

Table 1S. Absolute Energies (hartree) and Zero-Point Vibrational Energy (ZPVE) Corrections (kcal/mol) of Chemically Important Structures Located for the Reaction of HCCCH_2^+ with NH_3 .

Species	MP2-FULL/6-31+G(d,p)	ZPVE	CCSD(T)/6-311+G(2df,2p)// MP2-FULL/6-31+G(d,p)
<i>Reactants</i>			
$\text{HCCCH}_2^+ + \text{NH}_3$	-171.731094	49.7	-171.925244
<i>Minimum Structures</i>			
M1	-171.763846	51.2	-171.956725
M2	-171.766732	52.5	-171.962166
M3	-171.846409	56.1	-172.038918
M4	-171.825650	55.5	-172.012829
M5	-171.789306	52.6	-171.985336
M6	-171.892851	56.5	-172.082282
M7	-171.885466	56.4	-172.075158
M8	-171.802237	53.6	-171.993653
M9	-171.803752	53.6	-171.994819
M10	-171.878278	54.5	-172.065027
M11	-171.801500	54.8	-171.988851
M12	-171.871524	57.1	-172.058872
M13	-171.809491	51.1	-171.998922
M14	-171.837356	56.3	-172.022583
M15	-171.812092	52.8	-171.997216
M16	-171.803239	52.5	-171.989507
<i>Transition States</i>			
TS1-2	-171.762347	49.3	-171.955916
TS1-3	-171.756406	51.0	-171.949876
TS3-4	-171.756786	51.6	-171.950110
TS3-14	-171.716937	54.0	-171.910287
TS4-5	-171.777774	52.3	-171.973330
TS5-6	-171.783508	52.6	-171.976776
TS6-7	-171.875624	55.9	-172.065427
TS7-8	-171.789873	51.4	-171.980048
TS8-9	-171.788625	52.9	-171.978407
TS9-10	-171.777076	51.5	-171.973056
TS9-11	-171.774632	52.6	-171.967871
TS11-12	-171.794265	55.0	-171.981720
TS11-13	-171.787871	52.2	-171.978557
TS14-15	-171.805953	52.4	-171.991543
TS15-16	-171.803153	51.0	-171.988995
<i>Products</i>			
$\text{H}_2\text{CCC} + \text{NH}_4^+$	-171.717696	51.7	-171.914632
$c\text{-C}_3\text{H}_2 + \text{NH}_4^+$	-171.748787	52.6	-171.935839
$c\text{-C}_3\text{H}_3^+ + \text{NH}_3$	-171.783006	51.1	-171.970088
$\text{C}_2\text{H}_4 + \text{HCNH}^+$	-171.792111	50.0	-171.981335

MP2-FULL/6-31+G(d,p) (CCSD(T)/6-311+G(2df,2p)//MP2-FULL/6-31+G(d,p) in parentheses) absolute energies in hartree for the reactants, HCCCH_2^+ and NH_3 are -115.335280 (-115.367375) and -56.395814 (-56.410657), respectively, and for the products, H_2CCC , $c\text{-C}_3\text{H}_2$, NH_4^+ , $c\text{-C}_3\text{H}_3^+$, C_2H_4 , and HCNH^+ are -114.979438 (-115.016033), -115.010529 (-115.035885), -56.738258 (-56.754906), -115.387192 (-115.411739), -78.333262 (-78.361433), and -93.458849 (-93.473474), respectively.

Table 2S. Absolute Energies (hartree) and Zero-Point Vibrational Energy (ZPVE) Corrections (kcal/mol) of Chemically Important Structures Located for the Isomerization Reaction of H₂CCC into *c*-C₃H₂.

Species	MP2(FULL)/6-31+G(d,p)	ZPVE	CCSD(T)/6-311+G(2df,2p)// MP2-FULL/6-31+G(d,p)
H ₂ CCC	-114.979438	19.8	-115.107708
TSC1A	-114.846292	15.9	-114.977676
MC1A	-114.957940	18.3	-115.087712
TSC2A	-114.869759	17.2	-115.004228
TSC1B	-114.926815	18.5	-115.049480
MC1B	-114.926818	18.7	-115.049194
TSC2B	-114.915255	17.7	-115.034523
<i>c</i> -C ₃ H ₂	-115.010529	20.7	-115.128915