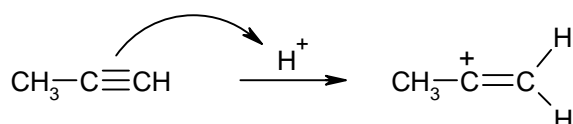


Energia di formazione dei carbocationi

Calcolo eseguito con ArgusLab (PM3)

Energia calcolata delle molecole
kcal/mol

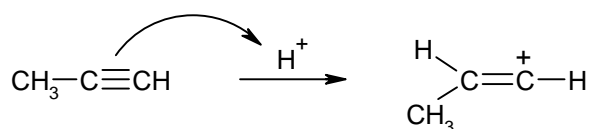
Aumento di energia
kcal/mol



Propino
40,2172

Carbocatione Vinilico 2°
238,2349

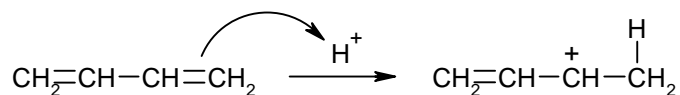
+198,0177



Propino
40,2172

Carbocatione Vinilico 1°
256,4040

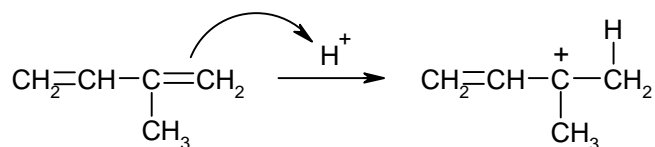
+216,1868



1,3-butadiene
31,0434

Carbocatione Allilico 2°(1°)
211,9280

+180,8846



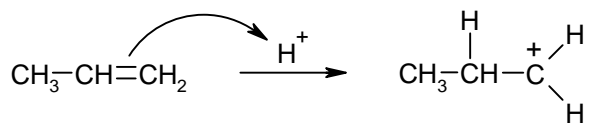
2-metil-1,3-butadiene
22,6257

Carbocatione Allilico 3°(1°)
195,6985

+173,0728

Energia calcolata delle molecole
kcal/mol

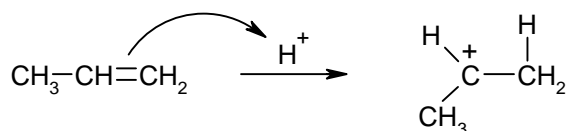
Aumento di energia
kcal/mol



Propene
6,4124

Carbocatione 1°
215,3980

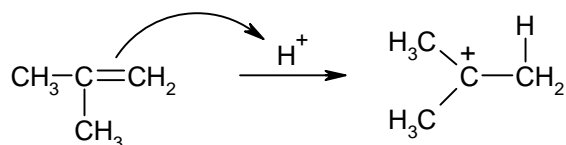
+208,9856



Propene
6,4124

Carbocatione 2°
197,2727 kcal/mol

+190,8646



2-metilpropene
-3,3025

Carbocatione 3°
177,8767

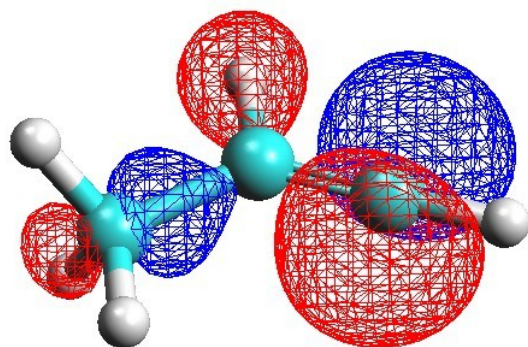
+181,1782

Ricapitolando, le energie necessarie per formare i diversi carbocationi nelle reazioni citate sono:

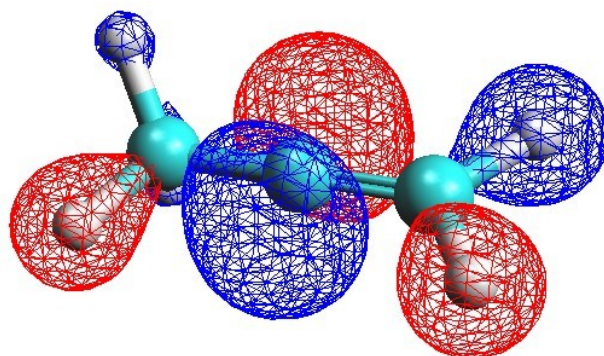
Carbocationi più stabili

Carbocationi meno stabili

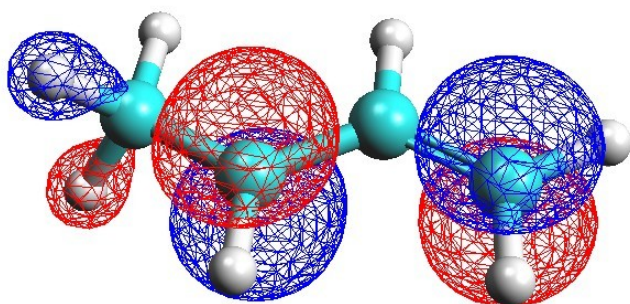
170	175	180	185	190	195	200	205	210	215	220	ΔH
.	
		3°		2°				1°			
<u>A3°</u>	<u>A2°</u>					<u>V2°</u>			<u>V1°</u>		
(1°)	(1°)										



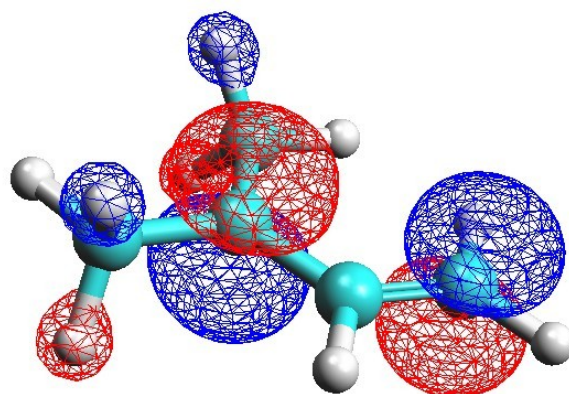
Carbocatione Vinilico 1°
Orbitale LUMO



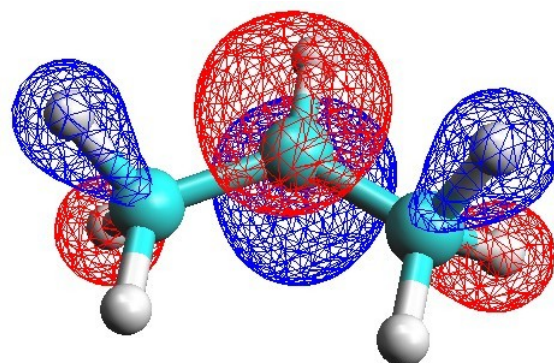
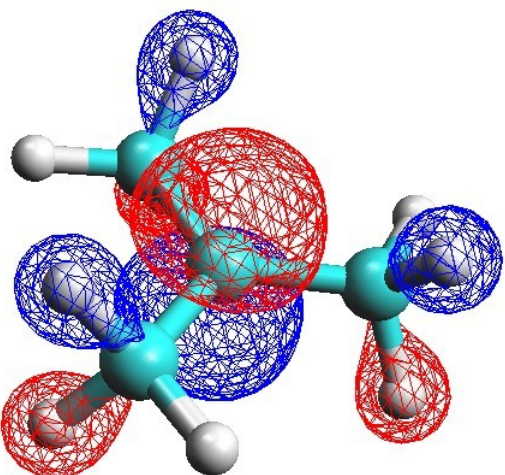
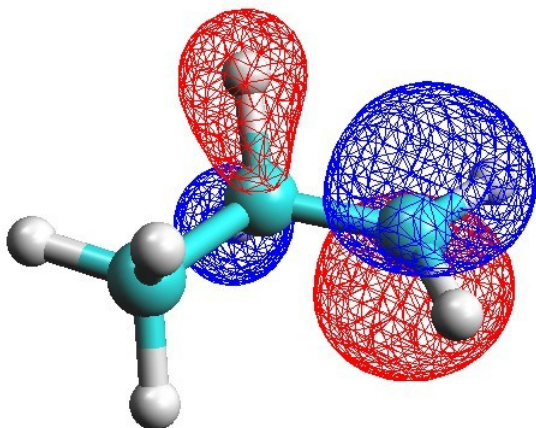
Carbocatione Vinilico 2°
Orbitale LUMO



Carbocatione Allilico 2°(e 1°)
Orbitale LUMO



Carbocatione Allilico 3°(e 1°)
Orbitale LUMO



Carbocationi 1°, 2° e 3°
Orbitali LUMO