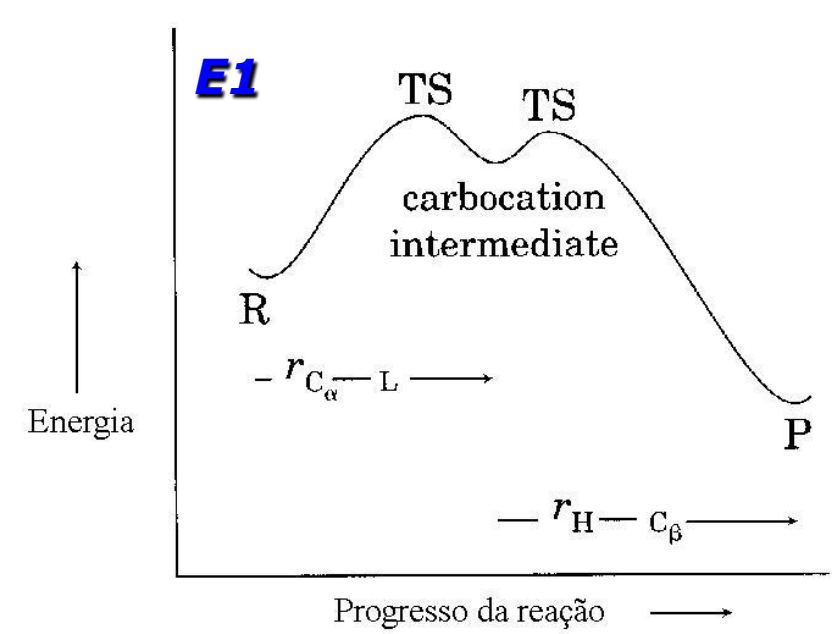
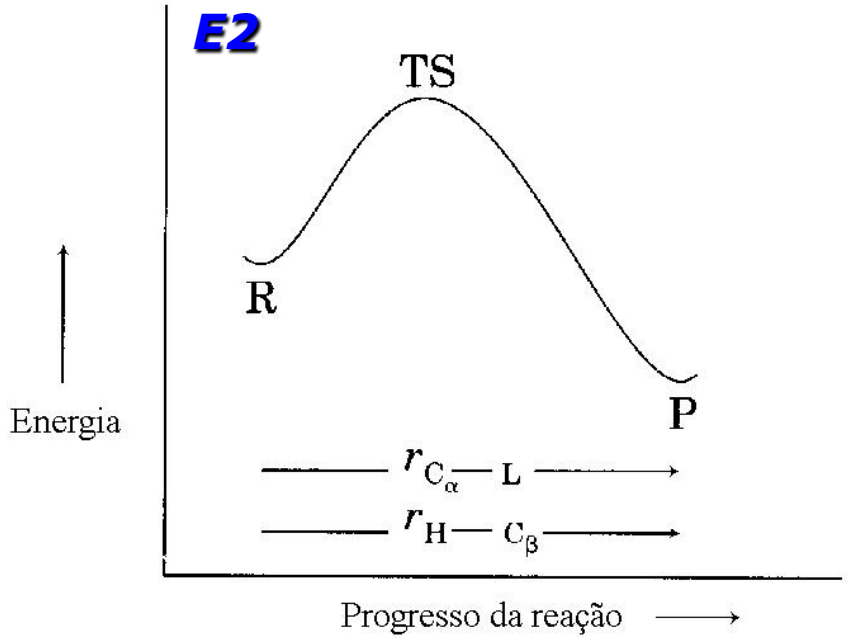
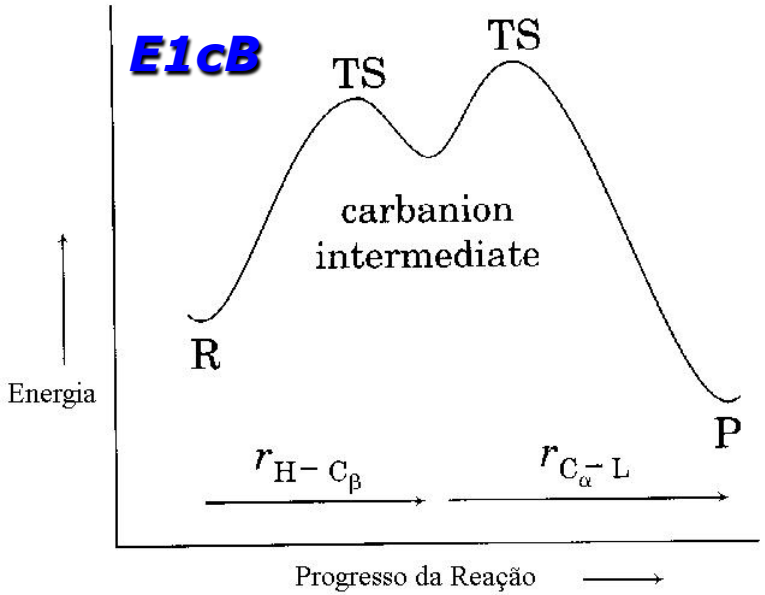
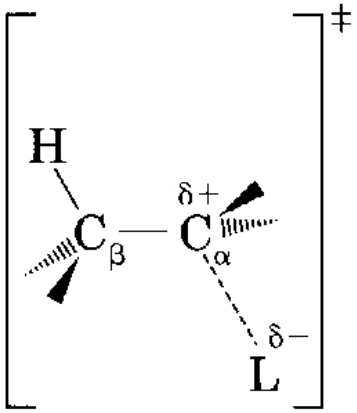
Diagramas de Energia Potencial da Reação



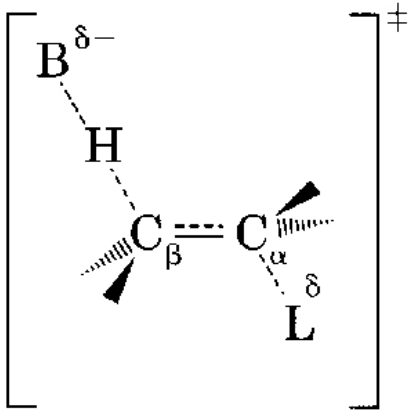




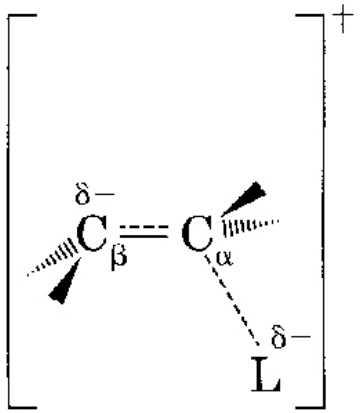
Estados de Transição para os Mecanismos de Eliminações-1,2



E1



E2



E1cb

Diagrama bidimensional de coordenada de reação de More O´Ferrall-Jencks para os Mecanismos de Eliminações-1,2

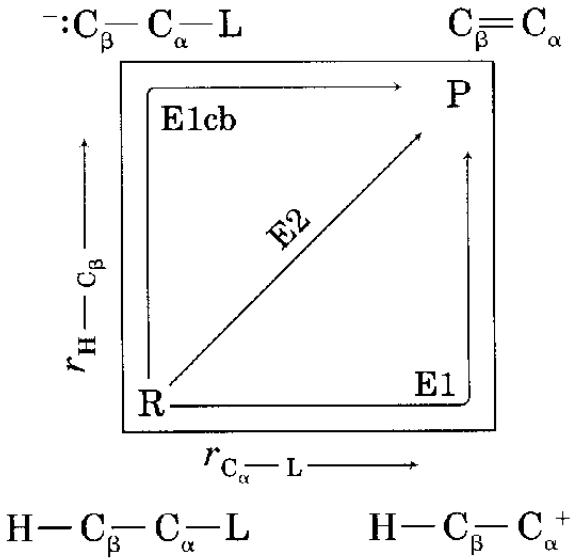
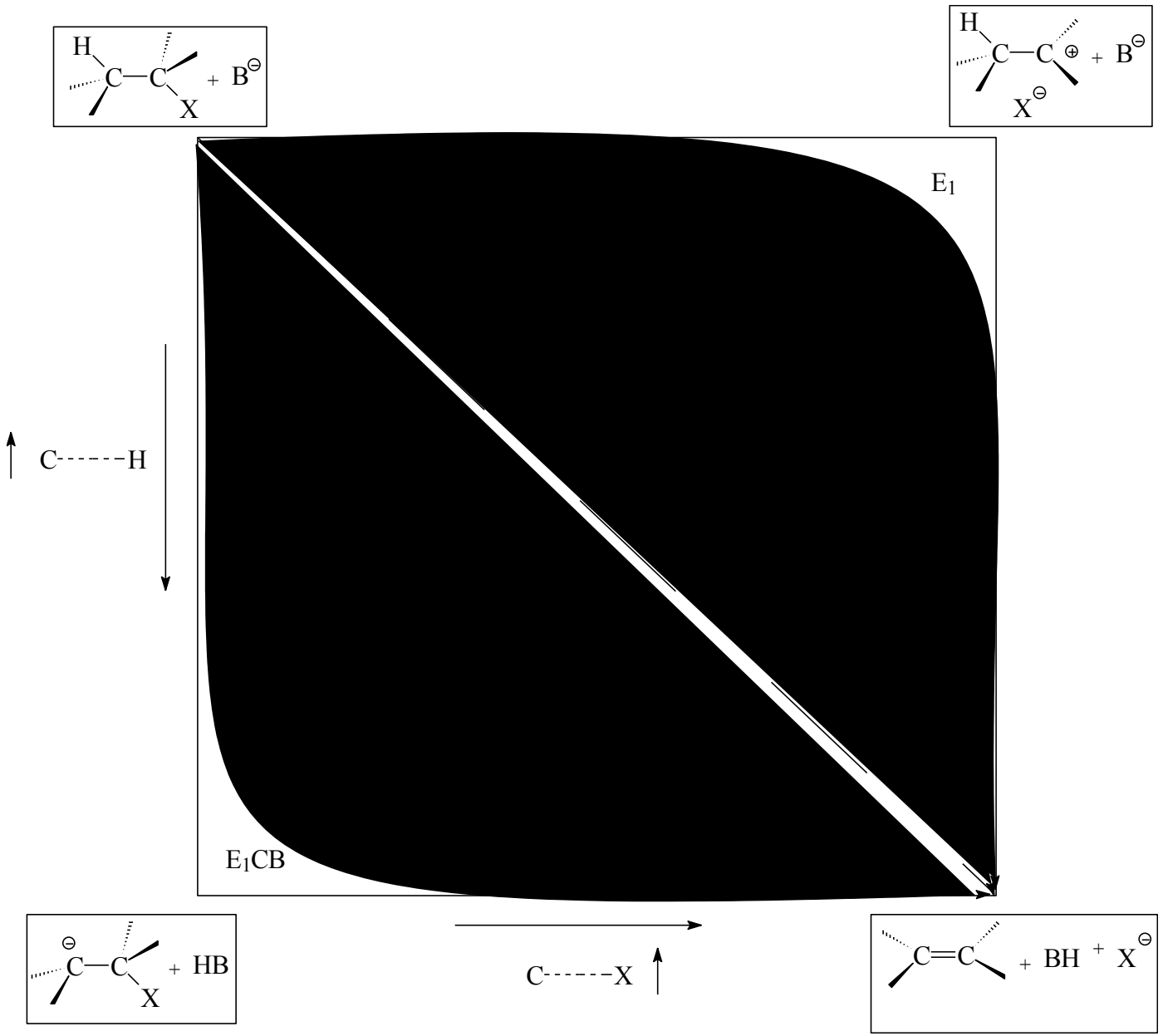


Diagrama bidimensional da reação: More O'Ferrall - Jencks



Substituição Nucleofílica

Carey, Cap. 5, Carroll, Cap. 8 e March, Cap. 10

envolve as seguintes possíveis combinações

a) $RX + Y: \longrightarrow RY^{+} + X^{-}:$

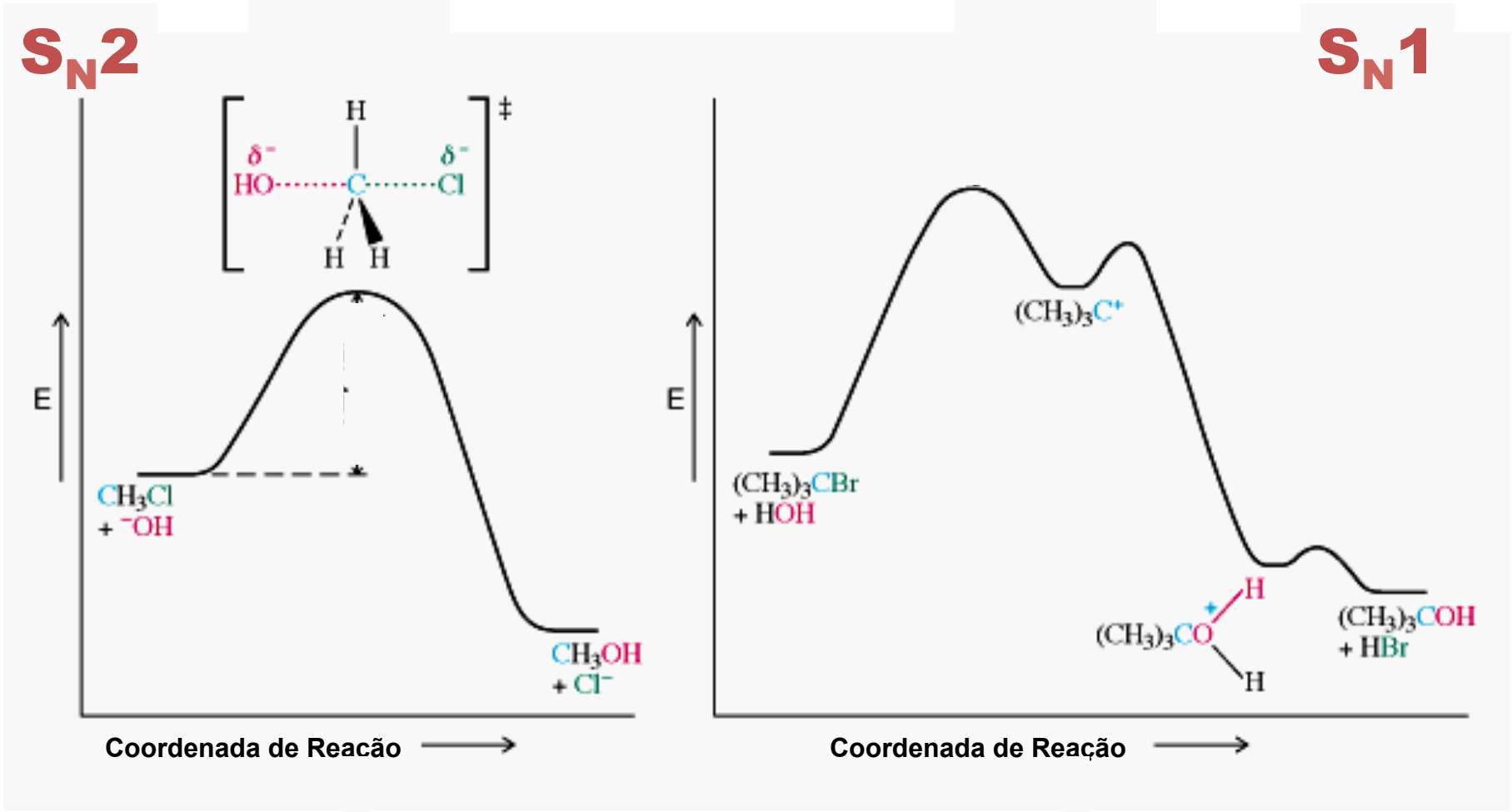
b) $RX + Y:^{-} \longrightarrow RY + X^{-}:$

c) $RX^{+} + Y: \longrightarrow RY^{+} + X:$

d) $RX^{+} + Y:^{-} \longrightarrow RY + X:$

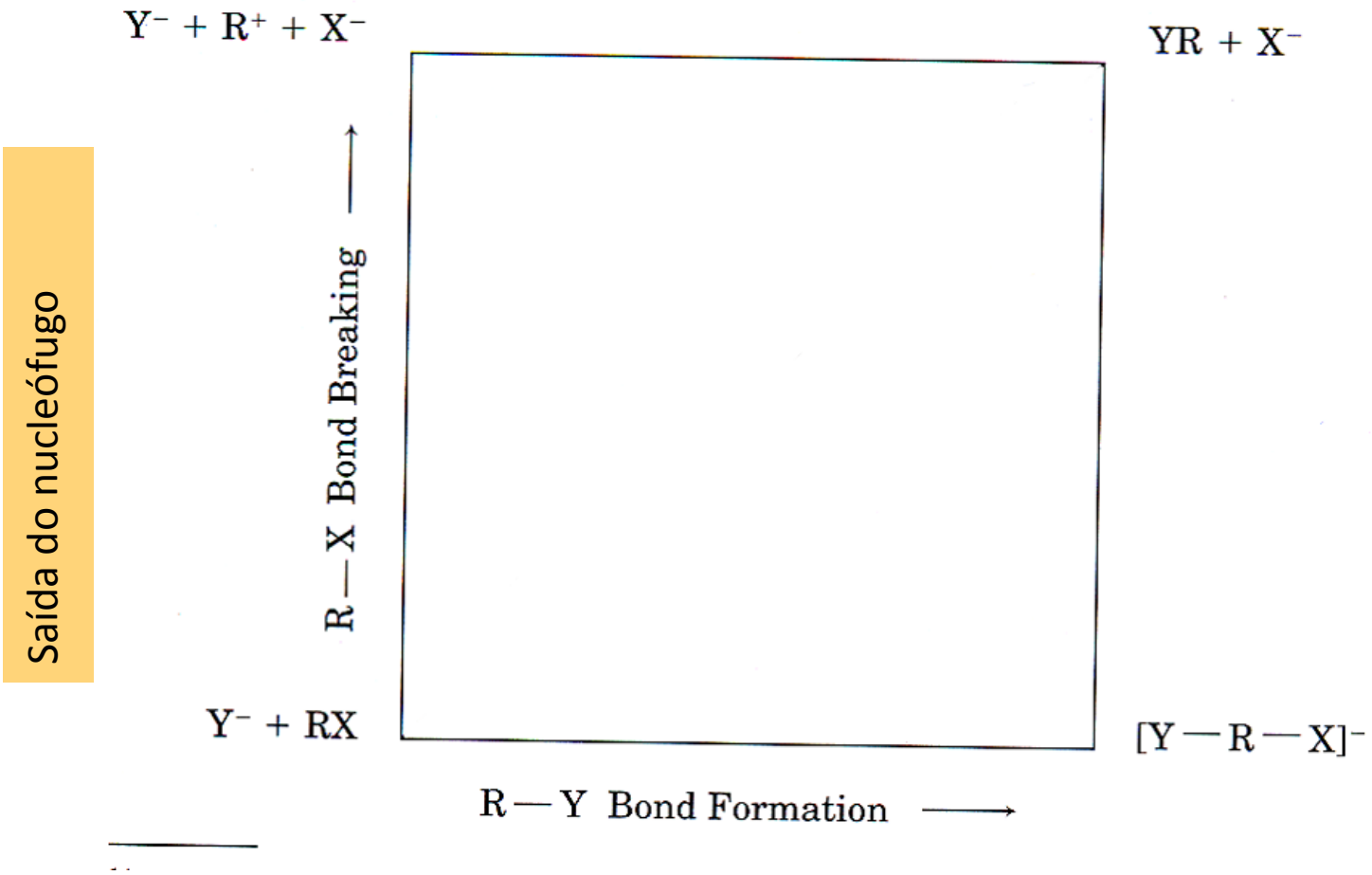
- sempre Y deve conter um par de elétrons não emparelhados
- Y é denominado nucleófilo
- X é denominado nucleófugo
- quando Y é o solvente é chamado *solvólise*

Diagramas da Coordenada de Reação para S_N2 e S_N1



O que representa a "C.R." em cada um dos mecanismos???

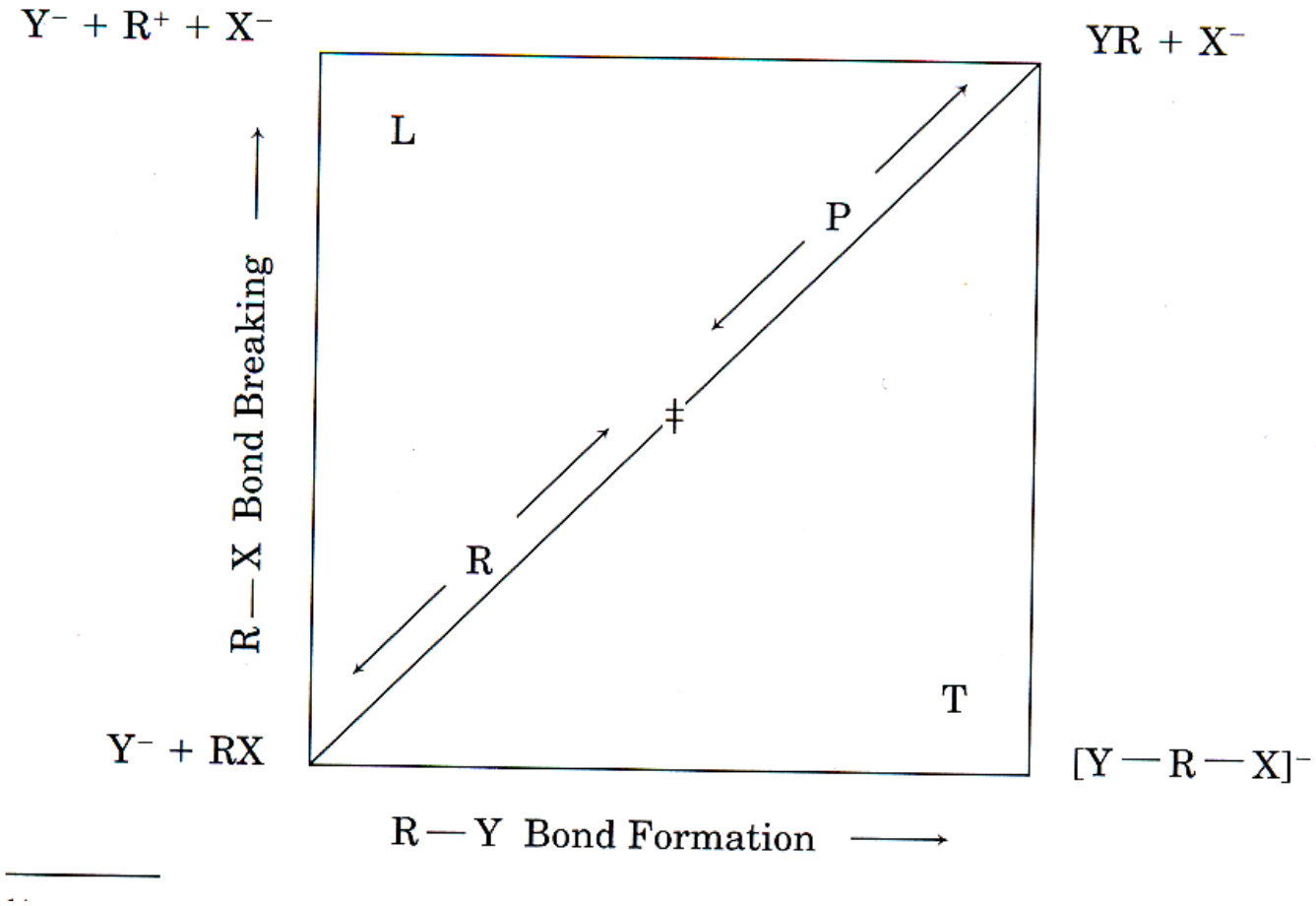
Coordenada de reação bi-dimensional



Saída do nucleófugo

Ataque do nucleófilo

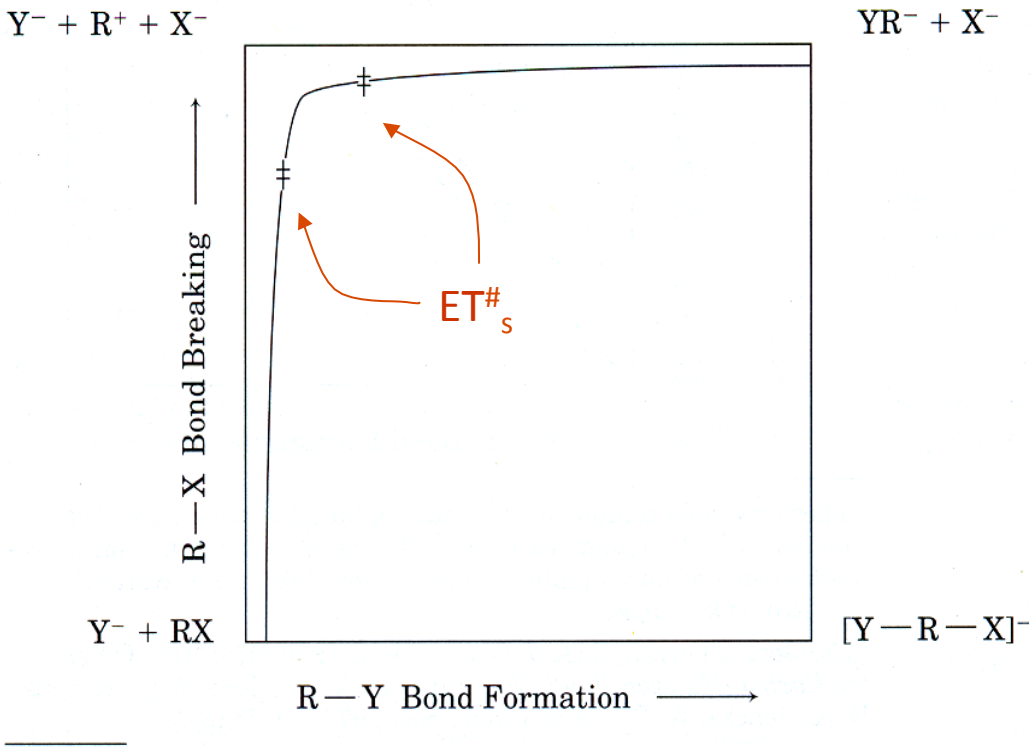
Ex: S_N2

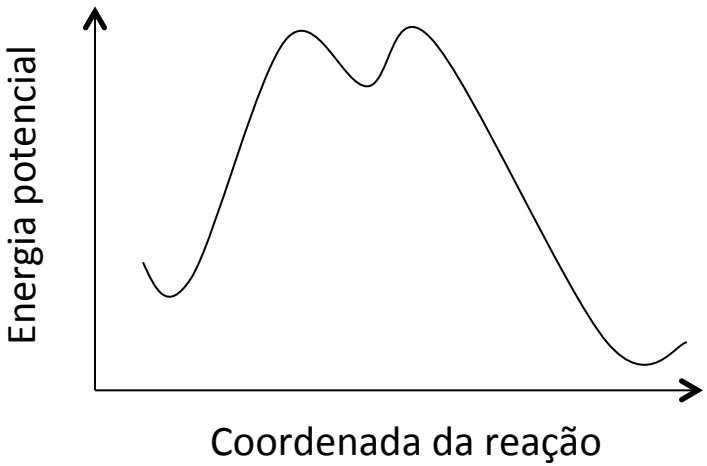


L denota ET solto"(*loose*)
T denota ET apertado (*tight*)

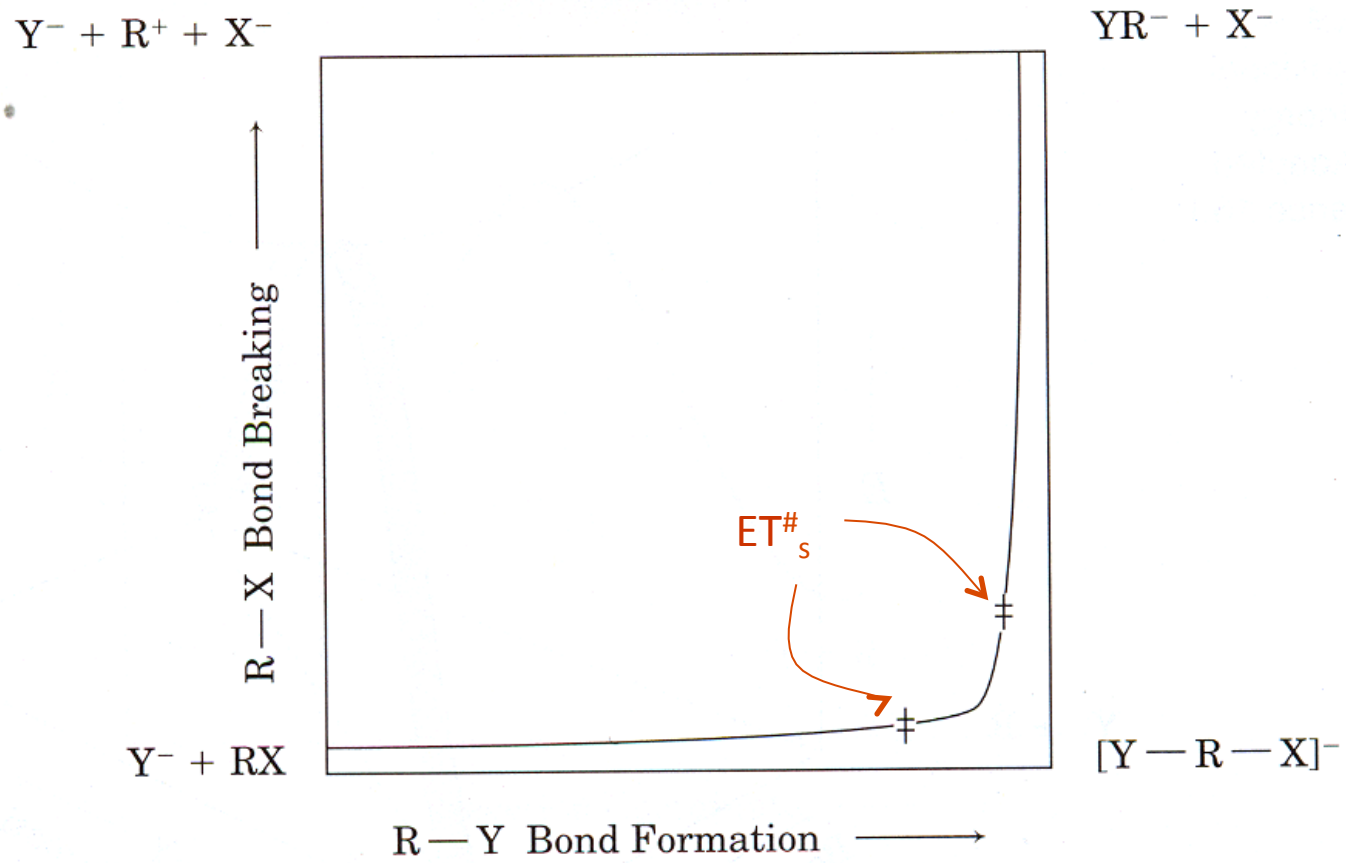
R denota ET similar a reagentes
P denota ET similar a produtos

Ex: S_N1


Y⁻ + R⁺ + X⁻
YR⁻ + X⁻
R—X Bond Breaking
ET#s
Y⁻ + RX
[Y—R—X]⁻
R—Y Bond Formation

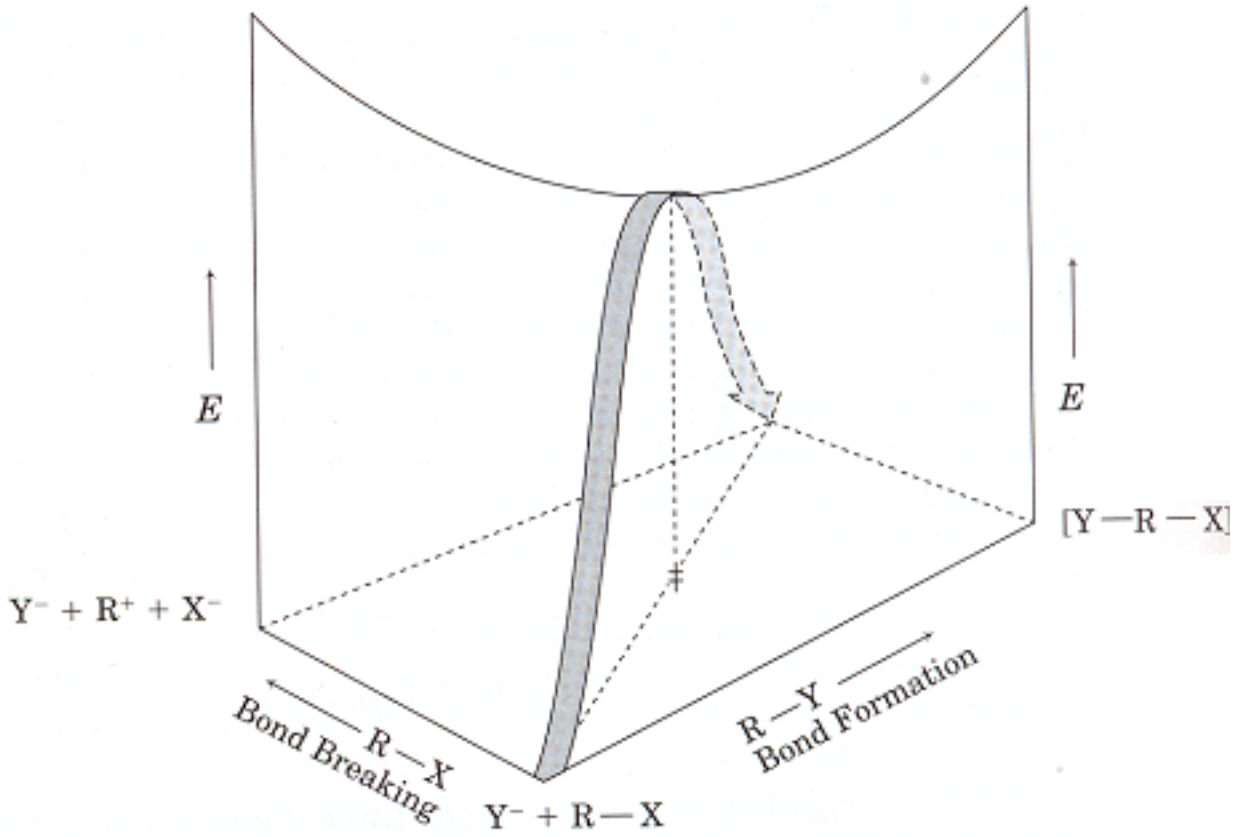

Energia potencial
Coordenada da reação

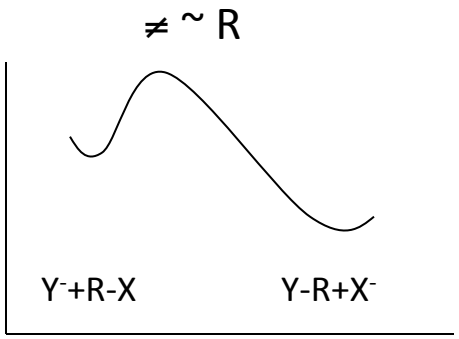
Ex: S_NAr

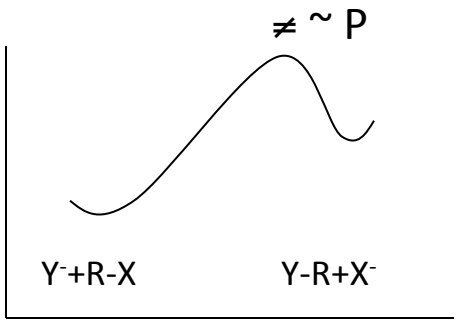


Efeito da estabilização de reagentes ou produtos

S_N2

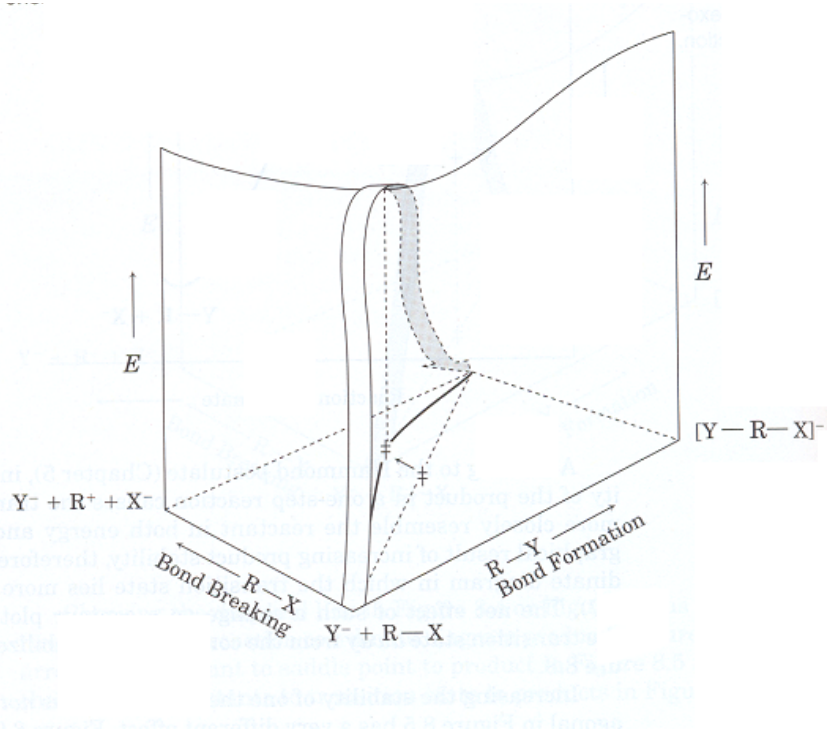






S_N2

Efeito da estabilização do intermediário



Efeito da estabilização do grupo de partida

