
6	1	0	-2.4198	-1.46729	0.000527
7	6	0	-2.87936	0.572662	0.000075
8	1	0	-3.95335	0.417031	0.000367

9	1	0	-2.52633	1.601216	-0.000222
10	6	0	2.500095	0.028433	-0.000044
11	6	0	3.699415	0.168675	0.00014
12	1	0	4.760131	0.292532	0.000278

PRC1 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0.524624	-0.31063	-0.000079
2	1	0	0.090379	-0.79433	0.88054
3	1	0	0.090579	-0.79393	-0.881018
4	1	0	0.230065	0.741536	0.000113
5	6	0	2.018695	-0.44975	0.000041
6	1	0	2.40645	-1.46588	0.000127
7	6	0	2.871145	0.567906	0.00002
8	1	0	3.942853	0.409337	0.000078
9	1	0	2.521945	1.595845	-0.000052
10	6	0	-2.4898	0.027573	0.000039
11	6	0	-3.68178	0.167379	0.000015
12	1	0	-4.73957	0.292544	-0.000005

PRC2 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	-0.82684	1.154827	0.001107
2	1	0	-0.22228	1.401159	-0.88089
3	1	0	-0.22274	1.401183	0.883373
4	1	0	-1.70735	1.803869	0.000741
5	6	0	-1.21707	-0.29386	0.000992
6	1	0	-0.39794	-1.01459	0.002214
7	6	0	-2.46966	-0.73784	-0.000468
8	1	0	-2.70118	-1.79821	-0.000517
9	1	0	-3.31297	-0.05108	-0.001675
10	6	0	2.057011	0.065145	-0.005359
11	6	0	3.186185	-0.35701	0.00199
12	1	0	4.186694	-0.72992	0.007182

PRC2 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-0.82808	1.150436	0.00122

2	1	0	-0.22342	1.391419	-0.881553
3	1	0	-0.22387	1.390833	0.884417
4	1	0	-1.70422	1.804962	0.001131
5	6	0	-1.22984	-0.29568	0.000641
6	1	0	-0.41918	-1.02613	0.001016
7	6	0	-2.48847	-0.73081	-0.000228
8	1	0	-2.72364	-1.79016	-0.000587
9	1	0	-3.32536	-0.03624	-0.000668
10	6	0	2.074478	0.063157	-0.006083
11	6	0	3.207168	-0.35504	0.002313
12	1	0	4.208206	-0.72709	0.009069

PRC2 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-0.82346	1.150425	0.000975
2	1	0	-0.21983	1.390156	-0.88074
3	1	0	-0.22015	1.390488	0.882775
4	1	0	-1.69898	1.802582	0.000578
5	6	0	-1.22302	-0.29515	0.001136
6	1	0	-0.4128	-1.02305	0.002813
7	6	0	-2.47706	-0.73082	-0.00059
8	1	0	-2.70982	-1.78892	-0.000427
9	1	0	-3.31377	-0.039	-0.002243
10	6	0	2.065367	0.064229	-0.004488
11	6	0	3.189594	-0.35568	0.001456
12	1	0	4.186778	-0.73028	0.006309

PRC3 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0.947663	1.287329	0.181262
2	1	0	0.128051	1.669119	-0.43849
3	1	0	1.711738	2.071304	0.224976
4	1	0	0.560357	1.124281	1.19104
5	6	0	1.512424	0.022834	-0.39427
6	1	0	1.918165	0.089579	-1.40351
7	6	0	1.543942	-1.14923	0.237913
8	1	0	1.966666	-2.03722	-0.22136
9	1	0	1.155914	-1.2548	1.249116
10	6	0	-3.09549	0.066872	0.032383

11	6	0	-1.98413	-0.37892	-0.11678
12	1	0	-0.98737	-0.75557	-0.24478

PRC3 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	1.03179	-1.28619	-0.18031
2	1	0	0.235008	-1.71039	0.44117
3	1	0	1.836093	-2.02812	-0.22205
4	1	0	0.63801	-1.14485	-1.19057
5	6	0	1.530815	0.005737	0.395791
6	1	0	1.933946	-0.03811	1.407408
7	6	0	1.509387	1.179428	-0.2381
8	1	0	1.887132	2.08469	0.226236
9	1	0	1.12235	1.265793	-1.2516
10	6	0	-3.15401	-0.0776	-0.02842
11	6	0	-2.0239	0.327262	0.110924
12	1	0	-1.01708	0.679186	0.230084

PRC3 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0.940653	1.284614	0.175086
2	1	0	0.168957	1.674731	-0.49512
3	1	0	1.702873	2.062202	0.27442
4	1	0	0.487899	1.114458	1.153555
5	6	0	1.539924	0.025832	-0.37481
6	1	0	2.001833	0.099339	-1.35719
7	6	0	1.5417	-1.14868	0.248928
8	1	0	1.994579	-2.02721	-0.19496
9	1	0	1.098191	-1.26347	1.234161
10	6	0	-3.08879	0.07411	0.074797
11	6	0	-2.00373	-0.38239	-0.16461
12	1	0	-1.03285	-0.78098	-0.37122

TSabs1 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	-0.91785	-1.20315	0.000015
2	1	0	-1.05707	-1.82559	-0.889907
3	1	0	-1.05686	-1.82551	0.890027
4	1	0	0.175104	-0.88498	-0.000126
5	6	0	-1.78862	0.0129	0.000063

6	1	0	-2.86291	-0.17556	0.000189
7	6	0	-1.34529	1.265494	-0.000038
8	1	0	-2.02783	2.109112	0.000002
9	1	0	-0.28028	1.488384	-0.000161
10	6	0	1.750754	-0.25306	-0.0002
11	6	0	2.847938	0.251051	0.000094
12	1	0	3.828294	0.674731	0.000368

TSabs1 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-0.94409	-1.20932	0.000002
2	1	0	-1.06099	-1.83579	-0.889669
3	1	0	-1.06093	-1.83576	0.889706
4	1	0	0.128324	-0.84902	-0.000043
5	6	0	-1.86686	-0.03152	0.000013
6	1	0	-2.93261	-0.26382	0.000037
7	6	0	-1.4798	1.242294	-0.000005
8	1	0	-2.20193	2.05212	0.000004
9	1	0	-0.42575	1.512802	-0.00003
10	6	0	1.732813	-0.18412	-0.000036
11	6	0	2.867215	0.234741	0.000021
12	1	0	3.871232	0.599441	0.000057

TSabs1 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-0.89676	-1.20313	0.00003
2	1	0	-1.02217	-1.82577	-0.888865
3	1	0	-1.0218	-1.82554	0.889137
4	1	0	0.186205	-0.86086	-0.000229
5	6	0	-1.79825	-0.0113	0.000067
6	1	0	-2.86536	-0.22844	0.000179
7	6	0	-1.39496	1.253054	-0.000032
8	1	0	-2.10569	2.070399	0.000002
9	1	0	-0.33948	1.510125	-0.000143
10	6	0	1.756603	-0.18597	-0.000293
11	6	0	2.881409	0.239097	0.000133
12	1	0	3.880039	0.60958	0.000481

TSabs2 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	0.631438	0.968335	-0.070292
2	1	0	0.600381	1.872525	0.545391
3	1	0	-0.42568	0.567777	-0.053417
4	1	0	0.847954	1.234553	-1.107918
5	6	0	1.573038	-0.058	0.461557
6	1	0	1.460159	-0.3231	1.511649
7	6	0	2.516485	-0.65232	-0.26532
8	1	0	3.184934	-1.39278	0.161985
9	1	0	2.654801	-0.41286	-1.316851
10	6	0	-2.1246	-0.00718	-0.051546
11	6	0	-3.26968	-0.38763	-0.029741
12	1	0	-4.2826	-0.72536	-0.008784

TSabs2 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	0.702024	0.974196	-0.070959
2	1	0	0.670215	1.875272	0.548422
3	1	0	-0.34605	0.567164	-0.05183
4	1	0	0.91654	1.244952	-1.107552
5	6	0	1.651944	-0.04862	0.456669
6	1	0	1.539677	-0.3231	1.504645
7	6	0	2.603949	-0.63283	-0.271623
8	1	0	3.274299	-1.37071	0.156853
9	1	0	2.743118	-0.38537	-1.321248
10	6	0	-2.09316	-0.00274	-0.055663
11	6	0	-3.24567	-0.3668	-0.034493
12	1	0	-4.26239	-0.69368	-0.014223

TSabs2 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	0.635318	0.961956	-0.077216
2	1	0	0.606007	1.871833	0.525822
3	1	0	-0.41395	0.552861	-0.039841
4	1	0	0.838303	1.211804	-1.119128
5	6	0	1.586929	-0.05058	0.461413

6	1	0	1.487089	-0.29905	1.514999
7	6	0	2.523679	-0.65407	-0.263507
8	1	0	3.195678	-1.38336	0.172599
9	1	0	2.649574	-0.43248	-1.318619
10	6	0	-2.14445	0.001287	-0.048651
11	6	0	-3.28079	-0.38916	-0.027029
12	1	0	-4.28681	-0.73826	-0.005892

TSabs3 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	1.71388	-1.1836	0.000006
2	1	0	1.46213	-1.78179	-0.881758
3	1	0	1.462497	-1.78155	0.882044
4	1	0	2.792715	-1.00107	-0.000236
5	6	0	0.964358	0.11002	-0.000008
6	1	0	-0.16345	0.005611	-0.000012
7	6	0	1.457476	1.339883	0.000009
8	1	0	0.814013	2.21351	0.000018
9	1	0	2.531887	1.511874	0.000006
10	6	0	-1.86167	-0.03626	-0.000061
11	6	0	-3.06808	-0.07359	0.000027
12	1	0	-4.13555	-0.10531	0.000095

TSabs3 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	1.779704	-1.2081	-0.000053
2	1	0	1.517927	-1.80121	-0.881752
3	1	0	1.518835	-1.80096	0.882081
4	1	0	2.860573	-1.04069	-0.000646
5	6	0	1.047692	0.096162	0.000141
6	1	0	-0.07564	0.009519	0.000505
7	6	0	1.561385	1.320594	-0.000057
8	1	0	0.929529	2.202517	0.00009
9	1	0	2.638554	1.473995	-0.000388
10	6	0	-1.81299	-0.03477	0.000109
11	6	0	-3.02104	-0.08296	-0.000113
12	1	0	-4.08831	-0.12584	-0.000213

TSabs3 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-1.86226	-1.09756	-0.000005
2	1	0	-1.68661	-1.71972	0.880815
3	1	0	-1.68655	-1.71975	-0.880796
4	1	0	-2.90678	-0.77866	-0.000047
5	6	0	-0.95612	0.090205	0.00001
6	1	0	0.14954	-0.15217	0.000037
7	6	0	-1.28245	1.372241	-0.000004
8	1	0	-0.52641	2.14815	0.000011
9	1	0	-2.32332	1.683485	-0.00003
10	6	0	1.854227	-0.13562	0.000017
11	6	0	3.0564	-0.12074	-0.000011
12	1	0	4.121365	-0.11255	-0.000034

TSabs4 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	-2.76803	-0.25006	-0.000043
2	1	0	-3.17559	-0.75675	-0.88138
3	1	0	-3.12349	0.783461	-0.00054
4	1	0	-3.17559	-0.7559	0.881782
5	6	0	-1.26759	-0.30873	0.000001
6	1	0	-0.81295	-1.29885	0.000525
7	6	0	-0.4801	0.755965	-0.00056
8	1	0	0.652111	0.611183	-0.00046
9	1	0	-0.81255	1.79085	-0.00098
10	6	0	2.19751	0.124519	0.002264
11	6	0	3.3355	-0.27908	-0.00103
12	1	0	4.34431	-0.62974	-0.00276

TSabs4 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-2.87436	-0.25	0.000101
2	1	0	-3.28165	-0.75532	-0.88149
3	1	0	-3.2265	0.784354	0.000335
4	1	0	-3.28143	-0.75565	0.881613
5	6	0	-1.37395	-0.31406	-0.0001

6	1	0	-0.92254	-1.30583	-0.00034
7	6	0	-0.57993	0.749034	-2.4E-05
8	1	0	0.544352	0.602275	-0.00019
9	1	0	-0.91285	1.78391	0.000205
10	6	0	2.12686	0.113065	-0.00015
11	6	0	3.272114	-0.27606	0.000144
12	1	0	4.285003	-0.61546	0.000274

TSabs4 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-2.72447	-0.30558	0.000081
2	1	0	-3.09935	-0.83451	-0.879776
3	1	0	-3.13585	0.704438	0.000095
4	1	0	-3.09913	-0.83446	0.880062
5	6	0	-1.22436	-0.28383	-0.000098
6	1	0	-0.71726	-1.24608	-0.000241
7	6	0	-0.49287	0.817382	-0.000138
8	1	0	0.643029	0.723223	-0.000373
9	1	0	-0.87213	1.834141	0.000051
10	6	0	2.171523	0.158571	0.000296
11	6	0	3.27438	-0.32159	-0.000042
12	1	0	4.255423	-0.73646	-0.00041

TSabs5 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	1.412427	-1.20882	-0.000068
2	1	0	1.841661	-1.69793	-0.881048
3	1	0	0.331532	-1.37641	-0.000489
4	1	0	1.840973	-1.69802	0.881194
5	6	0	1.728699	0.257007	0.000143
6	1	0	2.785243	0.530837	0.000515
7	6	0	0.83099	1.230619	-0.000116
8	1	0	1.043514	2.294622	0.000097
9	1	0	-0.27807	0.959013	-0.000526
10	6	0	-1.77035	0.294912	0.000005
11	6	0	-2.83178	-0.28174	0.000058
12	1	0	-3.78475	-0.76397	0.000124

TSabs5 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	1.553372	-1.21433	0.000097
2	1	0	2.002646	-1.68334	-0.881161
3	1	0	0.481235	-1.42944	0.000502
4	1	0	2.003245	-1.68301	0.881225
5	6	0	1.806221	0.263752	-0.000253
6	1	0	2.849744	0.583696	-0.000792
7	6	0	0.86684	1.201009	0.00009
8	1	0	1.04221	2.271683	-0.000169
9	1	0	-0.22434	0.888899	0.000674
10	6	0	-1.74131	0.192948	0.000323
11	6	0	-2.84824	-0.29515	-0.000224
12	1	0	-3.83114	-0.7134	-0.000672

TSabs5 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-1.45721	-1.19612	-0.000062
2	1	0	-1.90177	-1.6684	0.879615
3	1	0	-0.38462	-1.39737	-0.000434
4	1	0	-1.90237	-1.66829	-0.879495
5	6	0	-1.73106	0.276784	0.000135
6	1	0	-2.77831	0.578968	0.000485
7	6	0	-0.81324	1.228358	-0.000097
8	1	0	-1.00325	2.294764	0.000096
9	1	0	0.289138	0.936089	-0.000505
10	6	0	1.771675	0.226475	-0.000037
11	6	0	2.869028	-0.26639	0.000073
12	1	0	3.846016	-0.69038	0.000167

TSadd1 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	1.320235	-1.13025	0.147376
2	1	0	2.380147	-1.37965	0.022563
3	1	0	0.734727	-1.88021	-0.391205
4	1	0	1.064599	-1.18709	1.208035
5	6	0	1.042904	0.232977	-0.400545

6	1	0	1.187973	0.374609	-1.469823
7	6	0	0.677546	1.296964	0.346275
8	1	0	0.515791	2.272108	-0.099663
9	1	0	0.526092	1.203353	1.417722
10	6	0	-1.3455	0.208088	-0.444811
11	6	0	-2.24399	-0.36732	0.14769
12	1	0	-3.1165	-0.84586	0.536466

TSadd1 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	1.525043	-1.064496	0.186666
2	1	0	2.602777	-1.207226	0.052157
3	1	0	1.015579	-1.880275	-0.33334
4	1	0	1.288188	-1.126683	1.250941
5	6	0	1.108327	0.25163	-0.384907
6	1	0	1.233044	0.387645	-1.457351
7	6	0	0.625722	1.285795	0.342803
8	1	0	0.363521	2.228492	-0.123962
9	1	0	0.486984	1.197545	1.416273
10	6	0	-1.294602	0.032293	-0.414284
11	6	0	-2.282796	-0.404675	0.156772
12	1	0	-3.200094	-0.796696	0.540162

TSadd1 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	1.394806	-1.09399	0.157417
2	1	0	2.46177	-1.2905	0.016915
3	1	0	0.842773	-1.8768	-0.366083
4	1	0	1.158995	-1.14997	1.220367
5	6	0	1.046993	0.244715	-0.403954
6	1	0	1.168827	0.37847	-1.475414
7	6	0	0.640769	1.301012	0.331999
8	1	0	0.429934	2.257926	-0.128083
9	1	0	0.508015	1.215969	1.404872
10	6	0	-1.34918	0.138709	-0.42103
11	6	0	-2.29756	-0.37623	0.136087
12	1	0	-3.18529	-0.82041	0.52431

TSadd2 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	-1.67759	-0.68844	-0.195319
2	1	0	-2.67661	-0.23318	-0.26087
3	1	0	-1.78874	-1.65729	0.300144
4	1	0	-1.33182	-0.87304	-1.218018
5	6	0	-0.71708	0.195192	0.532092
6	1	0	-0.7516	0.255128	1.614051
7	6	0	0.098667	1.218422	-0.190712
8	1	0	0.363055	2.119163	0.364532
9	1	0	-0.21268	1.444546	-1.212681
10	6	0	1.023521	0.106315	-0.053662
11	6	0	1.939491	-0.72904	-0.052644
12	1	0	2.396293	-1.67002	0.174308

TSadd2 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-1.67845	-0.6889	-0.19521
2	1	0	-2.67678	-0.2319	-0.25175
3	1	0	-1.78582	-1.65917	0.297485
4	1	0	-1.33842	-0.86863	-1.220394
5	6	0	-0.71622	0.194022	0.532002
6	1	0	-0.74484	0.250219	1.614554
7	6	0	0.097856	1.219744	-0.19097
8	1	0	0.366497	2.11764	0.365801
9	1	0	-0.21222	1.442949	-1.213555
10	6	0	1.019749	0.105703	-0.053347
11	6	0	1.939598	-0.72881	-0.052067
12	1	0	2.416355	-1.66164	0.165412

TSadd2 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-1.67051	-0.68836	-0.194497
2	1	0	-2.66927	-0.2359	-0.241596
3	1	0	-1.77009	-1.66023	0.292724
4	1	0	-1.33553	-0.85945	-1.220729
5	6	0	-0.70832	0.193889	0.531711
6	1	0	-0.73289	0.249135	1.612052
7	6	0	0.099664	1.223907	-0.191564
8	1	0	0.37276	2.116809	0.366218

9	1	0	-0.21006	1.445421	-1.211857
10	6	0	1.012172	0.104014	-0.052645
11	6	0	1.921891	-0.73328	-0.051282
12	1	0	2.415706	-1.6568	0.152846

TSadd2a (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	-1.62018	-0.71326	-0.204464
2	1	0	-2.59511	-0.23353	-0.078534
3	1	0	-1.66429	-1.7219	0.213916
4	1	0	-1.40729	-0.79548	-1.274114
5	6	0	-0.54218	0.10894	0.481539
6	1	0	-0.70735	0.218703	1.556157
7	6	0	-0.08875	1.360828	-0.193581
8	1	0	0.290485	2.194711	0.381701
9	1	0	-0.26366	1.486732	-1.255002
10	6	0	0.83991	-0.19556	0.143654
11	6	0	1.972381	-0.64563	-0.078222
12	1	0	2.980063	-0.64116	-0.437676

TSadd2a (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	1.621972	-0.7126	0.204068
2	1	0	2.596544	-0.23401	0.072689
3	1	0	1.66134	-1.72182	-0.212628
4	1	0	1.412213	-0.79109	1.274359
5	6	0	0.544305	0.110245	-0.481586
6	1	0	0.704477	0.221148	-1.556418
7	6	0	0.083679	1.360864	0.194742
8	1	0	-0.30211	2.190846	-0.382092
9	1	0	0.2558	1.484372	1.257144
10	6	0	-0.83738	-0.19132	-0.142144
11	6	0	-1.97057	-0.64805	0.07773
12	1	0	-2.98032	-0.6643	0.430087

TSadd2a (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-1.62395	-0.70392	-0.20453

2	1	0	-2.595	-0.22021	-0.08003
3	1	0	-1.67197	-1.71008	0.21399
4	1	0	-1.40834	-0.78603	-1.271446
5	6	0	-0.5459	0.113148	0.483697
6	1	0	-0.70389	0.228272	1.555676
7	6	0	-0.06793	1.354868	-0.196875
8	1	0	0.32547	2.180113	0.377468
9	1	0	-0.23784	1.474993	-1.25776
10	6	0	0.832951	-0.19205	0.143334
11	6	0	1.958876	-0.65046	-0.078198
12	1	0	2.967311	-0.69655	-0.42246

Rad1 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	1.222594	0.197022	0
2	1	0	2.156081	-0.35173	0.000002
3	1	0	1.279477	1.28075	0.000001
4	6	0	-0.000001	-0.44767	-0.000001
5	1	0	0	-1.53631	0.000002
6	6	0	-1.222593	0.197022	0
7	1	0	-2.156082	-0.35173	0.000003
8	1	0	-1.279477	1.28075	0.000001

Rad1 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	1.224242	-0.19767	0
2	1	0	1.279943	-1.28153	-0.000001
3	1	0	2.156167	0.353544	0
4	6	0	0	0.448492	0
5	1	0	0	1.537084	0.000001
6	6	0	-1.22424	-0.19767	0
7	1	0	-2.15617	0.353543	-0.000001
8	1	0	-1.27994	-1.28153	0.000001

Rad1 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	1.221718	0.197279	0.000076
2	1	0	2.151809	-0.35405	0.000061

3	1	0	1.277664	1.279484	-0.000233
4	6	0	-3.4E-05	-0.44738	-0.000118
5	1	0	-3.7E-05	-1.53411	0.000174
6	6	0	-1.22169	0.197295	-0.000002
7	1	0	-2.15177	-0.35404	0.000089
8	1	0	-1.27763	1.27955	0.000166

Rad2 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	1.222936	0.196943	0.000017
2	1	0	2.155868	-0.35301	-0.000164
3	1	0	1.281383	1.280658	0.000113
4	6	0	-1.9E-05	-0.44714	-0.000057
5	1	0	0.000004	-1.53591	0.000365
6	6	0	-1.22293	0.196924	-0.000041
7	1	0	-2.15598	-0.35278	-0.000009
8	1	0	-1.28118	1.280656	0.00018

Rad2 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-1.22424	-0.19767	0
2	1	0	-2.15617	0.353543	0
3	1	0	-1.27994	-1.28153	0
4	6	0	0	0.448492	0
5	1	0	0	1.537084	0
6	6	0	1.224241	-0.19767	0
7	1	0	2.156168	0.353543	0.000001
8	1	0	1.279942	-1.28153	-0.000001

Rad2 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	1.221722	0.197307	0.000021
2	1	0	2.15178	-0.35413	-0.000165
3	1	0	1.277836	1.27953	0.000076
4	6	0	-0.000021	-0.44742	-0.000049
5	1	0	0.000004	-1.53409	0.00032
6	6	0	-1.221711	0.197281	-0.000033
7	1	0	-2.151909	-0.35388	-0.000032

8	1	0	-1.277653	1.279522	0.000163

Rad3 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	-1.26596	0.080972	0.000001
2	1	0	-1.80706	-0.27344	0.883301
3	1	0	-1.80708	-0.27349	-0.883266
4	1	0	-1.29931	1.180157	-0.000031
5	6	0	0.127064	-0.40273	-0.000002
6	6	0	1.336408	0.104894	-0.000001
7	1	0	2.227329	-0.51849	0.000007
8	1	0	1.501066	1.186422	0.000001

Rad3 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	1.267133	0.080924	0
2	1	0	1.805378	-0.27452	-0.883415
3	1	0	1.805378	-0.27452	0.883415
4	1	0	1.296513	1.180019	-0.000001
5	6	0	-0.12587	-0.40144	0
6	6	0	-1.33822	0.104676	0
7	1	0	-2.22569	-0.5226	0
8	1	0	-1.49981	1.18667	0

Rad3 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	1.265254	0.080149	0
2	1	0	1.800868	-0.27706	-0.882387
3	1	0	1.800868	-0.27706	0.882387
4	1	0	1.296845	1.177435	0
5	6	0	-0.12658	-0.3976	0
6	6	0	-1.3353	0.103575	0
7	1	0	-2.22101	-0.52384	0
8	1	0	-1.49784	1.18378	0

Rad4 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	-1.14089	-0.19691	0
2	1	0	-1.71851	0.097603	0.882624
3	1	0	-1.04141	-1.285	-0.000005
4	1	0	-1.71851	0.09761	-0.882622
5	6	0	0.212556	0.474621	0.000004
6	1	0	0.208479	1.566237	-0.000009
7	6	0	1.362356	-0.15759	-0.000001
8	1	0	1.665818	-1.1972	-0.000002

Rad4 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	1.143759	-0.1981	0
2	1	0	1.717947	0.09944	-0.882973
3	1	0	1.046382	-1.28593	0
4	1	0	1.717946	0.09944	0.882973
5	6	0	-0.21083	0.473314	0
6	1	0	-0.20899	1.564838	0
7	6	0	-1.36383	-0.1566	0
8	1	0	-1.68789	-1.18948	0.000001

Rad4 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	1.141851	-0.19772	0
2	1	0	1.714561	0.100375	-0.881651
3	1	0	1.043447	-1.28349	-0.000007
4	1	0	1.714556	0.100364	0.881657
5	6	0	-0.21217	0.472717	0.000001
6	1	0	-0.21104	1.562667	-0.000002
7	6	0	-1.35919	-0.15702	0
8	1	0	-1.68445	-1.18775	-0.000001

Rad5 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	1.187524	-0.15388	0
2	1	0	1.740063	0.18653	-0.882221
3	1	0	1.172146	-1.24583	-0.000005
4	1	0	1.740061	0.186523	0.882226

5	6	0	-0.2129	0.399673	0
6	1	0	-0.30195	1.491689	0
7	6	0	-1.30503	-0.3276	0
8	1	0	-2.36791	-0.1281	-0.000001

Rad5 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	1.189513	-0.15439	0
2	1	0	1.738688	0.188802	-0.882354
3	1	0	1.17584	-1.246	-0.000003
4	1	0	1.738686	0.188796	0.882358
5	6	0	-0.21137	0.398484	0
6	1	0	-0.30467	1.49022	0
7	6	0	-1.30766	-0.32554	0
8	1	0	-2.37141	-0.13314	0.000001

Rad5 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-1.18785	-0.15432	0
2	1	0	-1.73512	0.18977	0.881092
3	1	0	-1.17487	-1.24399	-0.000003
4	1	0	-1.73512	0.189775	-0.881088
5	6	0	0.212379	0.397567	-0.000001
6	1	0	0.306295	1.487652	0.000002
7	6	0	1.304024	-0.32375	0
8	1	0	2.367505	-0.14024	0.000001

Adduct1 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	1.745434	-0.79592	0.150545
2	1	0	2.729331	-0.99609	-0.281766
3	1	0	1.109797	-1.67315	-0.048155
4	1	0	1.854899	-0.72876	1.23995
5	6	0	1.141621	0.447183	-0.405457
6	1	0	1.334227	0.70845	-1.440822
7	6	0	-0.09379	1.013325	0.237622
8	1	0	-0.33067	1.999378	-0.17633
9	1	0	0.075036	1.152006	1.314763

10	6	0	-1.25376	0.121495	0.059695
11	6	0	-2.17039	-0.64391	-0.102806
12	1	0	-2.9873	-1.31491	-0.245232

Adduct1 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-1.75979	-0.79078	0.148891
2	1	0	-1.14081	-1.67811	-0.057099
3	1	0	-2.74858	-0.97267	-0.279138
4	1	0	-1.86122	-0.72566	1.238954
5	6	0	-1.13979	0.444364	-0.406314
6	1	0	-1.35082	0.731956	-1.431066
7	6	0	0.096031	1.005965	0.239661
8	1	0	0.336199	1.991445	-0.172045
9	1	0	-0.07139	1.139331	1.317318
10	6	0	1.257805	0.117021	0.060202
11	6	0	2.184034	-0.64027	-0.104119
12	1	0	3.006875	-1.30406	-0.246849

Adduct1 (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	1.745796	-0.7968	0.147649
2	1	0	2.73844	-0.97771	-0.266982
3	1	0	1.125226	-1.67526	-0.08055
4	1	0	1.828893	-0.74698	1.238307
5	6	0	1.140569	0.447345	-0.400164
6	1	0	1.373954	0.754938	-1.412022
7	6	0	-0.09752	1.009326	0.238739
8	1	0	-0.33905	1.990168	-0.177532
9	1	0	0.064173	1.145859	1.315045
10	6	0	-1.25357	0.117438	0.058765
11	6	0	-2.1695	-0.64127	-0.10618
12	1	0	-2.98628	-1.3073	-0.24912

Adduct1a (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	-1.17385	-1.16365	-0.142019
2	1	0	-2.239102	-1.09889	0.096454

3	1	0	-0.768101	-2.08476	0.283008
4	1	0	-1.062569	-1.20965	-1.229458
5	6	0	-0.439285	0.066973	0.409978
6	1	0	-0.559586	0.087426	1.501417
7	6	0	-0.995014	1.339189	-0.162223
8	1	0	-0.82277	2.281271	0.343518
9	1	0	-1.252854	1.368393	-1.215223
10	6	0	1.006425	-0.02264	0.125053
11	6	0	2.182037	-0.0869	-0.134016
12	1	0	3.223098	-0.14165	-0.36035

Adduct1a (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-1.174753	-1.16558	-0.140634
2	1	0	-2.238305	-1.10115	0.104693
3	1	0	-0.765833	-2.08543	0.283467
4	1	0	-1.069517	-1.21179	-1.228445
5	6	0	-0.438871	0.066414	0.407899
6	1	0	-0.553345	0.088959	1.499534
7	6	0	-0.992444	1.340296	-0.163726
8	1	0	-0.846093	2.279076	0.355777
9	1	0	-1.269119	1.367882	-1.211973
10	6	0	1.006405	-0.02209	0.122053
11	6	0	2.185471	-0.08527	-0.133392
12	1	0	3.227356	-0.1402	-0.35625

Adduct1a (M06-2X/6-311++G(d,p))

			X	Y	Z
1	6	0	-1.171933	-1.16446	-0.140646
2	1	0	-2.234488	-1.09974	0.100914
3	1	0	-0.764525	-2.08222	0.284804
4	1	0	-1.062291	-1.21032	-1.226181
5	6	0	-0.437092	0.066514	0.408811
6	1	0	-0.550027	0.089791	1.498449
7	6	0	-0.988223	1.339564	-0.164047
8	1	0	-0.838423	2.278218	0.351535
9	1	0	-1.276988	1.363177	-1.207529
10	6	0	1.005591	-0.02247	0.123788
11	6	0	2.176932	-0.08541	-0.135018

12	1	0	3.215102	-0.14133	-0.359325

Adduct2 (M06-2X/6-31G(d))

			X	Y	Z
1	6	0	-1.68283	-0.61309	-0.205754
2	1	0	-2.63582	-0.08082	-0.122563
3	1	0	-1.80893	-1.6142	0.216003
4	1	0	-1.44111	-0.72402	-1.267228
5	6	0	-0.57981	0.137037	0.50654
6	1	0	-0.7282	0.285429	1.575255
7	6	0	0.159075	1.251144	-0.208732
8	1	0	0.474728	2.118761	0.364132
9	1	0	-0.1132	1.457423	-1.24152
10	6	0	0.823477	-0.0524	0.077157
11	6	0	1.847514	-0.83286	-0.018976
12	1	0	2.847969	-0.78156	-0.425492

Adduct2 (M06-2X/6-31+G(d,p))

			X	Y	Z
1	6	0	-1.68365	-0.61414	-0.20537
2	1	0	-2.63642	-0.08323	-0.114969
3	1	0	-1.80412	-1.61677	0.213573
4	1	0	-1.4458	-0.72014	-1.268053
5	6	0	-0.58027	0.136922	0.505841
6	1	0	-0.72272	0.283622	1.575498
7	6	0	0.158325	1.253738	-0.208849
8	1	0	0.478341	2.117952	0.36603
9	1	0	-0.11214	1.455899	-1.242619
10	6	0	0.822363	-0.0525	0.076814
11	6	0	1.848605	-0.83153	-0.019713
12	1	0	2.850624	-0.79228	-0.421794

Adduct2 (M06-2X/6-311++G(d,p)

			X	Y	Z
1	6	0	-1.68041	-0.61379	-0.205072

2	1	0	-2.63307	-0.08642	-0.114392
3	1	0	-1.79809	-1.61511	0.213283
4	1	0	-1.44184	-0.71829	-1.265724
5	6	0	-0.58017	0.139074	0.506016
6	1	0	-0.71919	0.286289	1.573413
7	6	0	0.158936	1.253122	-0.20981
8	1	0	0.481976	2.113976	0.363871
9	1	0	-0.10964	1.451726	-1.242151
10	6	0	0.821672	-0.05357	0.076882
11	6	0	1.842635	-0.82973	-0.01958
12	1	0	2.843834	-0.8028	-0.418915

Table S-IV: Vibartional frequencies (cm^{-1}) of reactants, pre-reaction complexes (PRCs), transition states (TSs), and products (Ps) at M06-2X level of theory using 6-31G(d), 6-31+G(d,p), and 6-311++G(d,p) basis sets.

$CH_4 + C_2H$

	CH_4	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
1380.7	1348.8093	1351.4837
1380.7	1348.8093	1351.4837
1380.7	1348.8093	1351.4837
1603.3295	1571.6606	1570.7744
1603.3296	1571.6607	1570.7744
3092.4607	3068.834	3057.6984
3215.855	3192.1135	3178.7587
3215.855	3192.1135	3178.7587
3215.855	3192.1135	3178.7587

	C_2H	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
498.058	498.058	527.6957
498.058	498.058	527.6957
2154.1031	2154.1031	2129.1792
3493.1184	3493.1184	3481.1605

	TS1	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
-452.409	-384.4045	-455.2644
84.2333	68.0603	86.8936

84.6699	68.5265	87.3462
294.1164	271.6967	215.7355
295.519	272.8521	216.9084
575.0281	579.6462	655.135
575.0327	579.6483	655.1355
1244.4372	1253.5423	1219.1624
1326.8316	1307.8064	1281.1816
1327.0746	1307.8896	1281.3419
1519.8931	1502.8978	1489.7681
1519.9148	1503.0565	1489.799
1729.7923	1914.4944	1763.0376
2169.1802	2183.2435	2151.363
3113.9206	3104.9615	3078.8321
3230.3209	3219.7556	3193.5439
3230.4086	3220.3879	3193.6217
3489.7127	3487.5175	3480.5703

	CH_3	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
388.5307	408.0541	495.743
1439.2555	1421.3224	1412.6109
1439.2918	1421.9838	1412.6735
3181.8166	3164.1231	3132.1117
3358.5855	3345.1354	3312.9154
3358.595	3346.691	3313.0428

	C_2H_2	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
640.5009	680.0443	716.2802
640.5009	680.0524	716.2802
802.7812	795.7557	805.9487
802.7812	795.764	805.9487
2125.4109	2105.9238	2099.1032
3449.2447	3429.6739	3433.6725
3557.0653	3535.5398	3542.7726

C_2H_6 + C_2H

	C_2H_6	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**

300.7232	311.3786	297.4391
820.6617	822.7083	814.3733
820.8707	824.1717	814.5011
1033.8225	1024.0674	1021.5491
1230.4481	1218.7774	1215.6688
1230.5028	1219.1522	1215.7353
1423.0911	1405.2786	1400.7122
1454.0149	1436.063	1425.8591
1534.1381	1513.2681	1508.9134
1534.1798	1513.3544	1508.9411
1537.0069	1513.3754	1509.1915
1537.0716	1513.6524	1509.2095
3076.916	3072.4445	3046.5421
3079.4157	3072.7778	3047.7954
3140.1158	3134.363	3105.367
3140.3615	3135.0262	3105.6149
3162.2576	3156.2314	3128.1347
3162.3837	3156.9468	3128.2594

	PRC	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
33.2848	51.3494	57.9257
62.8304	80.3979	78.6594
80.9198	96.4061	92.5069
100.8894	120.27	132.1001
126.5502	124.7218	153.1202
332.689	342.6653	356.1335
570.5314	584.5664	624.4445
611.9941	624.7556	662.1992
827.3151	824.969	831.9082
827.7236	828.6954	833.6148
1030.9776	1024.1994	1018.9872
1230.8557	1217.3174	1220.2959
1230.9	1220.1436	1222.3429
1425.4353	1407.4388	1408.9784
1455.4986	1438.6518	1433.8646
1530.9655	1508.4523	1508.3196
1531.4719	1510.7383	1509.039
1535.7712	1513.1136	1510.7119
1537.6341	1517.1242	1518.0946
2153.904	2139.5984	2127.356

3077.8137	3059.707	3053.0295
3082.6504	3062.9906	3058.2055
3136.7409	3122.5305	3111.1822
3141.3635	3122.9686	3113.7232
3162.5702	3143.6746	3135.0725
3169.151	3154.5325	3144.0166
3512.7916	3480.2834	3478.1175

	TS1	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
-384.0494	-294.5452	-373.984
42.343	26.7578	51.4039
66.167	49.8725	60.0007
104.92	89.2298	107.2801
133.5392	133.6376	134.9758
342.1918	337.5095	322.7442
577.3378	583.8172	636.1672
582.8834	584.2975	640.9228
801.6417	805.7987	768.7208
823.6863	822.0578	835.772
1039.3832	1030.0903	1025.2268
1182.8806	1182.1446	1161.3222
1226.3048	1215.382	1213.9691
1392.9759	1378.0455	1369.7692
1433.5601	1423.7372	1399.3027
1438.6227	1426.9612	1424.4989
1494.3487	1481.1709	1471.3877
1525.3666	1504.8889	1506.8249
1529.277	1508.566	1507.3257
1997.5299	2074.4875	2035.018
2226.8155	2348.5663	2261.2473
3085.8547	3072.8205	3061.8891
3110.8827	3103.9541	3080.5418
3157.5115	3145.1892	3131.1356
3162.1597	3148.2167	3134.7597
3180.9039	3171.823	3156.3122
3502.3251	3486.7775	3476.306

	C_2H_5	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
180.3535	131.5608	108.2502
440.2811	438.8721	439.2805
808.6763	810.3562	805.9392
999.8938	981.9979	984.7532
1094.7491	1085.2497	1082.2306
1207.0934	1194.2856	1191.7126
1430.8483	1408.4122	1403.8128
1498.1818	1477.1848	1471.435
1515.1138	1494.8884	1488.1882
1518.8842	1495.003	1488.9294
3022.0174	3014.031	2993.1661
3101.3162	3096.3804	3071.1968
3146.631	3141.7985	3117.0612
3196.6736	3190.9227	3162.4237
3297.7925	3294.402	3266.9743

C_3H_8 + C_2H

	C_3H_8	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
230.0535	217.2239	244.4172
286.3114	279.0453	299.5412
373.7757	372.7576	374.6337
755.6573	752.3492	756.0985
902.166	893.6033	892.9199
916.0176	911.6942	915.0733
945.6572	932.9713	941.6531
1091.7025	1081.9576	1080.5337
1196.083	1180.5766	1184.455
1228.3466	1212.566	1215.8769
1333.3515	1314.8092	1324.187
1386.3019	1364.3967	1371.8434
1438.9059	1415.0129	1414.1117
1449.4738	1426.1837	1425.2135
1523.6031	1497.0559	1499.4977
1526.3935	1499.2274	1501.7802
1530.6496	1503.9067	1503.6148
1545.3401	1515.7926	1520.4473
1547.1117	1519.4153	1520.5233

3079.5805	3060.7507	3053.5801
3079.5954	3062.2819	3054.8683
3084.2596	3065.9813	3062.4832
3115.0582	3097.1744	3090.6774
3149.2882	3130.8841	3120.6115
3158.6677	3140.0571	3131.4709
3161.4728	3143.5423	3134.4266
3163.1198	3145.0026	3136.3382

	PRC1	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
8.0786	43.5795	53.3831
25.3526	54.5253	61.482
41.5651	56.0807	80.2678
85.8783	69.6477	84.3594
118.8432	104.8686	108.4257
203.978	209.4662	210.284
272.2275	271.7952	271.3577
376.5236	368.1864	370.3147
544.5133	571.572	617.6744
558.2052	581.5119	635.1987
758.996	759.1255	760.3671
900.5194	890.8548	890.5372
911.4789	907.8074	908.526
935.266	924.8382	928.3126
1090.801	1085.963	1082.5454
1191.972	1178.699	1179.3575
1225.442	1212.283	1212.9668
1327.713	1314.749	1316.9187
1376.467	1359.61	1358.1168
1431.599	1408.445	1402.9869
1447.811	1422.09	1420.057
1516.425	1492.746	1490.3619
1518.062	1498.514	1496.5328
1526.263	1501.913	1500.2144
1536.205	1511.886	1509.4867
1541.781	1517.208	1516.4319
2153.948	2136.242	2124.9349
3053.972	3040.461	3023.8007

3068.469	3047.587	3034.349
3071.939	3055.692	3042.4502
3084.733	3071.417	3052.1364
3142.738	3123.153	3106.9216
3146.252	3127.512	3109.2076
3149.546	3134.517	3117.4446
3154.33	3136.952	3121.9129
3496.324	3478.424	3472.5423

	PRC2	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
44.5755	28.442	60.4094
47.0306	64.5393	66.5972
75.1985	73.8621	85.3643
92.8863	97.1072	102.65
92.9968	100.4891	109.0193
247.3834	257.4544	279.897
284.6447	293.4662	309.8506
382.5691	380.758	384.0113
567.1378	565.2037	623.4989
580.3665	585.3087	634.1979
760.2965	757.1431	761.892
900.5522	893.7614	892.1443
918.2575	912.0593	918.7438
938.7776	930.48	935.1547
1091.4699	1084.5664	1081.4375
1190.5217	1177.8616	1179.0934
1226.28	1212.8491	1215.033
1332.1411	1317.3495	1324.0178
1383.436	1365.9686	1369.8459
1430.9152	1410.489	1406.0932
1446.2468	1424.9989	1422.8231
1519.0516	1498.3504	1497.5738
1520.6138	1498.658	1498.9725
1521.0056	1499.5992	1499.7384
1540.1746	1517.6346	1517.8225
1541.0962	1517.6856	1518.0214
2152.7246	2136.2534	2126.9104
3065.5867	3048.7469	3039.9214

3069.3267	3052.6951	3044.0521
3083.8247	3067.889	3063.5022
3109.756	3094.4258	3084.2551
3130.2598	3115.8468	3102.6235
3144.4832	3129.6667	3120.3539
3155.208	3139.2728	3128.9457
3156.5392	3140.553	3130.5289
3497.3131	3478.866	3482.0428

	TS1	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
-346.8354	-249.0891	-357.5953
30.7443	25.9158	40.4938
43.7709	42.4455	65.707
91.5647	87.2164	85.5012
96.7678	91.4219	97.0103
244.6847	236.095	244.5794
340.969	318.96	306.0215
350.705	358.9663	340.2217
539.9331	577.9723	650.4322
551.5764	578.4335	653.8551
758.757	753.3759	763.8872
906.1417	897.5337	865.121
918.1171	908.3523	915.6348
928.5182	924.6525	920.2245
1084.4794	1078.0582	1074.4323
1162.5741	1158.3686	1145.9123
1223.436	1209.7186	1210.6492
1325.5789	1312.278	1323.0543
1369.9448	1353.0955	1352.2767
1400.3773	1382.771	1384.4967
1433.6455	1418.3094	1394.6212
1436.0393	1422.1137	1418.4901
1498.1266	1478.8713	1474.6859
1520.5078	1500.1244	1498.7494
1529.3067	1506.5918	1508.2883
1536.4495	1514.4137	1513.7408
1991.3868	2079.8529	2021.942
2224.6724	2358.1638	2247.1754

3076.4009	3064.0411	3051.7418
3087.9833	3072.8722	3069.4263
3110.6733	3092.6319	3078.8996
3122.2087	3107.8805	3102.5908
3150.9377	3139.3754	3126.6084
3165.3895	3147.2247	3130.4145
3174.9316	3155.9317	3142.6204
3478.943	3491.7924	3479.1964

	TS2	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
-404.4984	-324.7049	-384.1949
56.7644	39.8285	37.3642
78.5922	51.3688	59.2965
107.4258	76.3905	91.7477
115.3839	91.0414	107.7475
269.1113	240.5576	224.6342
333.4674	305.9731	286.5314
377.4633	371.3542	373.9994
574.7127	582.8259	638.0365
591.6593	586.1799	641.094
741.0685	736.92	723.9942
889.5944	884.5124	875.5092
905.1416	896.3821	894.754
937.2309	925.716	931.5608
1089.2717	1081.1342	1079.0164
1166.4676	1156.6744	1149.5069
1207.7586	1194.8303	1190.1836
1314.0665	1300.3464	1303.0952
1369.8917	1352.9871	1353.1944
1401.6513	1384.3654	1376.119
1430.8724	1413.8951	1398.5243
1448.973	1426.464	1423.3914
1490.8726	1471.4833	1464.5873
1512.9875	1492.0279	1488.9369
1535.3201	1507.8562	1507.4049
1536.9901	1510.4653	1509.2118
1994.7033	2067.4716	2020.8703
2228.0764	2333.0852	2249.8128

3071.8802	3058.2622	3042.965
3078.9844	3061.838	3049.2479
3104.8215	3091.1053	3075.8253
3117.4427	3103.1562	3090.9691
3151.5977	3134.7989	3116.8122
3168.2476	3147.0608	3135.7041
3175.3376	3161.2023	3143.1147
3497.9713	3488.7572	3466.6025

	TS3	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
-425.464	-310.224	-373.512
50.4435	43.7477	51.2597
52.1254	48.0692	55.1872
89.7456	81.4957	88.5117
127.4635	91.4485	119.5174
231.0243	218.0782	243.0818
275.8545	277.1178	285.5976
374.9306	373.3116	374.8968
593.9365	605.0561	641.0616
598.0823	605.7627	645.2192
683.087	691.5979	675.2904
903.666	896.0929	894.7017
914.7568	900.5235	907.3151
942.8225	928.9546	938.7471
1095.216	1085.711	1083.55
1175.24	1170.538	1161.754
1208.687	1193.881	1197.306
1279.182	1268.268	1261.674
1373.193	1353.279	1356.315
1431.673	1413.826	1413.194
1437.195	1423.981	1413.601
1446.505	1428.216	1425.041
1517.436	1493.594	1493.72
1520.341	1496.718	1496.081
1531.984	1507.206	1507.269
1538.438	1516.627	1515.349
2074.447	2098.246	2072.402
2331.388	2493.051	2405.798

3077.165	3057.346	3050.86
3079.089	3058.926	3052.734
3103.231	3084.801	3074.071
3149.936	3128.788	3120.456
3153.159	3132.704	3123.384
3164.129	3149.667	3136.942
3166.144	3150.701	3139.404
3500.182	3476.404	3468.689

	Rad1	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
67.9448	65.4045	62.769
240.5316	257.0249	238.4012
338.184	336.7371	342.1956
516.7801	504.7009	515.6644
744.3466	745.6274	740.8586
896.8269	892.651	890.4676
919.2485	911.9308	910.2975
1057.21	1046.285	1043.649
1118.018	1108.447	1106.785
1209.698	1196.824	1194.935
1322.537	1308.222	1308.342
1346.358	1330.472	1325.833
1429.731	1402.829	1403.731
1500.579	1475.468	1472.003
1516.252	1496.001	1489.56
1527.209	1503.495	1499.035
1536.237	1513.522	1508.414
3070.1	3060.093	3041.336
3076.633	3064.86	3047.063
3111.346	3102.433	3082.241
3153.402	3144.185	3122.234
3162.16	3149.364	3133.567
3203.849	3184.596	3158.172
3304.635	3288.36	3262.839

	Rad2	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
193.5306	133.3424	180.6849

234.3921	255.1586	234.8721
366.6497	372.8929	372.0367
458.4303	457.2289	458.5653
753.9351	753.7107	748.5586
901.5467	898.2615	894.4654
931.4817	927.1331	925.514
1064.746	1052.604	1051.519
1111.185	1103.228	1101.324
1189.849	1179.738	1175.965
1285.338	1269.904	1270.648
1375.542	1361.925	1357.745
1434.965	1415.671	1410.191
1490.826	1474.923	1467.315
1505.821	1481.355	1473.811
1527.846	1506.019	1501.52
1537.103	1512.557	1509.376
2999.731	2989.334	2977.214
3075.979	3067.44	3045.037
3086.29	3074.04	3049.334
3150.684	3142.459	3118.316
3159.706	3150.593	3126.934
3187.073	3181.759	3157.475
3288.706	3287.487	3262.61

	Rad3	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
121.1215	116.4203	102.6226
145.3428	135.2947	131.2784
357.2528	334.6266	344.5568
431.424	394.2952	396.53
907.5744	903.8782	900.289
943.5552	936.8697	935.7393
949.4859	944.5833	938.8812
1046.082	1028.599	1026.076
1172.008	1161.023	1158.619
1194.67	1183.154	1181.815
1387.044	1367.446	1365.291
1443.259	1421.057	1412.915
1447.365	1428.486	1421.395
1502.255	1477.182	1471.375
1513.48	1487.531	1483.581

1518.456	1488.599	1487.38
1529.422	1501.009	1500.043
3013.481	2998.827	2986.444
3016.825	3001.372	2989.26
3088.493	3072.907	3048.11
3088.737	3074.091	3049.167
3149.385	3142.615	3118.074
3149.877	3143.673	3118.747
3233.97	3215.451	3207.03

C_2H_4 + C_2H

	C_2H_4	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
836.1742	826.6008	838.319
993.4171	987.783	998.5852
999.3819	993.001	1008.461
1081.887	1060.3624	1072.887
1245.235	1234.819	1240.742
1401.774	1387.2367	1385.042
1492.05	1471.6171	1472.398
1742.168	1724.7103	1706.534
3182.2	3173.4679	3149.612
3199.159	3190.1262	3165.67
3260.651	3254.7506	3231.04
3283.651	3279.1782	3256.612

	TSabs	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
-452.822	-418.5284	-559.104
66.7369	48.2001	42.7905
70.1422	78.6217	97.6576
143.1051	132.9104	125.574
164.8023	215.5	197.2203
583.1172	573.5306	641.4183
585.6761	576.2123	645.6112
795.3437	793.6183	751.9666
948.2388	958.4206	928.579
962.6535	973.4102	973.9632
992.2758	996.0871	996.8025
1179.554	1177.328	1145.843

1350.098	1339.9654	1331.323
1444.17	1430.5382	1422.443
1643.408	1702.1034	1631.509
1756.292	1829.3194	1717.022
2168.479	2171.7031	2143.356
3173.421	3174.519	3146.347
3233.038	3232.4446	3203.943
3262.291	3266.0879	3237.906
3500.447	3484.1721	3467.54

	TSadd1	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
-227.276	-237.8836	-214.4588
58.0391	49.3836	43.6822
92.5171	70.5258	59.3172
243.1001	242.5582	171.5059
321.3611	306.9312	252.9339
663.3487	639.9254	637.8055
671.8199	666.4153	669.8197
844.1367	835.924	835.6723
986.1602	988.7458	987.6
1022.232	1008.4395	1008.9488
1028.635	1019.2532	1010.0307
1250.835	1239.7413	1241.1989
1387.744	1373.2641	1369.3819
1492.653	1473.141	1470.7609
1686.661	1665.5483	1649.4205
2038.442	2029.8738	2030.8734
3203.267	3177.0965	3146.6265
3213.274	3187.0715	3156.6211
3290.363	3269.1201	3235.5665
3311.915	3291.4916	3259.3806
3484.988	3465.6189	3449.4863

	TSadd2	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
-799.012	-787.8735	-783.6244
317.5373	314.2449	315.6537
325.89	324.5461	321.8907

526.542	500.6096	468.4879
572.5157	582.6927	590.8473
694.3123	718.4324	721.1031
722.8764	719.1905	728.2272
809.8527	807.3208	807.2047
923.4738	917.4436	909.8255
1061.945	1050.1801	1049.5487
1131.007	1124.2363	1120.8444
1208.459	1192.9467	1181.0809
1219.441	1207.8924	1205.4224
1467.972	1449.0157	1444.6866
1497.798	1477.7962	1472.6306
1994.603	1979.6461	1964.3721
3121.582	3111.0769	3098.8565
3191.501	3185.0837	3174.1723
3212.931	3196.2335	3181.5641
3330.888	3318.5205	3302.8278
3460.292	3447.4834	3434.2161

	C_2H_3	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
746.7312	726.3689	729.868
861.3845	859.1497	863.2076
951.2984	942.2712	951.1943
1088.4732	1067.5941	1062.6039
1421.8705	1399.9998	1397.7813
1699.7733	1684.5832	1669.5504
3126.8064	3114.3821	3092.8306
3214.8035	3210.233	3184.3892
3282.4616	3281.5932	3252.2178

	Adduct1	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
205.2763	197.9283	176.6184
232.485	204.4153	204.9712
347.5752	350.4639	340.5001
490.7351	481.4794	478.5569
620.2643	600.0373	599.9002
659.1626	680.0964	712.0388
679.826	694.8818	729.1582

775.5372	771.7425	770.3917
933.6424	927.3085	924.611
1087.3864	1082.3396	1077.841
1097.363	1085.6224	1084.391
1288.5791	1273.3181	1275.733
1320.6455	1305.2994	1301.757
1484.3355	1464.1443	1460.007
1496.0242	1476.0924	1469.445
2278.1664	2257.6557	2250.191
3076.5325	3066.0969	3045.035
3118.2615	3110.1458	3086.66
3202.6878	3186.7672	3167.136
3308.7506	3298.4671	3279.109
3506.938	3490.6746	3493.173

	Adduct2	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
299.1435	197.9283	300.0695
331.2813	204.4153	327.8754
684.8683	350.4639	687.1139
768.3202	481.4794	766.1783
781.6845	600.0373	766.8118
836.1293	680.0964	808.0804
874.149	694.8818	865.9345
963.3967	771.7425	926.1173
1056.01	927.3085	1035.239
1072.117	1082.34	1058.231
1088.209	1085.622	1075.268
1133.118	1273.318	1118.37
1186.387	1305.299	1174.794
1472.03	1464.144	1446.871
1500.079	1476.092	1474.869
1851.685	2257.656	1827.532
3155.353	3066.097	3127.98
3160.189	3110.146	3138.385
3237.535	3186.767	3217.123
3250.746	3298.467	3233.862
3299	3490.675	3280.378

$C_3H_6 + C_2H$

	C_3H_6	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
212.4901	203.0349	176.1831
429.4966	427.0787	426.81
586.4548	591.9509	582.655
947.8341	939.5985	938.3461
954.6618	943.8712	940.5471
955.1821	960.6376	957.9581
1037.5532	1028.233	1029.904
1085.5207	1074.747	1073.394
1205.8457	1193.185	1193.886
1335.214	1324.501	1326.464
1432.7105	1410.093	1402.465
1475.3618	1455.237	1450.429
1512.6751	1488.447	1479.906
1527.6888	1501.087	1495.461
1768.421	1748.67	1740.214
3073.4672	3062.712	3035.817
3138.1959	3125.646	3092.677
3153.4505	3149.484	3129.436
3169.8128	3171.444	3139.199
3181.3164	3180.445	3163.677
3258.0115	3265.377	3227.462

	PRC1	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
52.283	54.0618	57.8114
62.4888	78.0181	79.7927
75.3685	96.3313	83.3028
75.488	96.8344	104.125
97.6299	107.8305	106.1531
197.2751	195.0981	199.5647
438.6911	437.438	442.6592
595.7917	601.3828	605.4825
597.1592	601.7733	636.5636
603.7371	610.2172	647.4318
947.5981	941.9626	941.037
964.5955	964.3989	968.3847

968.901	964.7851	969.1883
1039.763	1029.5833	1034.3168
1088.9797	1087.8384	1087.7478
1210.4904	1199.4217	1201.708
1335.3589	1323.7139	1328.9392
1433.2943	1421.2134	1416.4673
1472.1709	1454.6482	1451.5591
1511.0275	1492.5775	1490.4729
1525.6558	1503.2923	1501.624
1766.5065	1744.6808	1731.7461
2155.6489	2139.7928	2128.1652
3059.5655	3045.5166	3032.6715
3115.326	3104.5464	3087.042
3150.0018	3136.2974	3120.5685
3175.8316	3161.0154	3145.2679
3186.1335	3171.7157	3155.3621
3266.1546	3254.6451	3239.3009
3498.6607	3479.7367	3475.213

	PRC2	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
24.2097	38.3205	44.7179
34.4895	46.9276	60.3432
77.9846	62.9496	71.8266
102.036	100.0253	112.032
113.2569	112.9931	117.6929
247.3323	268.8977	275.4967
430.1394	430.4572	435.5327
551.0342	558.0737	594.9375
594.0718	592.8147	612.748
633.6436	626.3231	667.2919
944.2277	938.0333	935.4306
949.6821	940.8964	946.3036
964.8945	962.43	964.5566
1030.4455	1018.1081	1020.6091
1082.9059	1072.204	1075.8434
1201.0813	1191.1279	1192.7033
1350.1045	1330.3993	1337.2031
1429.9396	1409.0659	1407.5557
1473.7712	1454.5774	1451.8737
1512.8941	1493.5476	1493.2068

1516.822	1497.9839	1495.0807
1769.0968	1747.4957	1735.3378
2155.2894	2139.1831	2129.3396
3064.363	3050.0825	3043.0624
3115.576	3104.5336	3093.49
3156.1986	3140.5502	3125.1165
3173.2093	3156.8657	3139.6637
3181.0899	3163.8817	3145.5786
3269.1007	3258.013	3238.1969
3497.1401	3478.7264	3474.7537

	PRC3	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
34.3077	28.5741	43.404
64.6058	56.5599	61.6049
98.1311	95.2155	96.9668
125.6907	120.8579	116.9189
145.5988	126.4518	139.0853
207.4127	206.4254	226.4805
429.9227	428.4489	434.84
588.8339	569.8706	593.4923
612.9153	596.1473	610.4054
639.3385	607.0123	651.5635
946.0804	939.8453	938.7933
951.4819	942.9897	952.7302
969.5356	968.9952	975.7185
1043.4197	1031.0478	1039.7062
1085.7102	1075.0327	1081.7784
1204.8084	1194.56	1197.4106
1338.2981	1324.3357	1328.7531
1432.3888	1410.9136	1415.0589
1474.4724	1454.7386	1453.6739
1505.9301	1484.6117	1485.7365
1522.5954	1499.7001	1500.201
1756.1004	1737.2486	1724.5828
2140.4896	2125.601	2111.2816
3069.7401	3053.7106	3049.4401
3134.3826	3119.9291	3111.3596
3158.6662	3145.418	3135.8795

3173.9026	3158.1468	3144.9935
3186.7135	3172.2447	3159.245
3262.9435	3253.0543	3236.5804
3431.9652	3405.9602	3402.9502

	TSabs1	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
-411.7368	-339.8231	-396.5398
50.0638	46.5406	68.1103
56.4427	58.664	80.0005
116.3648	99.882	113.6113
122.443	106.4709	118.8961
268.564	265.2091	200.4095
437.165	435.711	433.7713
535.5764	575.4542	585.7812
559.9113	577.7517	644.4991
593.7513	588.5442	655.4073
936.7624	931.9786	918.726
948.7611	943.2319	941.9533
977.2975	970.2198	974.509
1021.5719	1008.6928	1012.9623
1073.4651	1065.2413	1059.7434
1174.8193	1167.2266	1157.9962
1327.7233	1316.7887	1320.9406
1377.9261	1365.8854	1344.4911
1399.6796	1388.8526	1357.2747
1465.5151	1451.2009	1442.4938
1480.0265	1464.2301	1458.2053
1758.3618	1742.2965	1729.4367
1850.4257	1987.0452	1865.0284
2179.8189	2219.1471	2168.8336
3097.3739	3091.3579	3062.5754
3152.639	3145.3934	3116.4135
3164.8108	3161.6474	3139.1659
3180.8117	3171.9007	3146.9504
3269.5526	3266.1196	3236.4392
3477.1565	3487.638	3474.5899

	TSabs2	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**

-315.3629	-236.161	-251.208
44.7743	38.9834	42.2091
55.9974	50.3404	49.8501
91.3005	89.0403	99.0716
106.7894	104.6705	110.8854
297.5026	275.5414	260.2843
429.6502	428.5095	430.012
553.6734	573.5262	594.8114
566.8138	575.7778	649.724
595.1238	593.9157	653.3629
945.2947	941.1132	938.6544
957.2438	947.4653	945.3147
971.1695	967.4354	973.9404
1028.6326	1017.694	1017.543
1067.5219	1060.812	1058.766
1203.5402	1191.841	1191.936
1326.9068	1320.472	1316.486
1373.2146	1364.316	1345.458
1430.39	1415.059	1398.535
1462.3313	1445.921	1441.509
1501.1797	1481.433	1479.826
1748.0004	1735.325	1718.521
2031.858	2086.97	2057.128
2253.4116	2385.316	2307.915
3114.8768	3098.958	3090.252
3176.5244	3163.574	3144.884
3182.9544	3175.026	3150.726
3193.1832	3187.294	3163.551
3272.7712	3268.302	3242.896
3492.5937	3490.06	3472.481

	TSabs3	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
-311.736	-259.861	-321.728
34.6997	30.2287	37.4189
76.9007	60.7624	67.4275
104.192	102.3071	101.5026
120.7464	135.5779	115.3376
216.7334	209.7571	197.9686
416.2444	418.8027	416.0582
549.142	566.0632	582.1377

550.7518	570.1715	648.356
607.1738	598.3037	650.4619
935.471	928.3957	914.6709
945.9319	937.6176	924.7689
953.9414	949.4418	944.4887
978.6116	981.738	960.2696
1083.847	1070.017	1065.138
1193.134	1182.276	1174.162
1272.388	1268.81	1225.159
1427.047	1403.648	1396.489
1463.117	1444.155	1436.449
1505.263	1479.913	1474.005
1521.554	1495.783	1490.339
1757.645	1750.182	1735.679
1881.13	2006.213	1884.163
2196.78	2247.634	2180.142
3078.605	3065.087	3044.357
3152.778	3136.373	3109.451
3160.288	3150.913	3134.115
3176.628	3169.39	3137.149
3275.446	3264.48	3226.181
3489.12	3488.584	3480.288

	TSabs4	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
-445.878	-396.113	-504.314
48.2108	37.7511	38.7153
49.091	60.4051	46.8565
108.1336	123.7155	106.3058
132.0063	123.9063	112.0228
189.6323	204.2734	203.0816
380.5312	386.1122	369.4657
545.5596	563.2378	542.4261
574.4566	576.9172	647.3948
584.0821	580.2378	648.0401
920.5602	917.5186	884.3515
927.5616	931.9322	907.8489
948.9949	940.0074	938.8339
976.2884	976.4517	970.8018
1075.907	1072.898	1073.531
1165.649	1159.432	1146.588

1317.682	1309.098	1311.797
1376.04	1366.969	1347.062
1432.293	1414.204	1408.188
1510.585	1487.391	1486.478
1516.407	1494.691	1492.146
1687.409	1733.761	1700.15
1782.397	1862.425	1769.689
2171.226	2178.784	2150.159
3072.393	3065.783	3060.64
3137.743	3131.54	3122.291
3163.26	3156.298	3146.332
3184.026	3182.416	3172.465
3233.533	3219.226	3203.966
3492.698	3488.364	3482.097

	TSabs5	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
-436.882	-395.854	-498.136
57.288	52.5509	49.7378
63.0861	62.5757	70.1989
91.3621	115.4211	116.9559
135.5487	134.0126	118.6268
191.6792	213.4552	193.709
429.0764	428.185	418.0751
543.1905	575.0939	569.9309
568.7258	583.333	637.0844
581.9044	584.6867	642.7094
907.0212	905.3883	887.8087
921.1454	922.4252	895.5009
949.8488	942.1415	942.1928
956.5089	951.1122	956.032
1083.64	1073.344	1075.684
1173.558	1163.947	1153.616
1288.002	1279.427	1273.137
1387.258	1371.103	1367.4
1443.433	1424.836	1420.039
1507.055	1485.367	1484.662
1515.379	1495.749	1487.927
1705.226	1724.721	1665.247
1803.977	1877.193	1752.179
2168.855	2178.915	2143.684

3069.677	3063.659	3044.862
3136.977	3131.451	3109.841
3156.838	3145.448	3128.028
3177.811	3162.957	3147.011
3245.823	3241.521	3212.96
3475.193	3486.414	3469.062

	TSadd1	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
-233.245	-236.5715	-241.796
69.8564	32.7554	37.9748
86.9366	74.1631	80.9269
142.8897	154.9177	150.2124
204.1288	204.7772	208.9942
304.2797	291.9167	296.5455
427.5582	425.3284	427.7116
606.5389	613.7217	604.0333
654.1808	647.5936	664.8153
681.1337	671.9836	692.904
942.6485	933.6865	933.847
956.8565	948.3812	949.5401
974.0149	975.2340	970.6907
1007.275	997.5045	996.0359
1070.223	1062.5623	1063.206
1211.407	1201.4690	1203.009
1331.766	1320.9476	1321.69
1424.12	1405.0399	1404.323
1471.261	1449.7147	1448.068
1502.533	1480.6485	1478.222
1518.663	1497.0112	1495.524
1694.122	1675.1460	1660.921
2041.69	2030.2871	2016.97
3077.461	3069.9397	3053.685
3149.823	3141.0263	3124.195
3179.125	3168.9756	3150.301
3201.744	3189.5691	3155.383
3213.22	3201.7691	3176.176
3302.208	3291.8012	3257.141
3478.008	3474.7995	3461.184

	TSadd2	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
-764.181	-755.363	-755.147
145.1069	144.8337	141.1936
169.2865	168.8531	162.5083
319.211	317.2446	317.7747
366.519	365.6931	367.0544
392.6427	392.4472	394.0666
522.3731	501.7048	479.8418
662.6231	666.5651	677.8479
713.6567	712.3848	727.5604
870.5518	863.7591	857.8103
921.2361	913.1552	913.3262
962.8819	955.304	951.7673
1038.748	1027.839	1028.845
1065.463	1052.808	1051.966
1173.033	1165.041	1159.2
1195.597	1184.424	1180.984
1217.021	1203.685	1201.048
1392.71	1376.665	1373.067
1446.261	1426.143	1420.116
1490.377	1468.814	1464.614
1513.565	1488.512	1485.197
1523.909	1498.901	1495.941
1993.848	1982.898	1963.287
3042.1	3026.725	3011.793
3114.326	3100.846	3084.899
3116.775	3103.903	3093.125
3154.539	3141.314	3125.695
3186.048	3178.412	3170.75
3238.285	3223.97	3209.488
3434.712	3426.808	3424.564

	TSadd2a	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
-775.102	-762.309	-761.324
195.3288	195.2732	195.3156
239.8217	240.615	235.2103
312.8616	312.1872	312.0309

362.5177	363.2201	364.0104
434.4595	438.473	441.0549
518.5453	504.0565	483.3453
633.6672	638.9899	645.9417
675.3715	700.7941	704.2065
717.959	713.4784	731.5986
846.6419	842.8304	841.0541
908.0692	902.4686	897.2023
934.4418	926.743	925.6584
1090.595	1078.792	1079.781
1173.333	1164.171	1163.294
1180.787	1171.255	1169.561
1236.385	1220.35	1215.02
1376.918	1362.449	1361.379
1435.992	1416.294	1414.012
1473.584	1456.214	1447.199
1523.669	1500.668	1498.099
1527.026	1502.682	1500.301
1990.965	1975.715	1959.747
3085.227	3067.943	3055.826
3128.144	3119.755	3108.213
3167.683	3153.268	3138.021
3172.265	3157.321	3141.638
3200.151	3182.344	3163.964
3317.987	3304.781	3286.458
3446.669	3434.343	3427.262

	Rad1	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
428.3567	428.6109	431.4531
543.7956	537.6054	538.5482
565.5988	559.0219	562.5673
794.8628	809.2175	812.1733
819.5485	834.2302	835.528
936.9147	931.5302	933.5375
1025.8611	1016.401	1020.115
1053.0366	1045.118	1046.197
1151.6321	1154.881	1164.252
1295.6973	1284.013	1282.923
1420.6851	1410.053	1412.847
1515.1384	1503.359	1502.412

1551.4377	1533.098	1526.518
3195.4758	3181.953	3156.342
3196.4136	3186.239	3158.013
3205.5514	3190.607	3165.834
3301.165	3290.818	3264.377
3303.0648	3292.596	3266.45

	Rad2	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
427.8404	428.6111	431.4854
541.2447	537.6054	538.5754
562.6317	559.022	562.5805
792.627	809.2175	812.2575
817.0963	834.2302	835.5822
936.4272	931.5303	933.4928
1022.304	1016.401	1019.944
1055.09	1045.118	1046.156
1170.885	1154.882	1164.112
1297.081	1284.014	1282.868
1422.062	1410.053	1412.774
1521.701	1503.359	1502.376
1552.432	1533.099	1526.541
3181.997	3181.952	3156.832
3188.538	3186.239	3157.947
3197.146	3190.607	3165.802
3292.171	3290.818	3264.244
3293.947	3292.596	3266.32

	Rad3	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
181.869	181.1293	186.8044
314.9207	318.0043	320.0654
517.0902	500.7339	519.1475
916.4172	904.6122	906.6508
916.9011	907.9158	918.5248
955.5924	947.1808	945.3314
1064.622	1051.9	1052.07
1127.177	1111.959	1111.468
1417.913	1395.255	1390.754
1451.428	1427.709	1423.527

1493.94	1469.33	1464.67
1508.533	1481.691	1480.64
1792.34	1776.776	1763.701
3039.191	3029.528	3009.055
3106.545	3098.251	3074.585
3120.032	3115.669	3091.576
3146.768	3142.208	3117.648
3228.273	3217.731	3198.491

	Rad4	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
204.2136	195.6878	211.4867
404.8381	386.9139	397.1728
663.8434	663.7413	670.2532
891.2114	859.3027	859.5905
893.4976	878.1245	881.1093
955.6276	940.371	941.8118
1071.196	1058.647	1063.248
1128.662	1107.811	1109.768
1290.963	1279.352	1277.23
1429.585	1404.6	1402.37
1514.37	1490.468	1490.499
1521.479	1493.489	1494.31
1728.558	1711.544	1698.64
3079.708	3067.386	3057.194
3146.915	3135.597	3113.929
3147.817	3147.325	3125.756
3171.801	3165.7	3147.282
3280.427	3269.91	3246.4

	Rad5	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
200.7498	194.6658	198.9965
405.342	411.323	405.4461
626.186	622.9715	627.1884
828.1928	824.9763	804.9477
859.2754	851.9412	859.4623
951.2593	943.2901	941.1973
1074.048	1064.679	1064.756
1137.756	1125.394	1120.775

1288.084	1272.322	1269.447
1430.576	1410.595	1404.476
1515.212	1491.802	1488.827
1517.938	1491.84	1490.723
1740.819	1719.754	1710.422
3075.612	3068.63	3047.338
3099.932	3092.899	3071.161
3141.462	3133.931	3112.768
3171.385	3168.712	3142.512
3276.854	3284.639	3255.546

	Adduct1	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
72.28	76.1535	82.4721
133.5556	138.6386	147.1298
199.0475	203.2386	200.7582
338.2775	340.7845	338.3791
358.8321	360.2199	356.0899
465.5813	460.7846	452.5273
573.3338	569.2132	570.3216
655.5408	672.6296	710.6342
665.0117	680.3024	718.8397
885.0393	877.7899	875.8104
907.7906	899.9999	899.5137
954.8711	949.089	946.0679
1013.012	998.6272	1000.292
1118.266	1106.821	1106.69
1169.81	1162.428	1158.262
1262.509	1247.69	1251.594
1326	1310.772	1310.734
1400.13	1382.609	1379.045
1444.241	1425.92	1420.291
1491.938	1467.955	1464.926
1510.204	1485.511	1482.262
1517.855	1492.9	1491.027
2272.93	2252.54	2245.367
3033.044	3015.969	3008.272
3059.722	3048.992	3036.146
3102.38	3086.35	3070.75
3119.106	3111.003	3094.199
3159.251	3148.135	3131.374

3233.227	3222.338	3205.294
3503.193	3483.894	3491.864

	Adduct1a	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
176.0588	177.5965	177.2418
213.7539	217.2181	214.584
233.4699	225.1325	222.9259
279.4289	274.6023	274.9919
354.9161	356.2629	356.9153
500.1619	499.2778	497.0385
537.5755	538.2309	535.718
614.9386	607.834	609.3677
661.6341	677.9035	709.941
670.3154	685.6362	714.3179
812.4219	808.0581	807.0203
925.5428	921.1199	922.0866
968.4959	963.4071	961.6963
1072.146	1063.322	1062.714
1151.349	1142.495	1141.962
1197.624	1187.322	1186.451
1328.761	1311.957	1314.634
1343.881	1328.373	1329.585
1428.514	1409.767	1406.303
1484.684	1466.485	1459.23
1523.139	1501.294	1497.779
1530.997	1507.034	1505.155
2267.431	2247.675	2237.732
3068.59	3060.679	3052.021
3086.278	3069.162	3056.657
3167.077	3152.36	3136.106
3178.589	3163.232	3149.463
3202.005	3187.109	3167.168
3309.663	3300.471	3280.5
3502.681	3485.978	3488.131

	Adduct2	
M06-2X/6-31G(d)	**M06-2X/6-31+G(d,p)**	**M06-2X/6-311++G(d,p)**
175.2291	176.2884	178.2318
191.0943	191.1904	197.8867
319.4142	319.5421	319.2779
359.8405	359.7326	359.956
448.1321	448.4003	449.113
697.5185	688.8419	695.3807
773.4842	764.6812	757.2401
779.1029	768.8625	764.2891
869.2792	860.0859	856.7364
914.4783	898.1279	886.9212
943.1121	933.0358	933.9028
974.0985	961.6434	954.3393
1052.91	1041.933	1033.549
1085.59	1073.846	1074.277
1141.83	1128.878	1127.538
1177.943	1168.489	1165.848
1189.228	1178.295	1177.211
1386.125	1370.263	1366.433
1442.062	1421.627	1419.598
1487.878	1467.069	1460.738
1520.49	1495.994	1494.604
1529.298	1504.789	1502.467
1844.691	1830.872	1818.446
3077.432	3060.218	3049.238
3149.92	3135.108	3119.889
3157.759	3143.565	3126.133
3162.348	3147.95	3134.848
3172.745	3160.884	3147.12
3246.461	3236.691	3221.384
3276.586	3271.244	3259.849

Table S-V: The variational effects (k_{TST}/k_{CVT}) and small curvature tunneling (SCT) effects ($k_{CVT/SCT}/k_{CVT}$) for the title reactions at CCSD(T)/cc-pVTZ//M06-2X/6-31+G(d,p) level of theory.

$CH_4 + C_2H$

T(K)	HO		HR	
	$k_{CVT/SCT}/k_{CVT}$	k_{TST}/k_{CVT}	$k_{CVT/SCT}/k_{CVT}$	k_{TST}/k_{CVT}
150	6.58	$3. \times 10^{05}$	6.58	2796
175	4.58	$5. \times 10^{04}$	4.58	812
200	3.52	$1. \times 10^{04}$	3.52	323
225	2.87	5005	2.87	157
250	2.44	2206	2.44	88
275	2.16	1133	2.15	55
298	1.96	679	1.96	39
300	1.94	651	1.95	38
325	1.79	410	1.79	27
350	1.67	274	1.67	20
375	1.58	195	1.58	16
400	1.49	144	1.50	13
500	1.31	59	1.31	7
1000	1.07	11	1.07	3
1500	1.03	6	1.03	2
2000	1.02	5	1.02	2
2500	1.01	4	1.01	2
3000	1.01	4	1.01	2
3500	1.00	3	1.01	2
4000	1.00	3	1.00	2
4500	1.00	3	1.00	2
5000	1.00	3	1.00	2

$C_2H_6 + C_2H$

T(K)	HO		HR	
	$k_{CVT/SCT}/k_{CVT}$	k_{TST}/k_{CVT}	$k_{CVT/SCT}/k_{CVT}$	k_{TST}/k_{CVT}
150	0.97	1.02×10^{12}	0.97	1.02×10^{12}
175	0.98	1.50×10^{10}	0.98	1.50×10^{10}
200	0.98	6.36×10^{08}	0.98	6.37×10^{08}
225	0.98	5.42×10^{07}	0.98	5.43×10^{07}
250	0.98	7.55×10^{06}	0.98	7.57×10^{06}
275	0.99	1.50×10^{06}	0.98	1.51×10^{06}
298	0.99	4.29×10^{05}	0.99	4.31×10^{05}
300	0.99	3.89×10^{05}	0.99	3.91×10^{05}
325	0.99	1.24×10^{05}	0.99	1.25×10^{05}
350	0.98	4.63×10^{04}	0.98	4.67×10^{04}
375	0.99	1.98×10^{04}	0.99	2.00×10^{04}
400	0.99	9449	0.98	9524
500	0.99	1000	0.99	1018
1000	1.00	11	1.00	12
1500	1.00	2	0.99	3
2000	1.00	1	1.00	1
2500	1.00	1	1.00	1
3000	1.00	0.40	1.00	1
3500	1.00	0.28	1.00	0.41
4000	1.00	0.21	1.00	0.32
4500	1.00	0.16	1.00	0.25
5000	1.00	0.12	1.00	0.20

$C_3H_8 + C_2H$

T(K)	HO		HR	
	$k_{CVT/SCT}/k_{CVT}$	k_{TST}/k_{CVT}	$k_{CVT/SCT}/k_{CVT}$	k_{TST}/k_{CVT}
150	0.97	2.37×10^{70}	0.97	3.10×10^{35}
175	0.98	4.11×10^{65}	0.98	9.67×10^{30}
200	0.98	1.04×10^{62}	0.98	4.04×10^{27}
225	0.98	1.61×10^{59}	0.98	9.60×10^{24}
250	0.99	8.86×10^{56}	0.98	7.74×10^{22}
275	0.98	1.22×10^{55}	0.99	1.50×10^{21}
298	0.99	4.38×10^{53}	0.99	7.17×10^{19}
300	0.99	3.38×10^{53}	0.99	5.64×10^{19}
325	0.99	1.59×10^{52}	0.99	3.53×10^{18}
350	0.99	1.15×10^{51}	0.99	3.29×10^{17}
375	0.99	1.16×10^{50}	0.99	4.24×10^{16}
400	0.99	1.54×10^{49}	0.99	7.06×10^{15}
500	0.99	3.40×10^{46}	0.99	3.35×10^{13}
1000	1.00	9.12×10^{40}	1.00	8.96×10^{08}
1500	1.00	7.90×10^{38}	0.73	3.05×10^{07}
2000	1.00	5.30×10^{37}	0.79	4.92×10^{06}
2500	1.00	8.24×10^{36}	0.83	1.43×10^{06}
3000	1.00	1.99×10^{36}	0.85	5.60×10^{05}
3500	1.00	6.32×10^{35}	0.87	2.60×10^{05}
4000	1.00	2.40×10^{35}	0.88	1.36×10^{05}
4500	1.00	1.04×10^{35}	0.89	7.71×10^{04}
5000	1.00	4.95 × 1034	0.90	4.62 × 1004

$C_2H_4 + C_2H$

T(K)	HO			
	$k_{absCVT/SCT}/k_{absCVT}$	$k_{addCVT/SCT}/k_{addCVT}$	k_{absTST}/k_{absCVT}	k_{addTST}/k_{addCVT}
150	5.19	1.00	6.61×10^{11}	9.31×10^{21}
175	3.74	1.00	1.50×10^{11}	8.81×10^{20}
200	2.94	1.00	4.94×10^{10}	1.50×10^{20}
225	2.46	1.00	2.09×10^{10}	3.74×10^{19}
250	2.14	1.00	1.04×10^{10}	1.22×10^{19}
275	1.91	1.00	5.91×10^{09}	4.91×10^{18}
298	1.76	1.00	3.79×10^{09}	2.41×10^{18}
300	1.74	1.00	3.67×10^{09}	2.27×10^{18}
325	1.63	1.00	2.46×10^{09}	1.18×10^{18}
350	1.54	1.00	1.74×10^{09}	6.71×10^{17}
375	1.46	1.00	1.29×10^{09}	4.12×10^{17}
400	1.40	1.00	9.88×10^{08}	2.67×10^{17}
500	1.25	1.00	4.49×10^{08}	7.19×10^{16}
1000	1.06	1.00	8.79×10^{07}	4.55×10^{15}
1500	1.03	1.00	4.92×10^{07}	1.59×10^{15}
2000	1.02	1.00	3.57×10^{07}	8.73×10^{14}
2500	1.01	1.00	2.87×10^{07}	5.75×10^{14}
3000	1.01	1.00	2.45×10^{07}	4.15×10^{14}
3500	1.00	1.00	2.15×10^{07}	3.19×10^{14}
4000	1.01	1.00	1.94×10^{07}	2.56×10^{14}
4500	1.01	1.00	1.76×10^{07}	2.11×10^{14}
5000	1.00	1.00	1.62×10^{07}	1.78×10^{14}

$C_3H_6 + C_2H$

T(K)	HO				HR			
	$k_{absCVT/SCT}/k_{absCVT}$	$k_{addCVT/SCT}/k_{addCVT}$	$k_{absCVT/SCT}/k_{absCVT}$	$k_{addCVT/SCT}/k_{addCVT}$	$k_{absCVT/SCT}/k_{absCVT}$	$k_{addCVT/SCT}/k_{addCVT}$	$k_{absCVT/SCT}/k_{absCVT}$	$k_{addCVT/SCT}/k_{addCVT}$
150	0.99	0.69	1.75×10^{15}	1.86×10^{22}	0.98	1.00	3.34×10^{15}	6.56×10^{16}
175	0.99	0.70	2.32×10^{14}	1.89×10^{21}	0.98	1.00	4.41×10^{14}	7.03×10^{15}
200	0.99	0.72	5.06×10^{13}	3.39×10^{20}	0.98	1.00	9.62×10^{13}	1.31×10^{15}
225	0.99	0.74	1.54×10^{13}	8.83×10^{19}	0.98	1.00	2.92×10^{13}	3.55×10^{14}
250	0.99	0.75	5.90×10^{12}	2.98×10^{19}	0.98	1.00	1.12×10^{13}	1.25×10^{14}
275	0.99	0.76	2.68×10^{12}	1.23×10^{19}	0.98	1.00	5.10×10^{12}	5.28×10^{13}
298	0.99	0.77	1.45×10^{12}	6.12×10^{18}	0.98	1.00	2.78×10^{12}	2.72×10^{13}
300	0.99	0.77	1.38×10^{12}	5.80×10^{18}	0.98	1.00	2.64×10^{12}	2.58×10^{13}
325	0.99	0.78	7.88×10^{11}	3.07×10^{18}	0.98	1.00	1.51×10^{12}	1.40×10^{13}
350	0.99	0.79	4.88×10^{11}	1.77×10^{18}	0.98	1.00	9.31×10^{11}	8.30×10^{12}
375	0.99	0.81	3.19×10^{11}	1.09×10^{18}	0.98	1.00	6.12×10^{11}	5.26×10^{12}
400	0.99	0.81	2.21×10^{11}	7.19×10^{17}	0.98	1.00	4.23×10^{11}	3.53×10^{12}
500	0.99	0.84	7.19×10^{10}	1.99×10^{17}	0.98	1.00	1.39×10^{11}	1.06×10^{12}
1000	1.00	0.91	7.04×10^{09}	1.29×10^{16}	0.99	1.00	1.36×10^{10}	8.58×10^{10}
1500	1.00	0.93	2.93×10^{09}	4.49×10^{15}	0.99	1.00	5.74×10^{09}	$3.38 \times 10^{+10}$
2000	1.00	0.95	1.71×10^{09}	2.44×10^{15}	0.99	1.00	3.49×10^{09}	1.97×10^{10}
2500	1.00	0.97	1.15×10^{09}	1.60×10^{15}	0.99	1.00	2.47×10^{09}	1.35×10^{10}
3000	1.00	0.97	8.45×10^{08}	1.15×10^{15}	1.00	1.00	1.90×10^{09}	1.02×10^{10}
3500	1.00	0.97	6.53×10^{08}	8.75×10^{14}	1.00	1.00	1.52×10^{09}	8.00×10^{09}
4000	1.00	0.98	5.25×10^{08}	6.96×10^{14}	1.00	1.00	1.27×10^{09}	6.55×10^{09}
4500	1.00	0.98	4.37×10^{08}	5.70×10^{14}	1.00	1.00	1.08×10^{09}	5.51×10^{09}
5000	1.00	0.98	3.70×10^{08}	4.77×10^{14}	1.00	1.00	9.39×10^{08}	4.71×10^{09}

Table S-VI. Rate coefficients (in cm^3 $molecule^{-1}$ sec^{-1}) for the reactions R3a and R3b in the temperature range of 150-5000 K at CCSD(T)/cc-pVTZ//M06-2X/6-31+G(d,p) level of theory.

T(K)	HO			HR		
	R3a		R3b	R3a		R3b
	k_{TS1}	k_{TS2}	k_{TS3}	k_{TS1}	k_{TS2}	k_{TS3}
150	5.86×10^{-12}	4.98×10^{-11}	5.15×10^{-11}	5.86×10^{-12}	4.96×10^{-11}	5.15×10^{-11}
175	5.25×10^{-12}	3.44×10^{-11}	3.22×10^{-11}	5.25×10^{-12}	3.42×10^{-11}	3.22×10^{-11}
200	5.04×10^{-12}	2.70×10^{-11}	2.36×10^{-11}	5.04×10^{-12}	2.68×10^{-11}	2.35×10^{-11}
225	5.03×10^{-12}	2.32×10^{-11}	1.91×10^{-11}	5.02×10^{-12}	2.28×10^{-11}	1.90×10^{-11}
250	5.14×10^{-12}	2.10×10^{-11}	1.65×10^{-11}	5.14×10^{-12}	2.06×10^{-11}	1.65×10^{-11}
275	5.35×10^{-12}	1.97×10^{-11}	1.50×10^{-11}	5.35×10^{-12}	1.93×10^{-11}	1.50×10^{-11}
298	5.60×10^{-12}	1.91×10^{-11}	1.42×10^{-11}	5.60×10^{-12}	1.86×10^{-11}	1.41×10^{-11}
300	5.63×10^{-12}	1.91×10^{-11}	1.41×10^{-11}	5.62×10^{-12}	1.86×10^{-11}	1.41×10^{-11}
325	5.96×10^{-12}	1.88×10^{-11}	1.36×10^{-11}	5.96×10^{-12}	1.82×10^{-11}	1.35×10^{-11}
350	6.35×10^{-12}	1.89×10^{-11}	1.33×10^{-11}	6.34×10^{-12}	1.82×10^{-11}	1.32×10^{-11}
375	6.78×10^{-12}	1.91×10^{-11}	1.33×10^{-11}	6.77×10^{-12}	1.83×10^{-11}	1.32×10^{-11}
400	7.25×10^{-12}	1.95×10^{-11}	1.34×10^{-11}	7.24×10^{-12}	1.86×10^{-11}	1.32×10^{-11}
500	9.55×10^{-12}	2.24×10^{-11}	1.46×10^{-11}	9.51×10^{-12}	2.08×10^{-11}	1.44×10^{-11}
1000	3.12×10^{-11}	5.66×10^{-11}	3.31×10^{-11}	3.04×10^{-11}	4.54×10^{-11}	3.07×10^{-11}
1500	7.11×10^{-11}	1.19×10^{-10}	6.62×10^{-11}	6.71×10^{-11}	1.07×10^{-11}	5.77×10^{-11}
2000	1.28×10^{-10}	2.07×10^{-10}	1.12×10^{-10}	1.17×10^{-10}	2.23×10^{-11}	9.08×10^{-11}
2500	2.00×10^{-10}	3.17×10^{-10}	1.68×10^{-10}	1.75×10^{-10}	3.84×10^{-11}	1.28×10^{-10}
3000	2.88×10^{-10}	4.49×10^{-10}	2.35×10^{-10}	2.42×10^{-10}	5.91×10^{-11}	1.68×10^{-10}
3500	3.92×10^{-10}	6.04×10^{-10}	3.13×10^{-10}	3.16×10^{-10}	8.39×10^{-11}	2.11×10^{-10}
4000	5.11×10^{-10}	7.83×10^{-10}	4.02×10^{-10}	3.96×10^{-10}	1.12×10^{-10}	2.56×10^{-10}
4500	6.51×10^{-10}	9.88×10^{-10}	5.05×10^{-10}	4.83×10^{-10}	1.45×10^{-10}	3.04×10^{-10}
5000	8.04×10^{-10}	1.22×10^{-09}	6.18×10^{-10}	5.75×10^{-10}	1.81×10^{-10}	3.55×10^{-10}

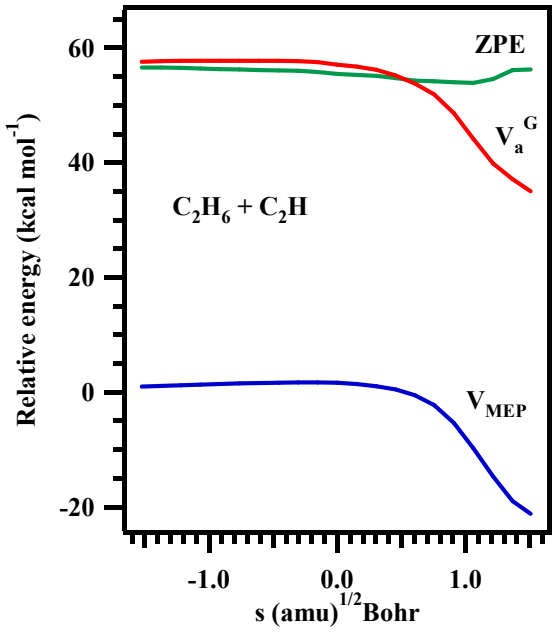
Table S-VII. Rate coefficients (in cm^3 $molecule^{-1}$ sec^{-1}) for the reactions R4a, and R4b in the temperature range of 150-5000 K at CCSD(T)/cc-pVTZ//M06-2X/6-31+G(d,p) level of theory.

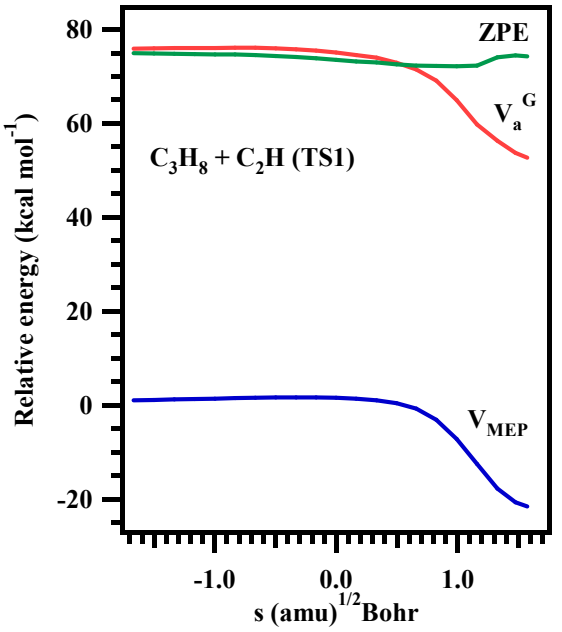
T(K)	k_{abs} (R4a)	k_{add} (R4b)
150	4.44×10^{-13}	8.00×10^{-09}
175	5.10×10^{-13}	2.14×10^{-09}
200	5.90×10^{-13}	8.20×10^{-10}
225	6.85×10^{-13}	3.98×10^{-10}
250	7.95×10^{-13}	2.27×10^{-10}
275	9.15×10^{-13}	1.46×10^{-10}
298	1.04×10^{-12}	1.05×10^{-10}
300	1.05×10^{-12}	1.03×10^{-10}
325	1.21×10^{-12}	7.75×10^{-11}
350	1.39×10^{-12}	6.15×10^{-11}
375	1.58×10^{-12}	5.05×10^{-11}
400	1.79×10^{-12}	4.31×10^{-11}
500	2.85×10^{-12}	2.84×10^{-11}
1000	1.52×10^{-11}	2.20×10^{-11}
1500	4.29×10^{-11}	2.96×10^{-11}
2000	8.77×10^{-11}	4.03×10^{-11}
2500	1.49×10^{-10}	5.29×10^{-11}
3000	2.27×10^{-10}	6.75×10^{-11}
3500	3.22×10^{-10}	8.42×10^{-11}
4000	4.35×10^{-10}	1.03×10^{-10}
4500	5.67×10^{-10}	1.24×10^{-10}
5000	7.16×10^{-10}	1.47×10^{-10}

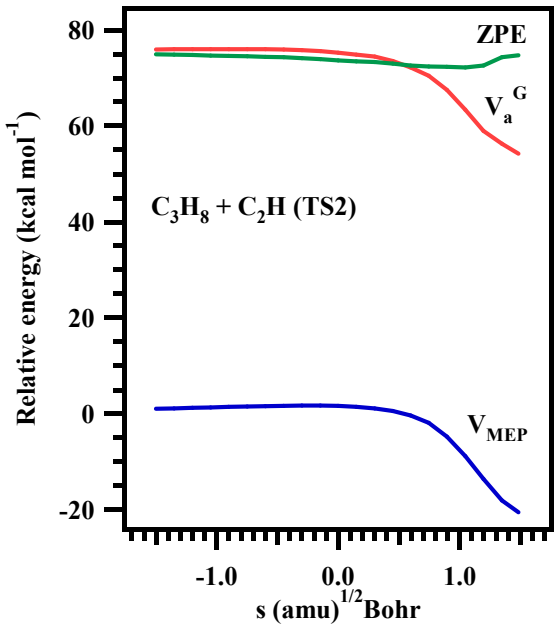
Table S-VIII. . Rate coefficients (in cm^3 $molecule^{-1}$ sec^{-1}) for the reactions R5a, R5b, R5c, and R5d in the temperature range of 150-5000 K at CCSD(T)/cc-pVTZ//M06-2X/6-31+G(d,p) level of theory.

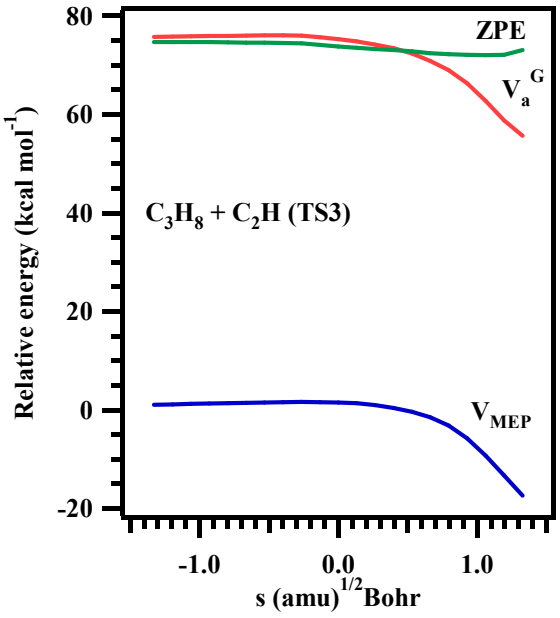
HO							
T(K)	R5a		R5b	R5c		R5a+R5b+R5c	R5d
	k_{TSabs1}	k_{TSabs2}	k_{TSabs3}	k_{TSabs4}	k_{TSabs5}	k_{abs}	k_{add}
150	1.76×10^{-12}	3.02×10^{-12}	9.30×10^{-15}	7.40×10^{-14}	2.39×10^{-13}	5.09×10^{-12}	4.51×10^{-07}
175	1.49×10^{-12}	2.79×10^{-12}	9.40×10^{-15}	9.35×10^{-14}	2.52×10^{-13}	4.64×10^{-12}	4.58×10^{-08}
200	1.36×10^{-12}	2.74×10^{-12}	9.90×10^{-15}	1.16×10^{-13}	2.73×10^{-13}	4.51×10^{-12}	8.50×10^{-09}
225	1.31×10^{-12}	2.79×10^{-12}	1.07×10^{-14}	1.43×10^{-13}	2.99×10^{-13}	4.56×10^{-12}	2.36×10^{-09}
250	1.31×10^{-12}	2.89×10^{-12}	1.17×10^{-14}	1.74×10^{-13}	3.30×10^{-13}	4.72×10^{-12}	8.70×10^{-10}
275	1.33×10^{-12}	3.04×10^{-12}	1.29×10^{-14}	2.08×10^{-13}	3.66×10^{-13}	4.96×10^{-12}	3.89×10^{-10}
298	1.36×10^{-12}	3.21×10^{-12}	1.42×10^{-14}	2.44×10^{-13}	4.02×10^{-13}	5.24×10^{-12}	2.13×10^{-10}
300	1.37×10^{-12}	3.23×10^{-12}	1.44×10^{-14}	2.47×10^{-13}	4.05×10^{-13}	5.27×10^{-12}	2.03×10^{-10}
325	1.42×10^{-12}	3.45×10^{-12}	1.60×10^{-14}	2.91×10^{-13}	4.49×10^{-13}	5.63×10^{-12}	1.18×10^{-10}
350	1.49×10^{-12}	3.69×10^{-12}	1.77×10^{-14}	3.39×10^{-13}	4.98×10^{-13}	6.05×10^{-12}	7.55×10^{-11}
375	1.57×10^{-12}	3.96×10^{-12}	1.97×10^{-14}	3.92×10^{-13}	5.50×10^{-13}	6.50×10^{-12}	5.20×10^{-11}
400	1.67×10^{-12}	4.26×10^{-12}	2.18×10^{-14}	4.51×10^{-13}	6.05×10^{-13}	7.01×10^{-12}	3.75×10^{-11}
500	2.12×10^{-12}	5.70×10^{-12}	3.24×10^{-14}	7.40×10^{-13}	8.80×10^{-13}	9.48×10^{-12}	1.53×10^{-11}
1000	6.63×10^{-12}	1.89×10^{-11}	1.47×10^{-13}	3.94×10^{-12}	3.66×10^{-12}	3.33×10^{-11}	4.66×10^{-12}
1500	1.51×10^{-11}	4.32×10^{-11}	3.98×10^{-13}	1.09×10^{-11}	9.31×10^{-12}	7.89×10^{-11}	4.68×10^{-12}
2000	2.73×10^{-11}	7.76×10^{-11}	8.03×10^{-13}	2.20×10^{-11}	1.79×10^{-11}	1.46×10^{-10}	5.53×10^{-12}
2500	4.32×10^{-11}	1.22×10^{-10}	1.36×10^{-12}	3.69×10^{-11}	2.94×10^{-11}	2.33×10^{-10}	6.74×10^{-12}
3000	6.23×10^{-11}	1.75×10^{-10}	2.09×10^{-12}	5.60×10^{-11}	4.37×10^{-11}	3.39×10^{-10}	8.13×10^{-12}
3500	8.48×10^{-11}	2.38×10^{-10}	2.98×10^{-12}	7.86×10^{-11}	6.09×10^{-11}	4.65×10^{-10}	9.77×10^{-12}
4000	1.11×10^{-10}	3.10×10^{-10}	4.05×10^{-12}	1.06×10^{-10}	8.11×10^{-11}	6.12×10^{-10}	1.16×10^{-11}
4500	1.42×10^{-10}	3.94×10^{-10}	5.33×10^{-12}	1.37×10^{-10}	1.04×10^{-10}	7.82×10^{-10}	1.38×10^{-11}
5000	1.76×10^{-10}	4.88×10^{-10}	6.83×10^{-12}	1.73×10^{-10}	1.31×10^{-10}	9.74×10^{-10}	1.61×10^{-11}
HR							
150	1.72×10^{-12}	2.98×10^{-12}	2.02×10^{-13}	8.05×10^{-14}	2.43×10^{-13}	5.23×10^{-12}	1.35×10^{-06}
175	1.45×10^{-12}	2.75×10^{-12}	2.01×10^{-13}	1.01×10^{-13}	2.57×10^{-13}	4.76×10^{-12}	1.38×10^{-07}
200	1.32×10^{-12}	2.68×10^{-12}	2.09×10^{-13}	1.26×10^{-13}	2.79×10^{-13}	4.61×10^{-12}	2.57×10^{-08}
225	1.26×10^{-12}	2.70×10^{-12}	2.23×10^{-13}	1.55×10^{-13}	3.06×10^{-13}	4.64×10^{-12}	7.15×10^{-09}
250	1.24×10^{-12}	2.78×10^{-12}	2.41×10^{-13}	1.87×10^{-13}	3.39×10^{-13}	4.79×10^{-12}	2.61×10^{-09}
275	1.25×10^{-12}	2.90×10^{-12}	2.63×10^{-13}	2.25×10^{-13}	3.76×10^{-13}	5.01×10^{-12}	1.16×10^{-09}
298	1.27×10^{-12}	3.03×10^{-12}	2.85×10^{-13}	2.63×10^{-13}	4.13×10^{-13}	5.27×10^{-12}	6.35×10^{-10}
300	1.27×10^{-12}	3.05×10^{-12}	2.87×10^{-13}	2.66×10^{-13}	4.17×10^{-13}	5.30×10^{-12}	6.05×10^{-10}
325	1.31×10^{-12}	3.22×10^{-12}	3.15×10^{-13}	3.13×10^{-13}	4.62×10^{-13}	5.63×10^{-12}	3.51×10^{-10}
350	1.36×10^{-12}	3.42×10^{-12}	3.46×10^{-13}	3.64×10^{-13}	5.10×10^{-13}	6.01×10^{-12}	2.23×10^{-10}
375	1.42×10^{-12}	3.64×10^{-12}	3.79×10^{-13}	4.21×10^{-13}	5.65×10^{-13}	6.43×10^{-12}	1.52×10^{-10}
400	1.49×10^{-12}	3.87×10^{-12}	4.16×10^{-13}	4.83×10^{-13}	6.25×10^{-13}	6.89×10^{-12}	1.09×10^{-10}

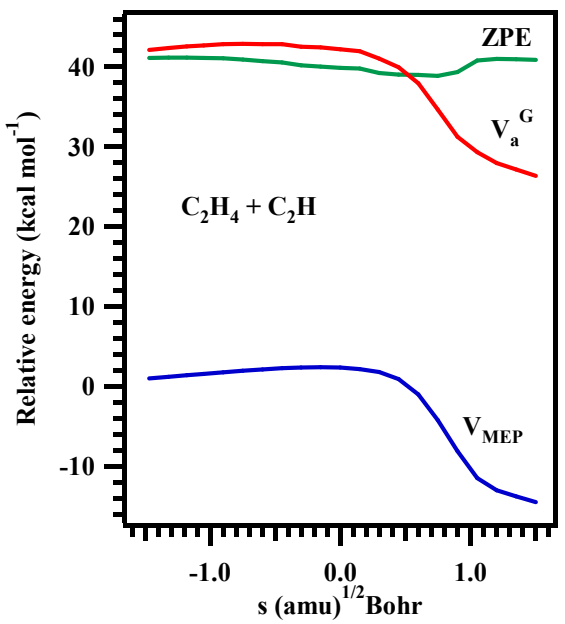
500	1.82×10^{-12}	4.97×10^{-12}	5.90×10^{-13}	7.90×10^{-13}	9.00×10^{-13}	9.08×10^{-12}	4.37×10^{-11}
1000	4.77×10^{-12}	1.41×10^{-11}	2.33×10^{-12}	4.16×10^{-12}	3.56×10^{-12}	2.89×10^{-11}	1.22×10^{-11}
1500	9.50×10^{-12}	2.82×10^{-11}	5.67×10^{-12}	1.14×10^{-11}	8.41×10^{-12}	6.32×10^{-11}	1.15×10^{-11}
2000	1.55×10^{-11}	4.60×10^{-11}	1.05×10^{-11}	2.25×10^{-11}	1.50×10^{-11}	1.10×10^{-10}	1.29×10^{-11}
2500	2.24×10^{-11}	6.58×10^{-11}	1.66×10^{-11}	3.72×10^{-11}	2.29×10^{-11}	1.65×10^{-10}	1.48×10^{-11}
3000	3.00×10^{-11}	8.77×10^{-11}	2.37×10^{-11}	5.52×10^{-11}	3.16×10^{-11}	2.28×10^{-10}	1.71×10^{-11}
3500	3.83×10^{-11}	1.12×10^{-10}	3.18×10^{-11}	7.62×10^{-11}	4.10×10^{-11}	2.99×10^{-10}	1.95×10^{-11}
4000	4.74×10^{-11}	1.38×10^{-10}	4.09×10^{-11}	1.00×10^{-10}	5.13×10^{-11}	3.77×10^{-10}	2.22×10^{-11}
4500	5.70×10^{-11}	1.66×10^{-10}	5.05×10^{-11}	1.27×10^{-10}	6.20×10^{-11}	4.63×10^{-10}	2.50×10^{-11}
5000	6.77×10^{-11}	1.95×10^{-10}	6.09×10^{-11}	1.57×10^{-10}	7.30×10^{-11}	5.55×10^{-10}	2.81×10^{-11}

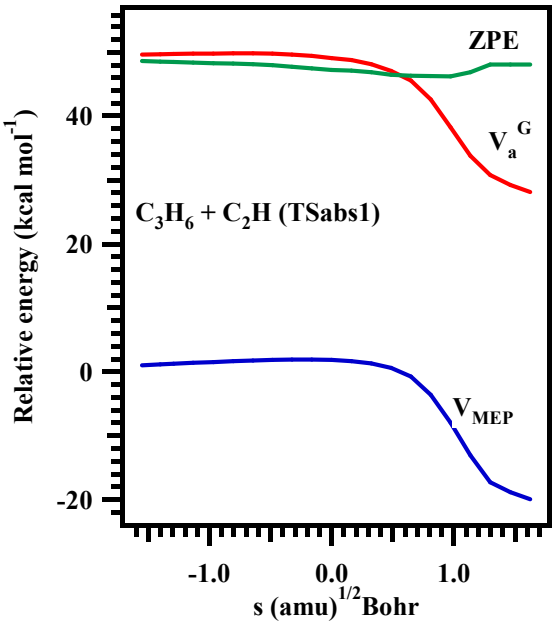

ZPE
V_a^G
$C_2H_6 + C_2H$
V_{MEP}
Relative energy (kcal mol^{-1})
s (amu)$^{1/2}$Bohr

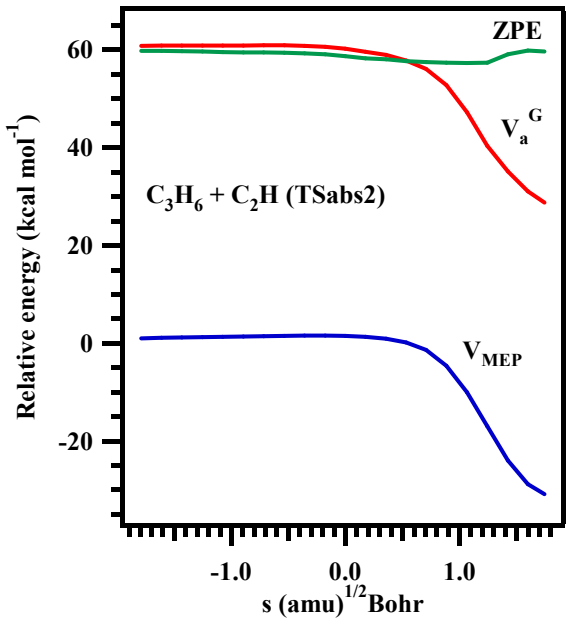

ZPE
V_a^G
$C_3H_8 + C_2H$ (TS1)
V_{MEP}
Relative energy (kcal mol^{-1})
s (amu)$^{1/2}$Bohr

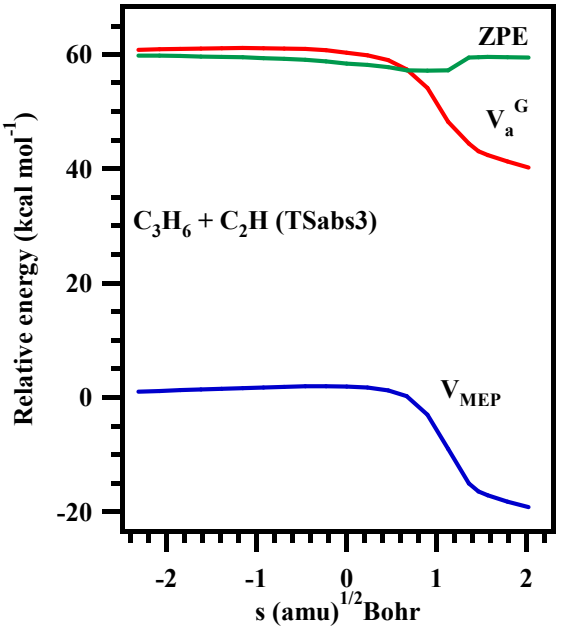

ZPE
V_a^G
$C_3H_8 + C_2H$ (TS2)
V_{MEP}
Relative energy (kcal mol^{-1})
s (amu)$^{1/2}$Bohr


ZPE
V_a^G
$C_3H_8 + C_2H$ (TS3)
V_{MEP}
Relative energy (kcal mol^{-1})
s (amu)$^{1/2}$Bohr


ZPE
V_a^G
$C_2H_4 + C_2H$
V_{MEP}
Relative energy (kcal mol^{-1})
s (amu)$^{1/2}$Bohr


ZPE
V_a^G
$C_3H_6 + C_2H$ (TSabs1)
V_{MEP}
Relative energy (kcal mol^{-1})
s (amu)$^{1/2}$Bohr


ZPE
V_a^G
$C_3H_6 + C_2H$ (TSabs2)
V_{MEP}
Relative energy (kcal mol^{-1})
s (amu)$^{1/2}$Bohr


ZPE
V_a^G
$C_3H_6 + C_2H$ (TSabs3)
V_{MEP}
Relative energy (kcal mol^{-1})
s (amu)$^{1/2}$Bohr

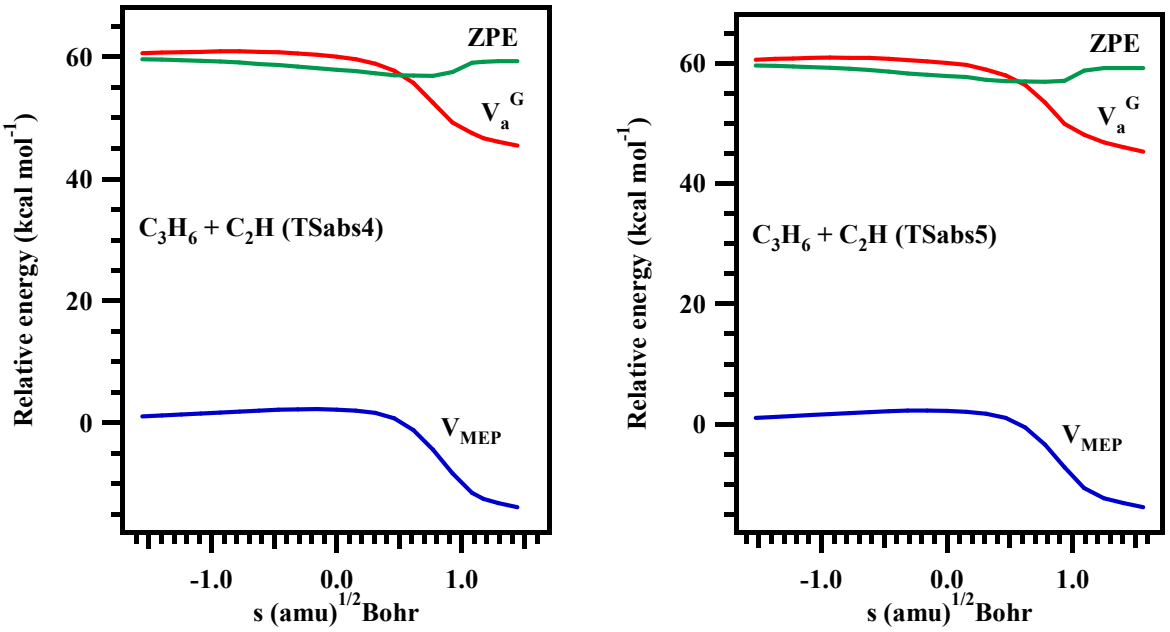


Figure S-I. Plots of the classical potential energy (V_{MEP}), vibrational ground state adiabatic potential energy (V_a^G) and zero-point energy (ZPE) of reacting system as functions of the intrinsic reaction coordinate s (amu)$^{1/2}$ Bohr at the M06-2X/6-31+G(d,p) level.