Heats of Combustion, Heats of Formation, Heats of Hydrogenation and Bond Dissociation Energies

Germain Henri Hess

(1802 - 1850)

Hess's Law (1840)

- The total heat liberated in a series of chemical reactions is equal to the sum of the heats liberated in the individual steps.

- The heat liberated, ΔH^o, (enthalpy) is a state function.

- State functions are independent of path.

The "Heat" Liberated in Either Route is the Same

The Standard State is the zero point for chemical reactions.

A temperature of 298°K and 1 atmosphere pressure

Carbon as graphite

Hydrogen as a gas

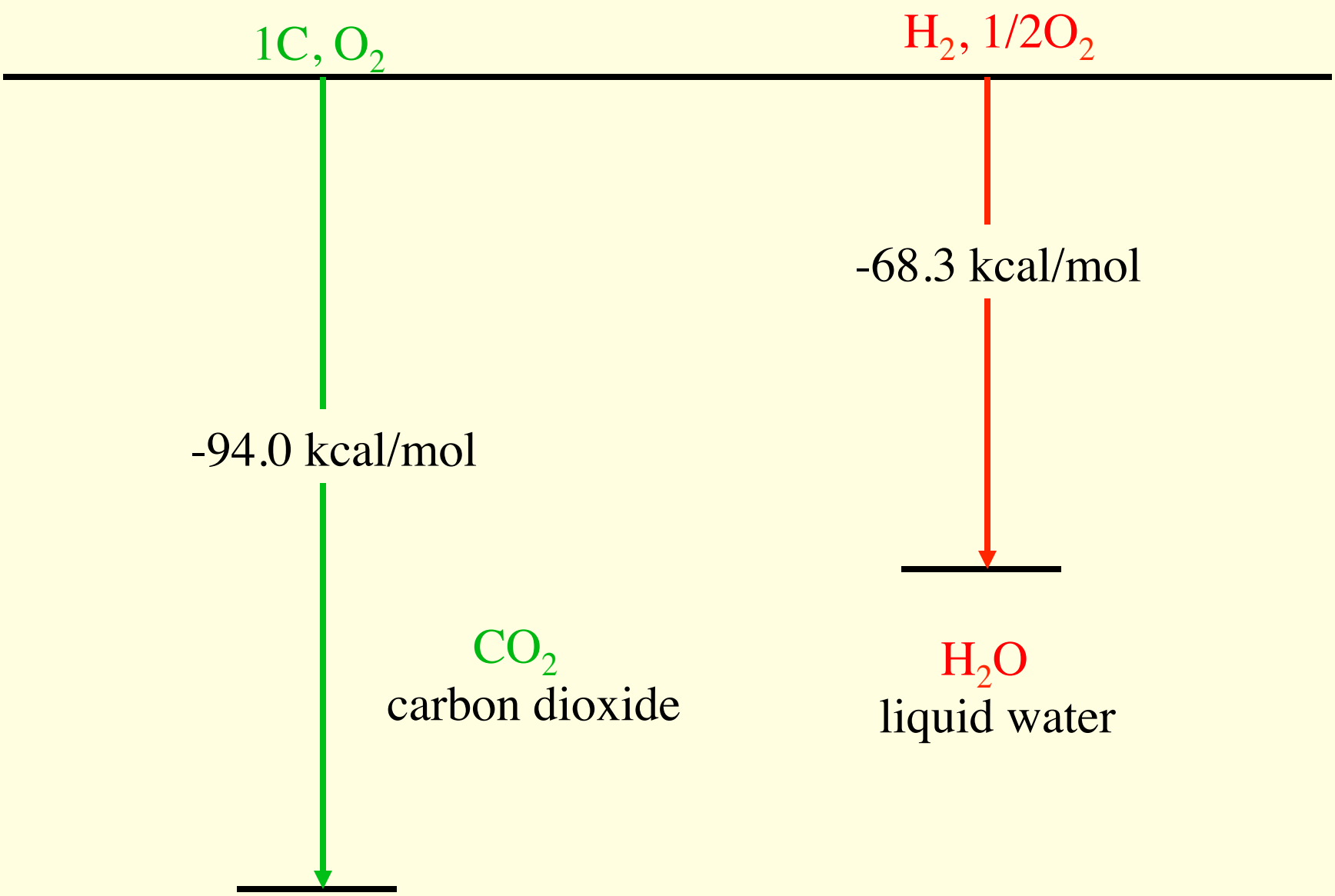
Oxygen as a gas

Chlorine as a gas

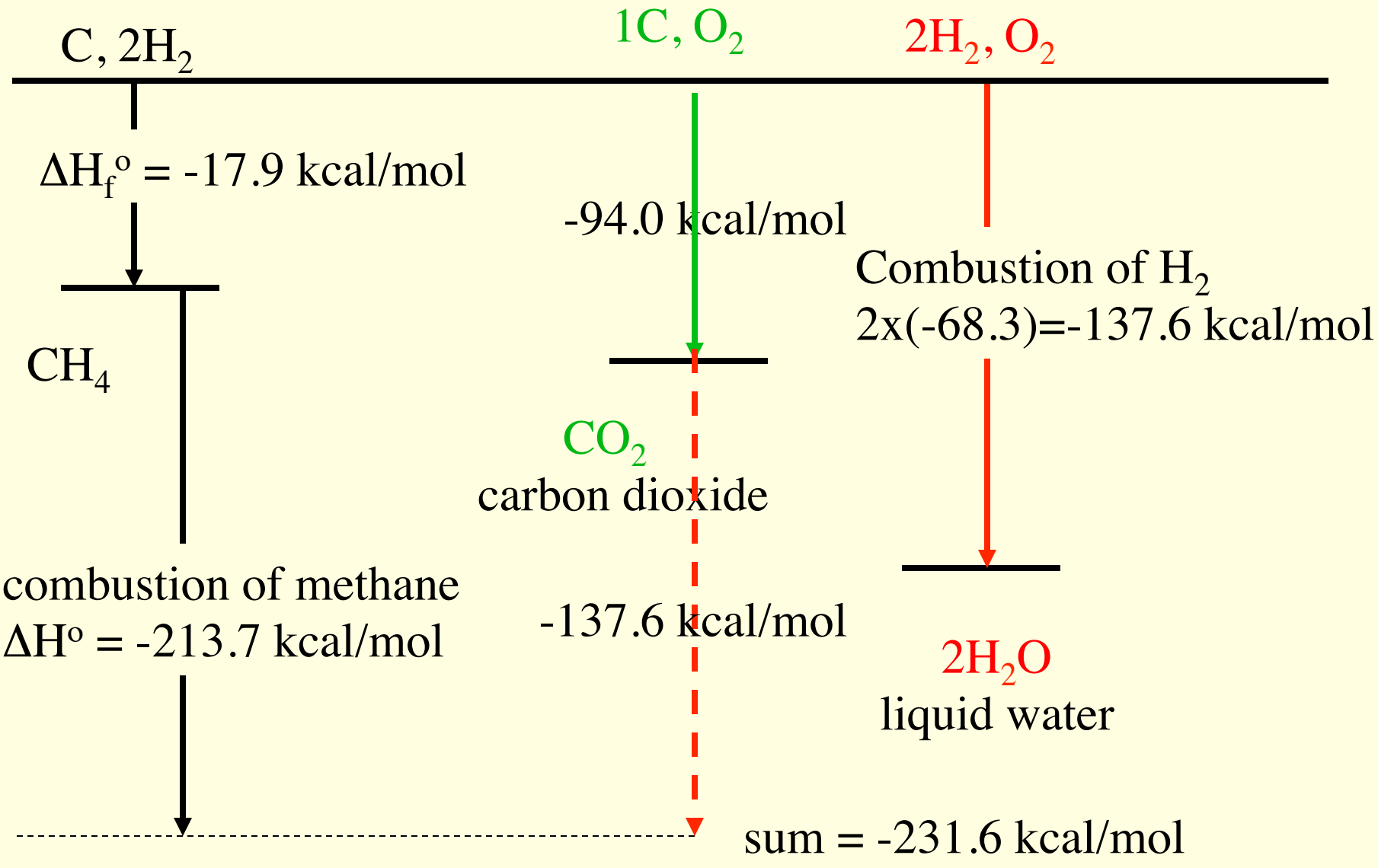
Bromine as a liquid

$\Delta H^{o} = 0$ kcal/mol

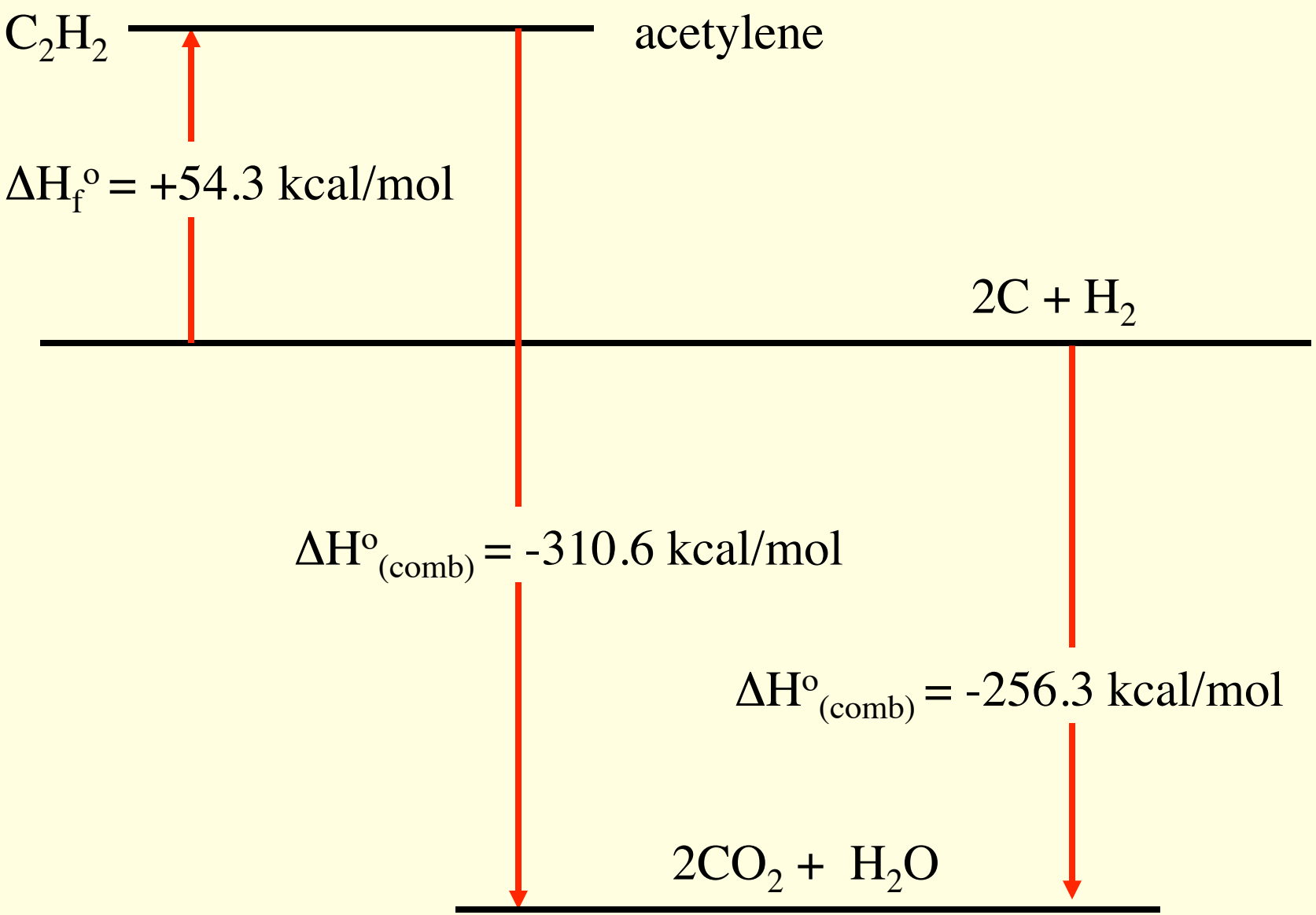
Combustion of Graphite and Hydrogen at 298°K



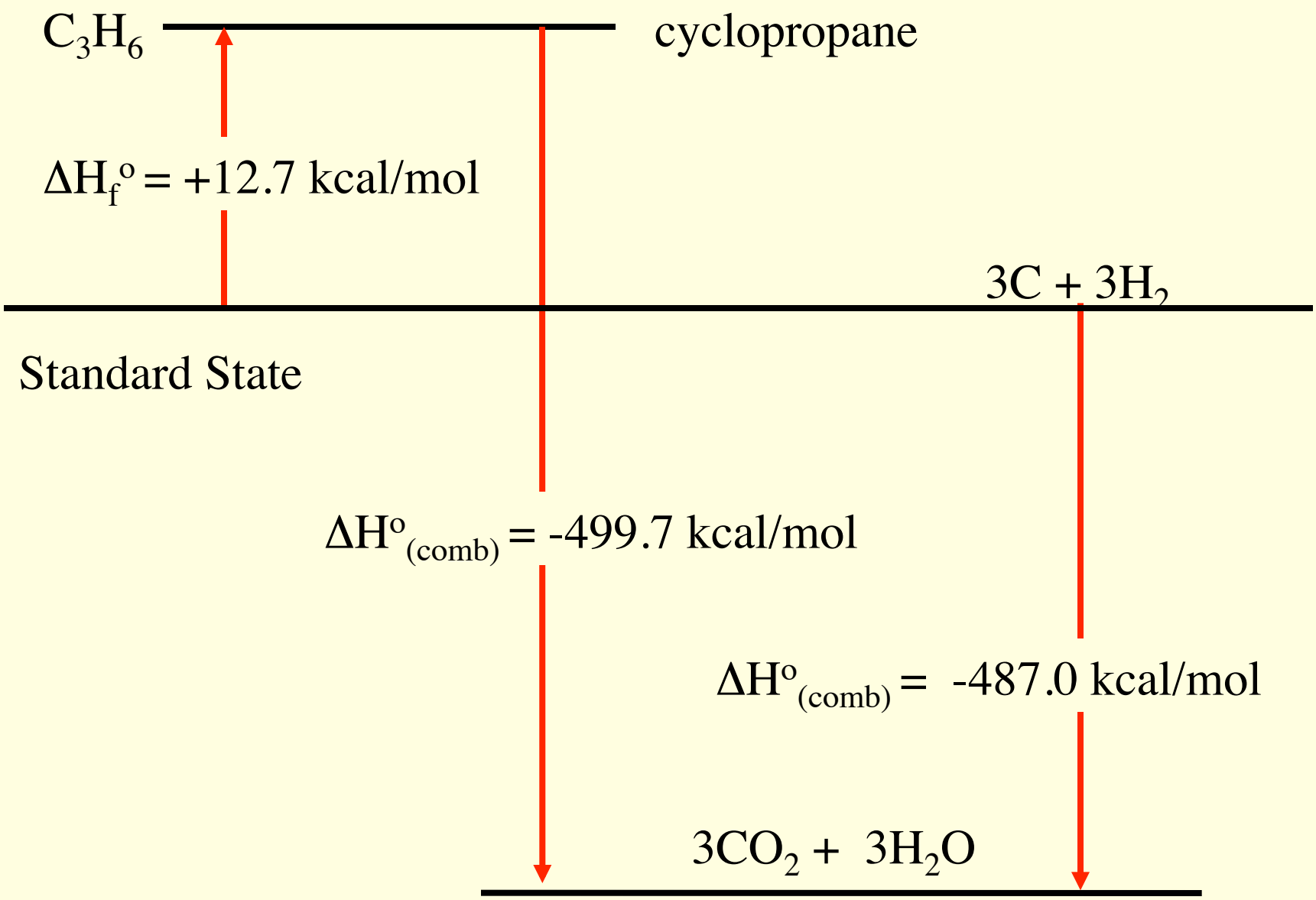
Combustion of Methane



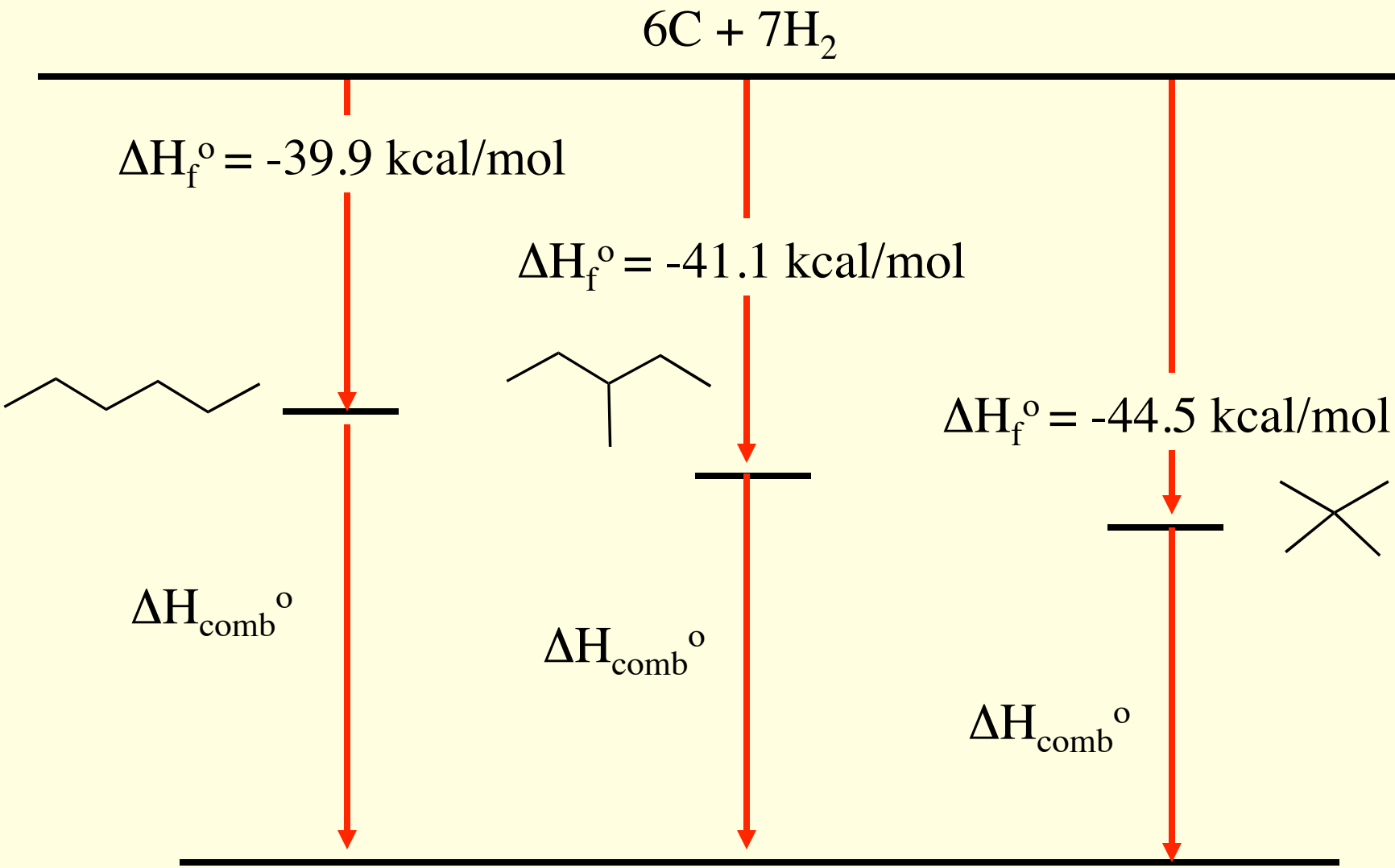
Not All Compounds Are More Stable Than Their Elements: Acetylene



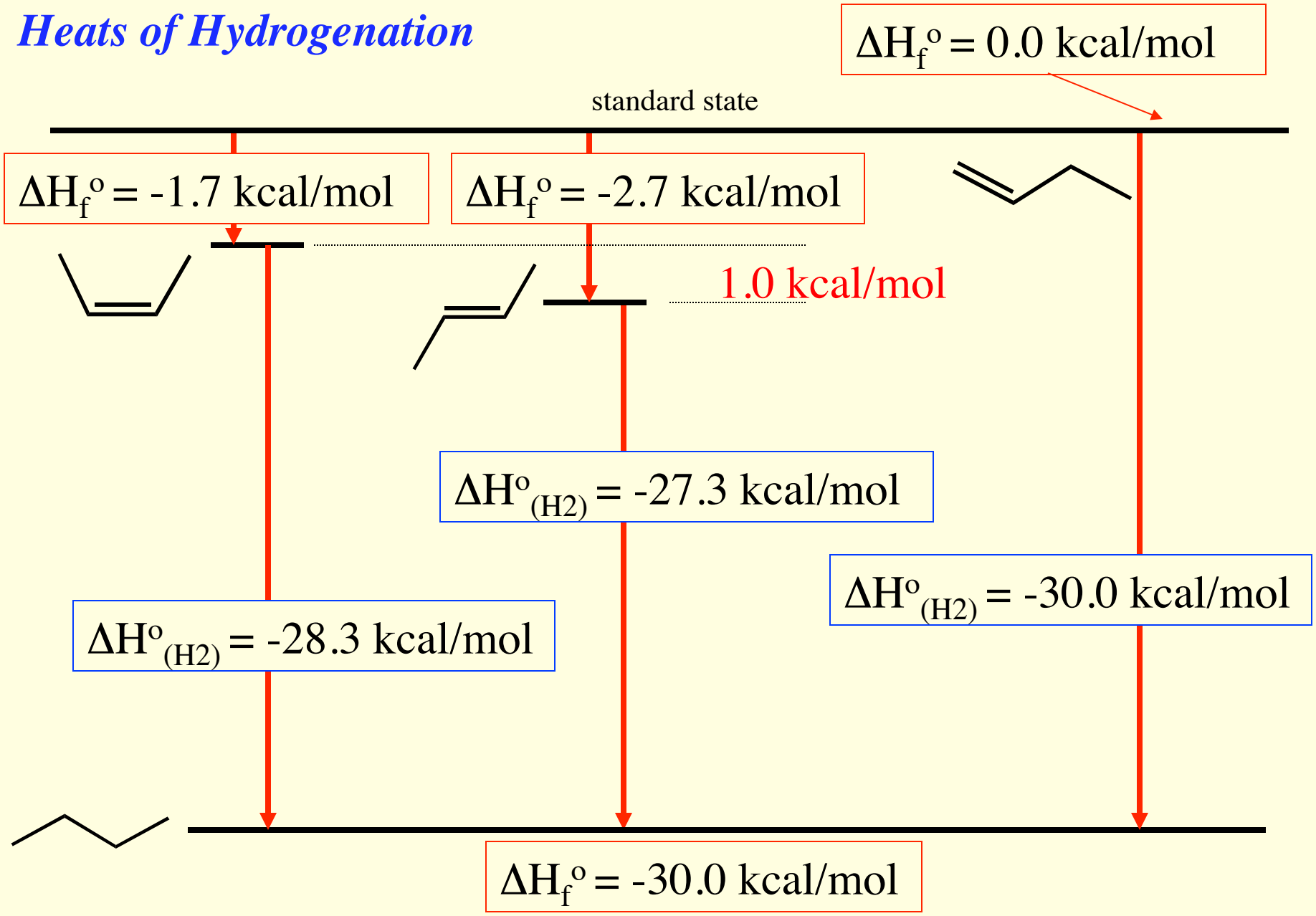
Not All Compounds Are More Stable Than Their Elements: Cyclopropane



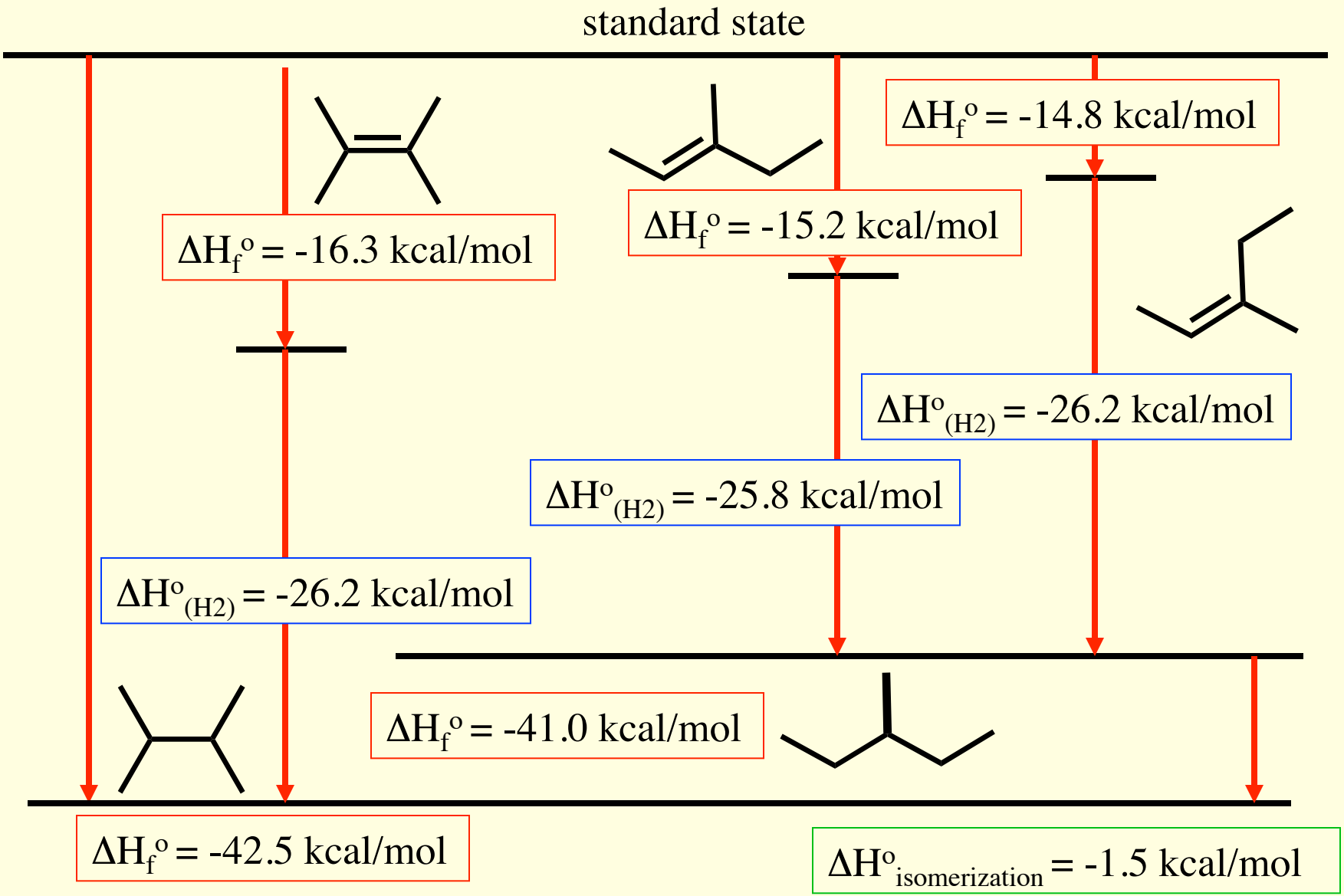
Combustion of Hexane Constitutional Isomers



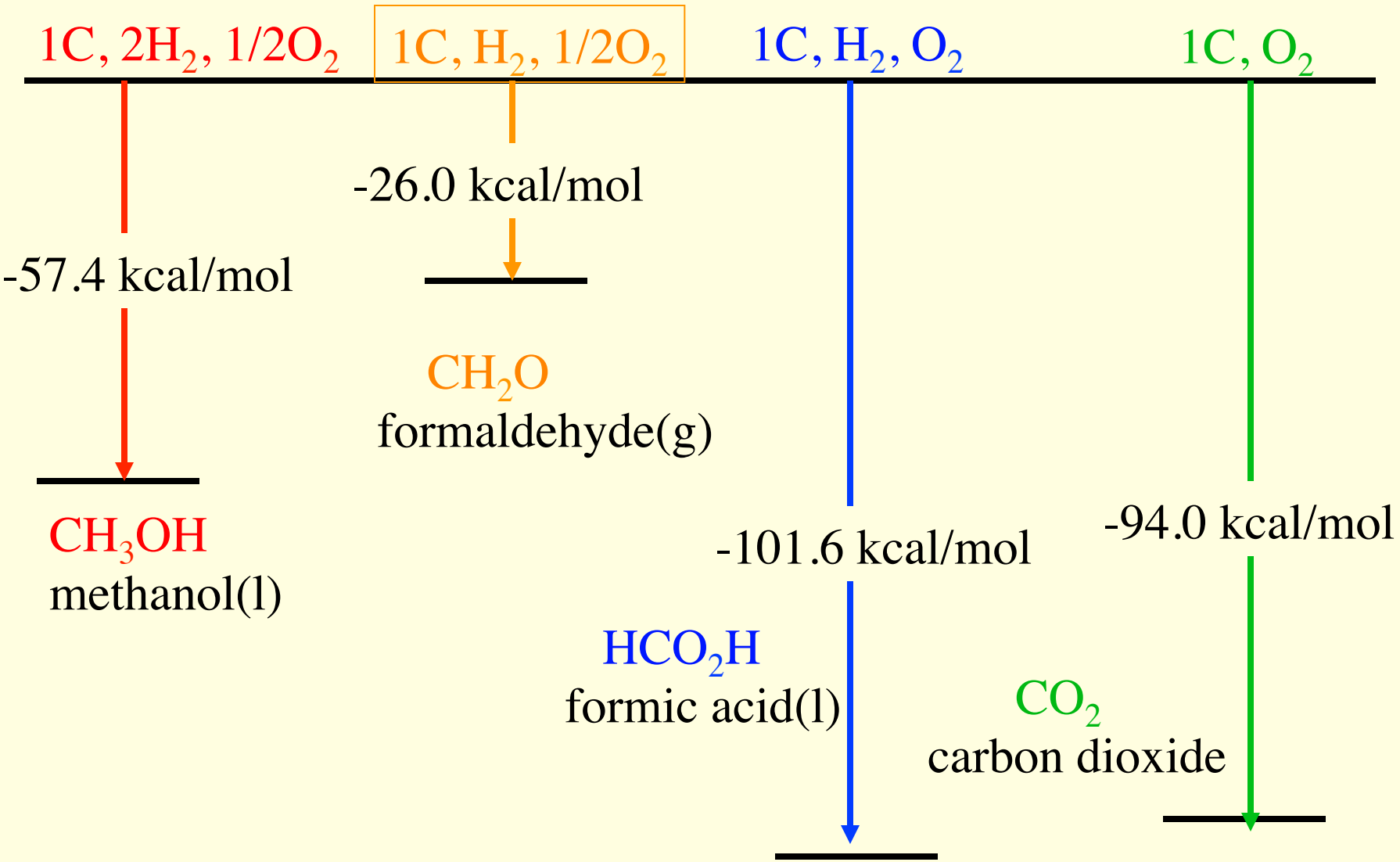
Heats of Hydrogenation



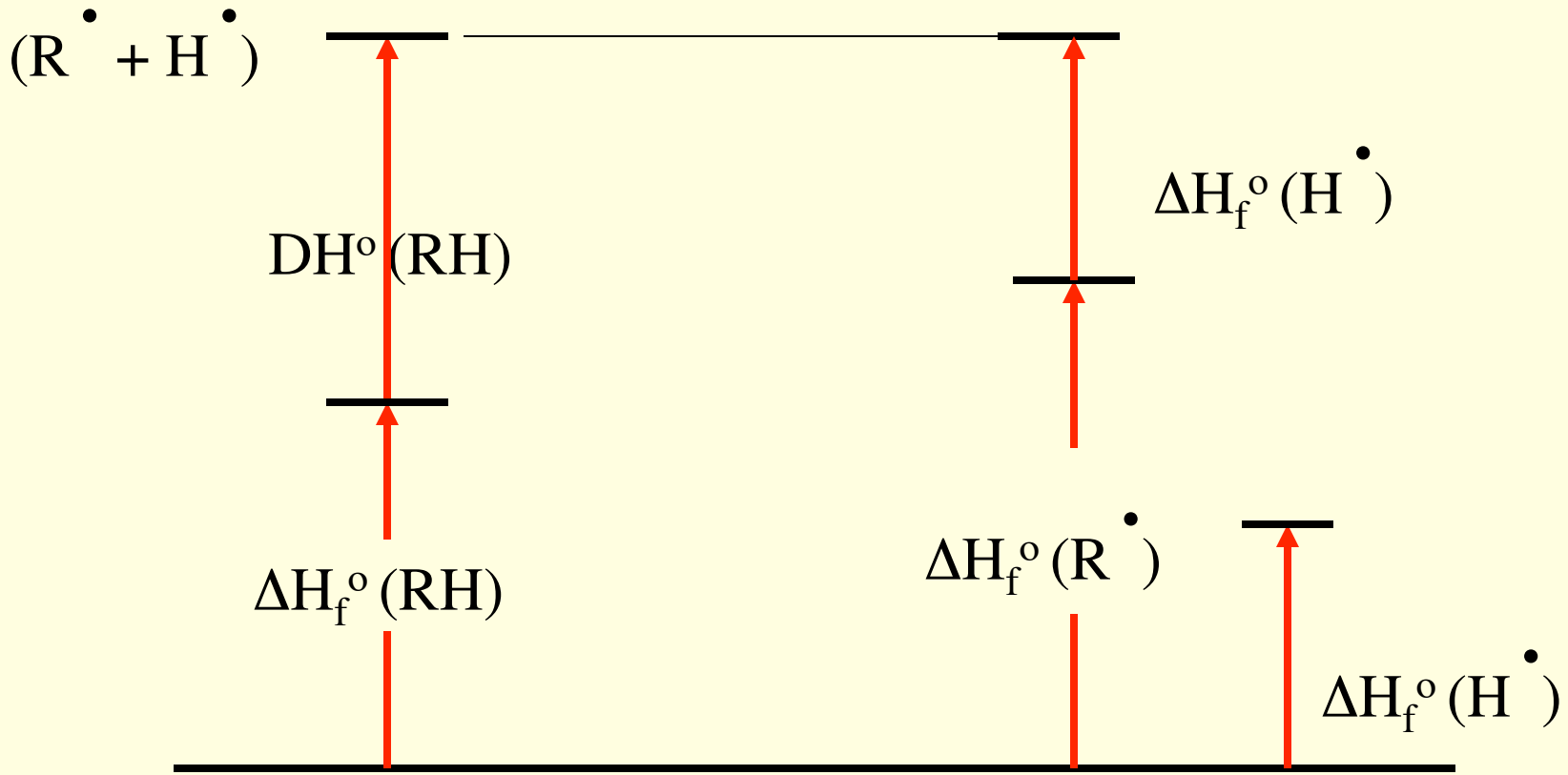
Heats of Hydrogenation - 2



ΔH_f^o of Methanol and Its Products of Oxidation

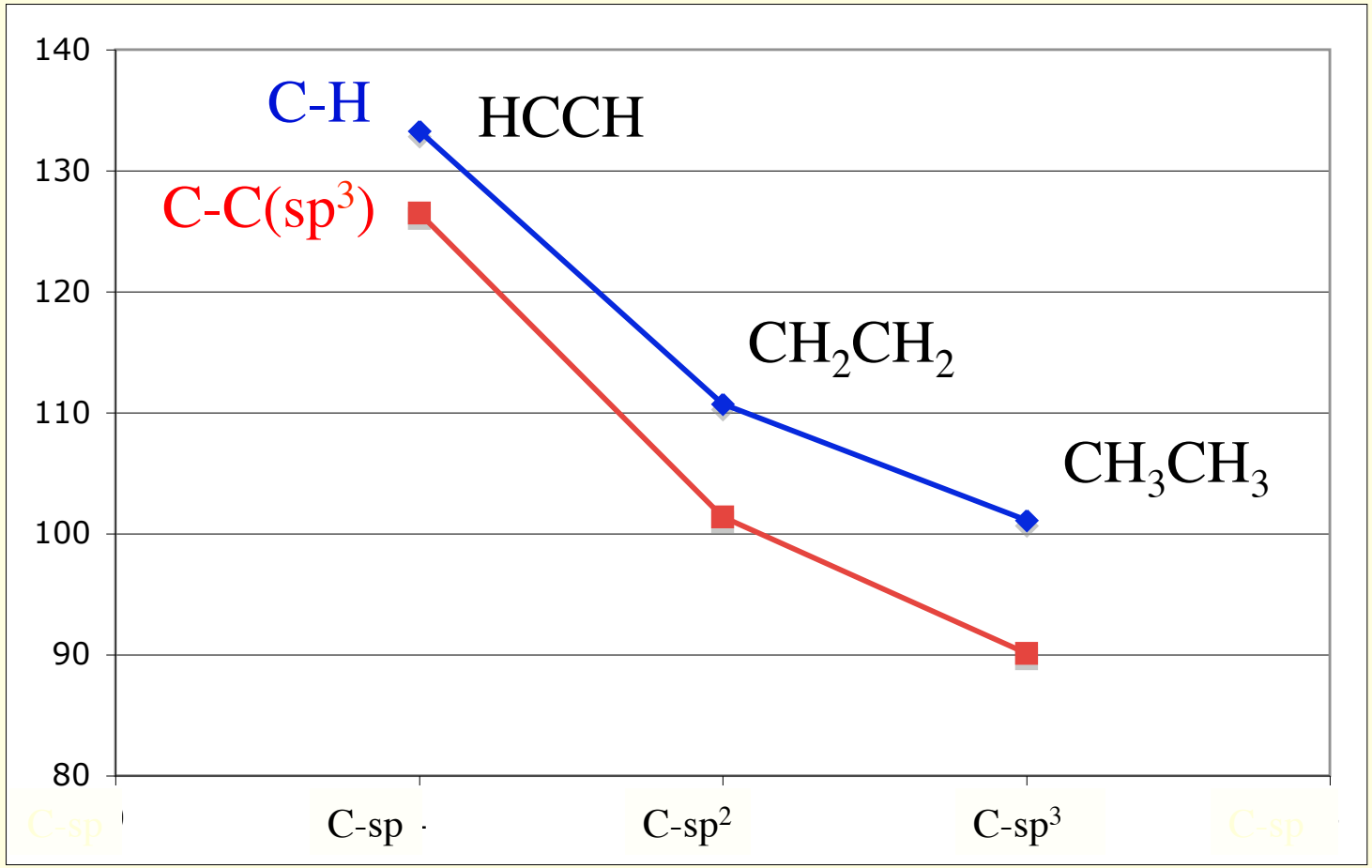


Bond Dissociation Energy (BDE)

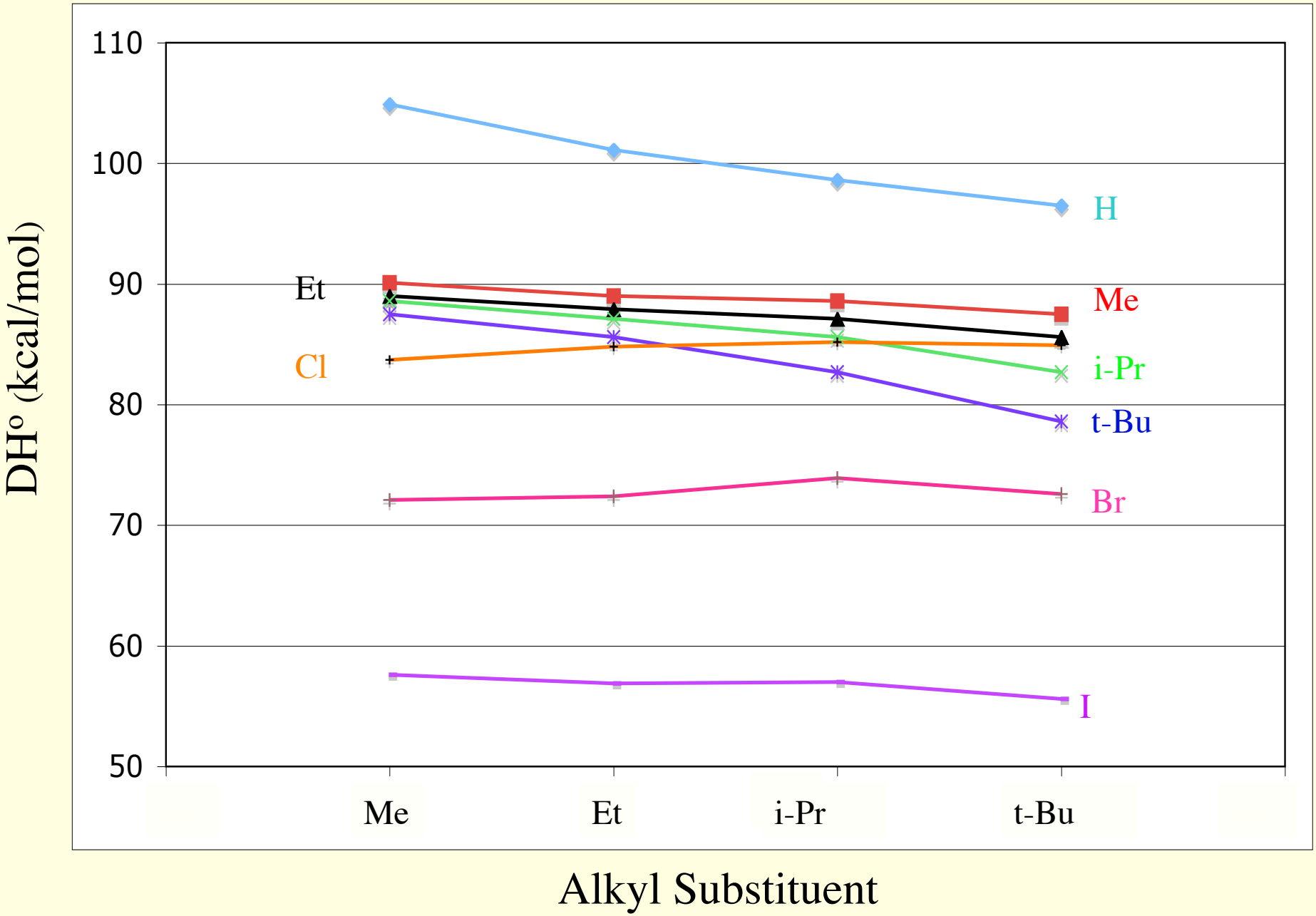


$$DH^{o}(RH) = \Delta H_f^{o}(H^{\bullet}) + \Delta H_f^{o}(R^{\bullet}) - \Delta H_f^{o}(RH)$$

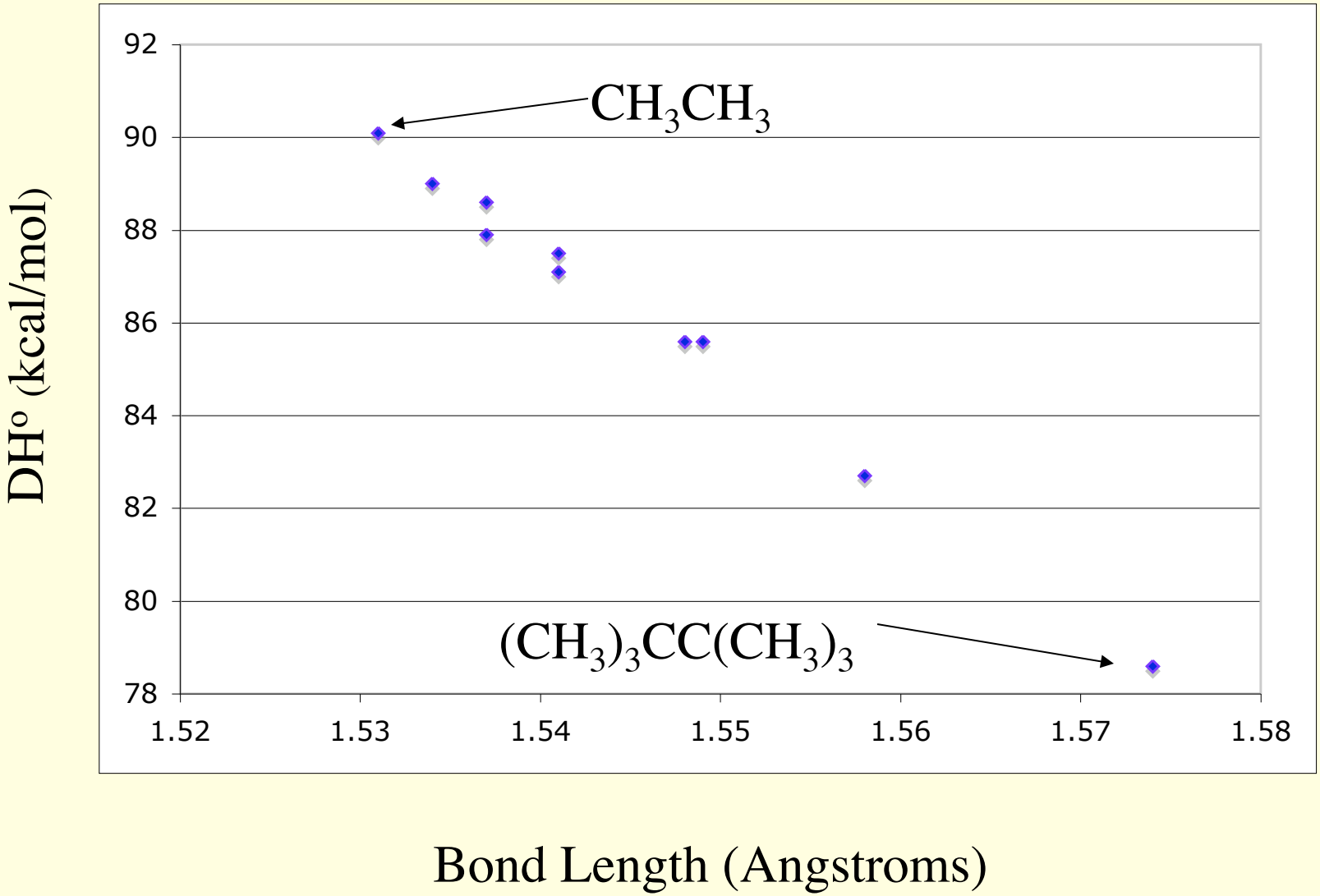
Bond Dissociation Energy and Hybridization



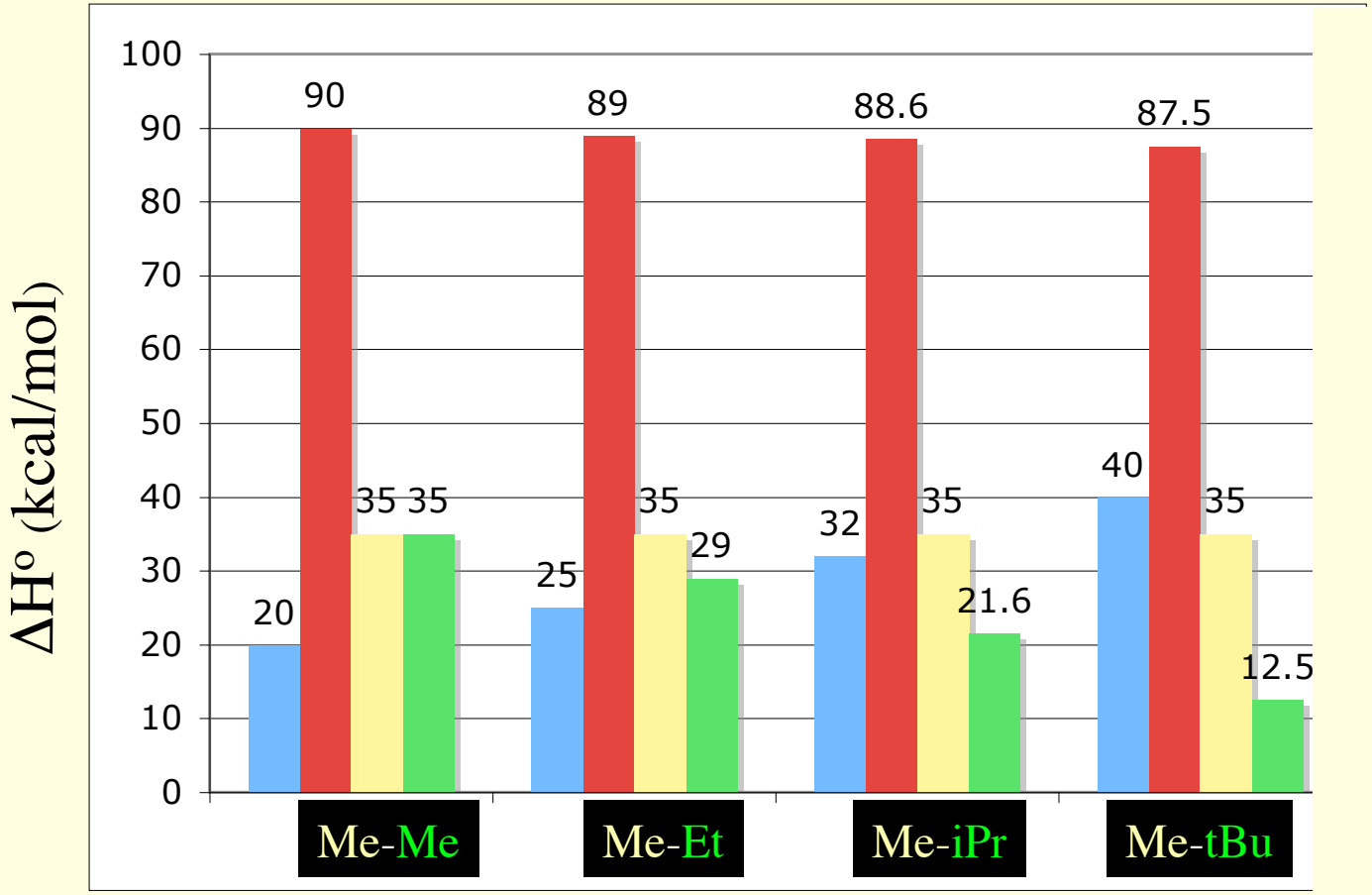
BDEs of C-C, C-X and C-H Bonds



C-C Bond Strength vs. Bond Length

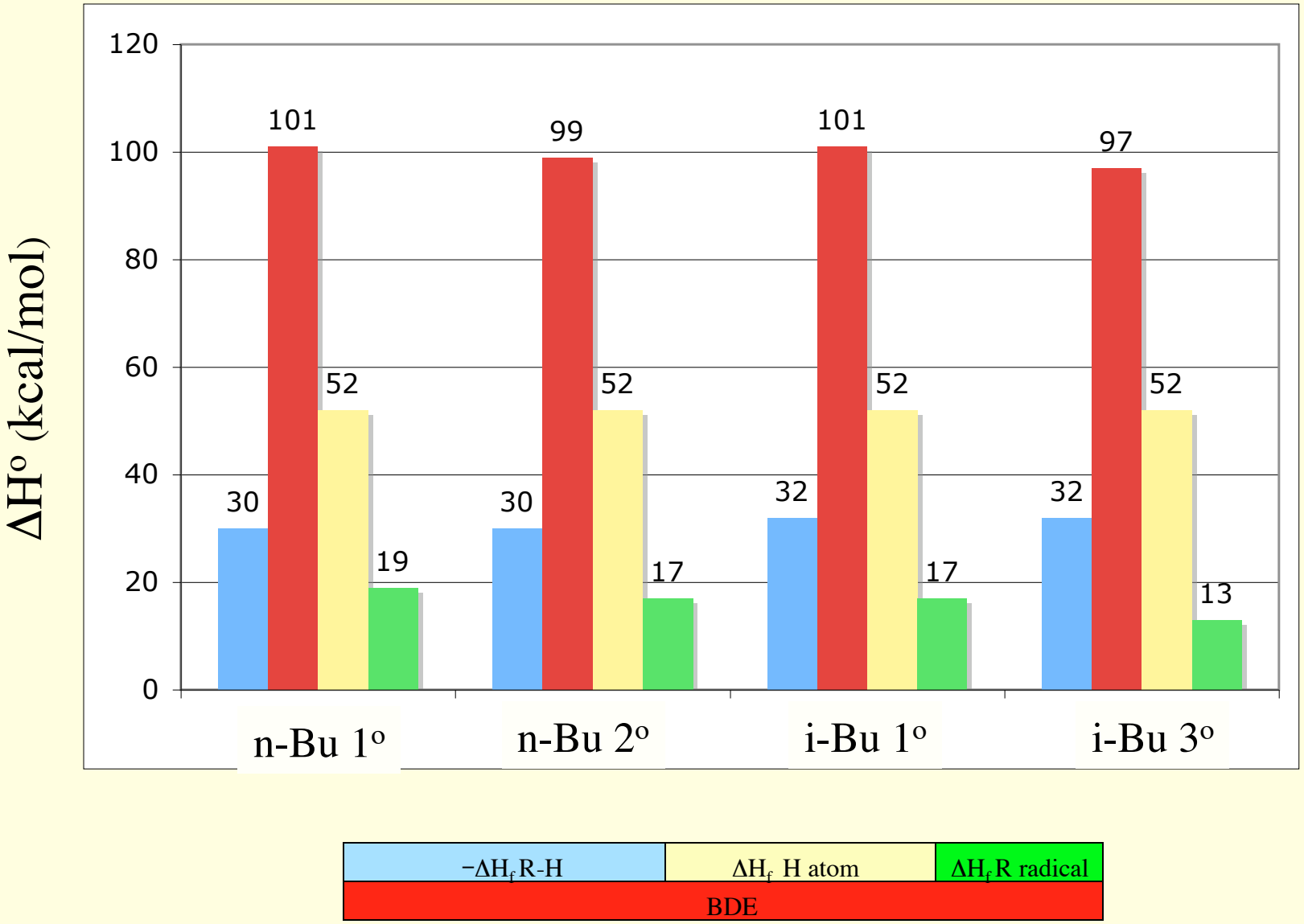


C-C Bonds

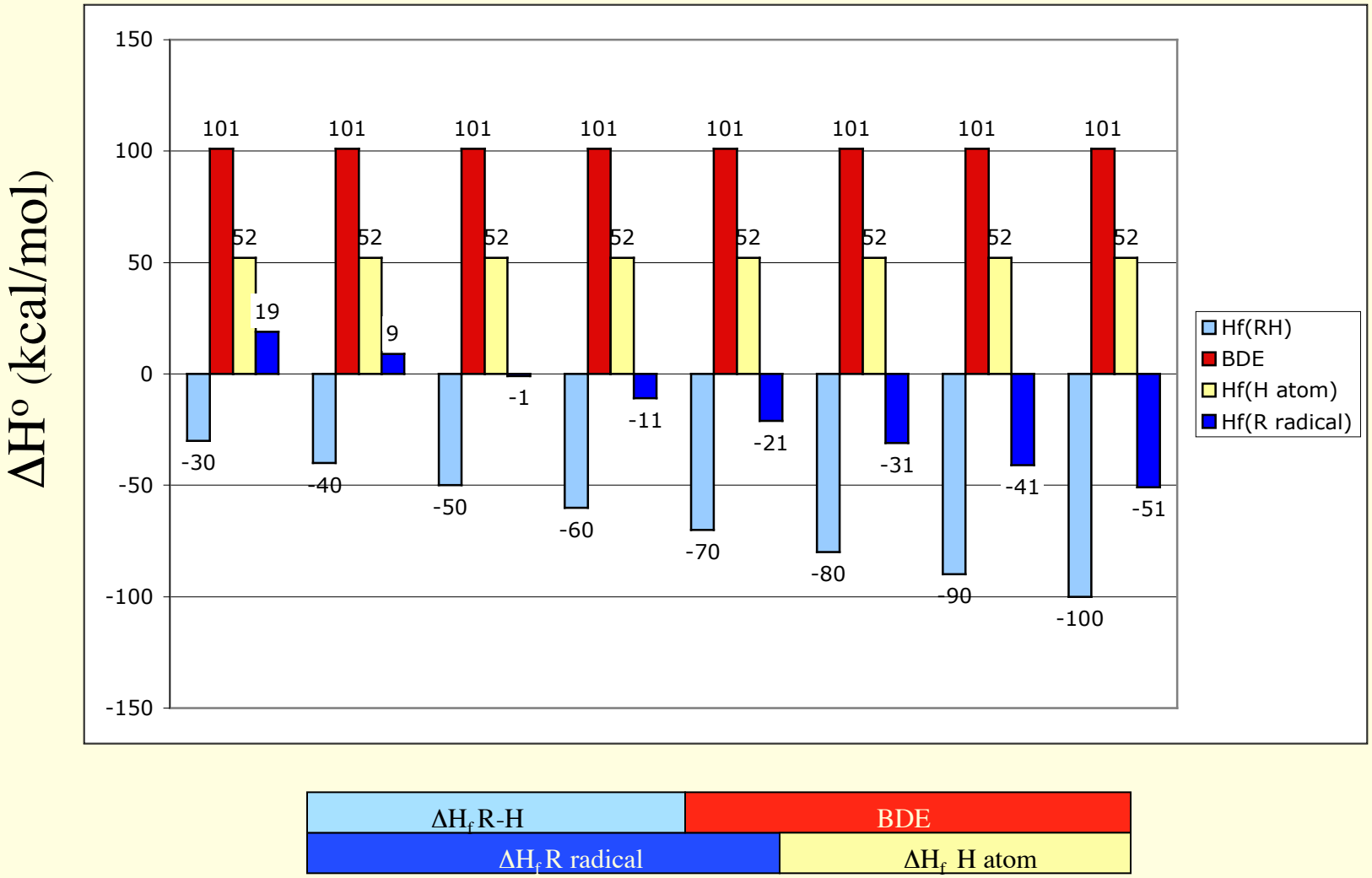

ΔH° (kcal/mol)
100
90
80
70
60
50
40
30
20
10
0
90
89
88.6
87.5
35 35
35
35
35
20
25
32
40
29
21.6
12.5
Me-Me
Me-Et
Me-iPr
Me-tBu


−ΔH$_f$ R-R'
ΔH$_f$ Radical 1
ΔH$_f$ Radical 2
BDE

Butane Isomers



Formation of C_4-C_{18} Even Primary Radicals from Their n-Alkanes



The End