

Supporting Information

Ab Initio Molecular Dynamics Study of the Reactions of Allene Cation Induced by Intense 7

Micron Laser Pulses

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Cartesian coordinate

allene cation (1)

Charge = 1 Multiplicity = 2

E(UB3LYP) = -116.323622518 A.U.

C	0.000000	0.000000	1.316786
H	0.324564	0.880113	1.880510
H	-0.324564	-0.880113	1.880510
C	0.000000	0.000000	-0.002977
C	0.000000	0.000000	-1.322520
H	-0.880361	-0.323891	-1.885940
H	0.880361	0.323891	-1.885940

vinylmethylene cation (2)

Charge = 1 Multiplicity = 2

E(UB3LYP) = -116.284317356 A.U.

C	-1.125422	0.229727	0.000000
H	-2.091283	-0.275391	0.000000
H	-1.128000	1.318571	0.000000
C	0.057963	-0.497228	0.000000
C	1.240905	0.184268	0.000000
H	1.602333	1.211241	0.000000
H	0.049897	-1.587042	0.000000

propyne cation (3)

Charge = 1 Multiplicity = 2

E(UB3LYP) = -116.296565330 A.U.

C	-1.232606	0.007937	-0.012568
H	-1.555199	-0.269217	1.018878
H	-1.651818	0.994844	-0.238586
C	0.183438	0.001154	-0.016132
C	1.435001	-0.014527	0.000786

H	2.513323	-0.025709	0.012611
H	-1.639002	-0.790833	-0.652666

cyclopropene cation (4)

Charge = 1 Multiplicity = 2

E(UB3LYP) = -116.284347247 A.U.

C	0.000000	0.000000	-0.817213
H	-0.806327	0.410499	-1.454475
H	0.806327	-0.410499	-1.454475
C	0.115376	0.657705	0.502092
C	-0.115376	-0.657705	0.502092
H	-0.096501	-1.621823	0.999396
H	0.096501	1.621823	0.999396

H₂CCCH⁺ (5)

Charge = 1 Multiplicity = 1

E(RB3LYP) = -115.697732958 A.U.

C	0.012642	-0.013350	1.379157
H	0.957529	0.299152	1.829316
H	-0.772513	-0.405994	2.029042
C	-0.180440	0.085048	0.048072
C	-0.357001	0.174928	-1.169241
H	-0.511362	0.253546	-2.233370

c-C₃H₃⁺ (6)

Charge = 1 Multiplicity = 1

E(RB3LYP) = -115.739761309 A.U.

C	-0.662123	-0.065121	0.311548
H	-1.715272	-0.103702	0.566697
C	0.464328	0.658376	0.038178
C	0.510801	-0.707182	0.030203
H	1.070753	-1.626345	-0.102217
H	0.957450	1.616394	-0.084269

HCCCH⁺ (7)

Charge = 1 Multiplicity = 2

E(UB3LYP) = -115.021974050 A.U.

C	1.011196	-0.478077	0.064348
H	2.061786	-0.726394	0.093116
C	-0.221959	-0.187602	0.031376
C	-1.455111	0.102229	-0.001432
H	-2.506267	0.348479	-0.028779

H

Charge = 0 Multiplicity = 2

E(UB3LYP) = -0.500272784186 A.U.

H	0.940644	0.500000	-1.901256
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H₂

Charge = 0 Multiplicity = 1

E(RB3LYP) = -1.17853935735 A.U.

H	-0.071397	0.000000	0.000000
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H	0.671397	0.000000	0.000000
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TS(1/2)

Charge = 1 Multiplicity = 2

E(UB3LYP) = -116.270340676 A.U.

C	-1.247153	0.072597	0.014844
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H	-1.985691	-0.719979	0.005164
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H	-1.562934	1.107266	-0.074508
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C	0.112388	-0.240911	0.005603
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C	1.298574	0.286199	0.130403
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H	2.341210	0.450297	-0.118759
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H	0.431100	-1.320456	-0.087834
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TS(1/3)

Charge = 1 Multiplicity = 2

E(UB3LYP) = -116.253976174 A.U.

C	1.273848	0.001784	0.108074
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H	1.816977	0.944958	0.053987
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H	1.815844	-0.943366	0.087353
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C	-0.126927	-0.000086	-0.045506
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C	-1.376855	0.003058	0.103376
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H	-2.450309	0.002251	0.019485
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H	0.187129	-0.019768	-1.173725
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TS(2/4)

Charge = 1 Multiplicity = 2

E(UB3LYP) = -116.278553618 A.U.

C	-0.934015	-0.272944	-0.006958
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H	-1.732135	-0.086473	0.715589
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H	-0.964813	-1.208288	-0.561959
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C	0.123511	0.680802	-0.120375
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C	1.000991	-0.257690	0.112936
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H	1.609225	-1.148326	0.167385
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H	0.111760	1.756089	0.053230
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TS(3/4)

Charge = 1 Multiplicity = 2

E(UB3LYP) = -116.203055284 A.U.

C	-0.906853	-0.188268	0.000000
H	-1.228332	-0.645598	0.935741
H	-1.228332	-0.645598	-0.935741
C	0.433401	0.814307	0.000000
C	0.877980	-0.340060	0.000000
H	1.391448	-1.289122	0.000000
H	-1.368624	0.843194	0.000000

TS(3/7)

Charge = 1 Multiplicity = 2

E(UB3LYP) = -116.201723652 A.U.

C	-1.036444	0.403046	-0.087127
H	-1.955290	0.923828	0.131001
H	-1.985503	-1.244560	-0.360471
C	0.226866	0.151403	-0.008461
C	1.463180	-0.055192	0.004868
H	2.528213	-0.219194	0.014204
H	-2.003664	-1.309375	0.401789

TS(4/6)

Charge = 1 Multiplicity = 2

E(UB3LYP) = -116.239268968 A.U.

C	-0.658285	-0.062690	0.124694
H	-1.702886	-0.116233	0.410489
H	-1.518125	0.041219	-1.657791
C	0.519238	0.656501	0.110449
C	0.561269	-0.698031	0.010752
H	1.131062	-1.616189	-0.071828
H	1.030748	1.610330	0.165631