Doorway mechanism for Dissociative Electron attachment

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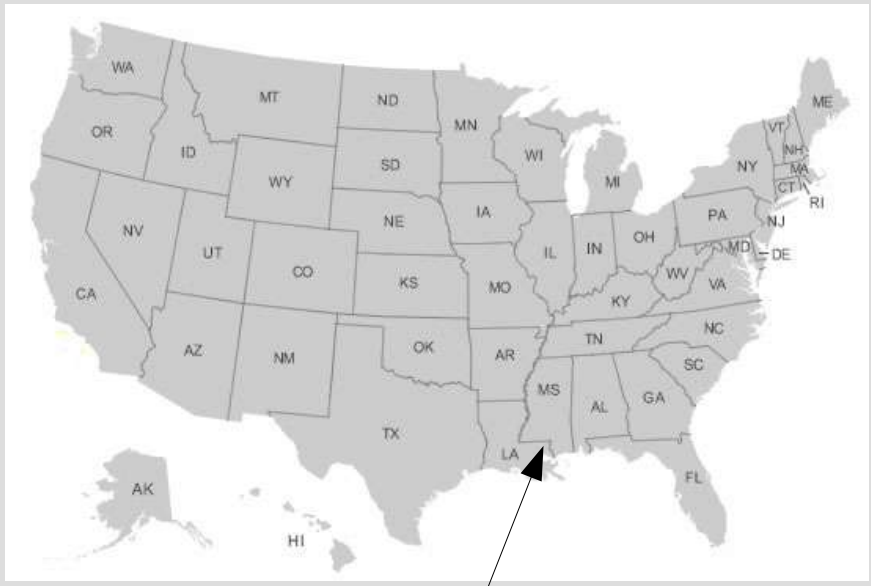
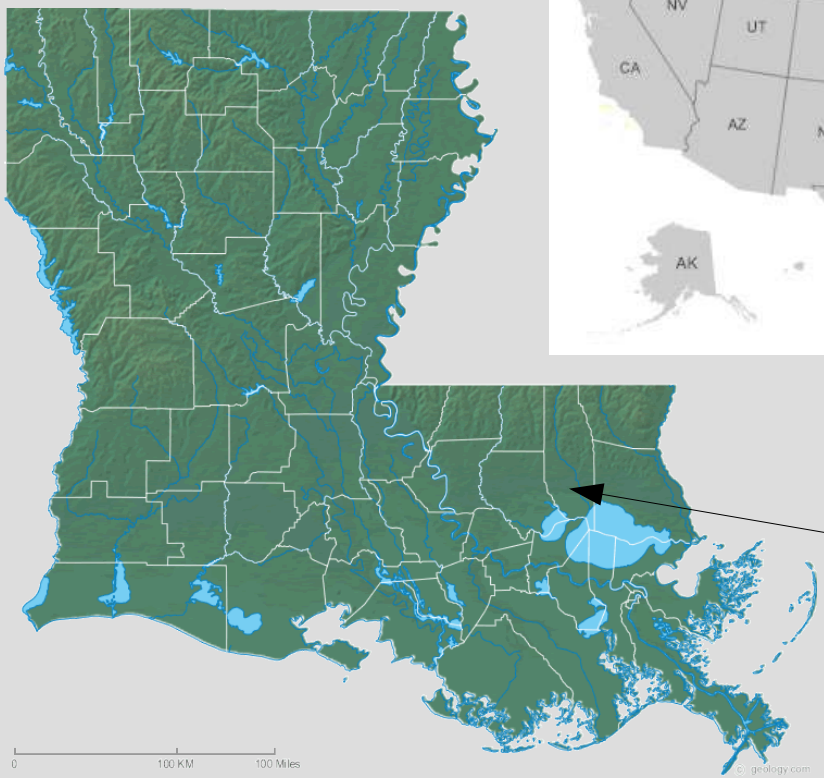




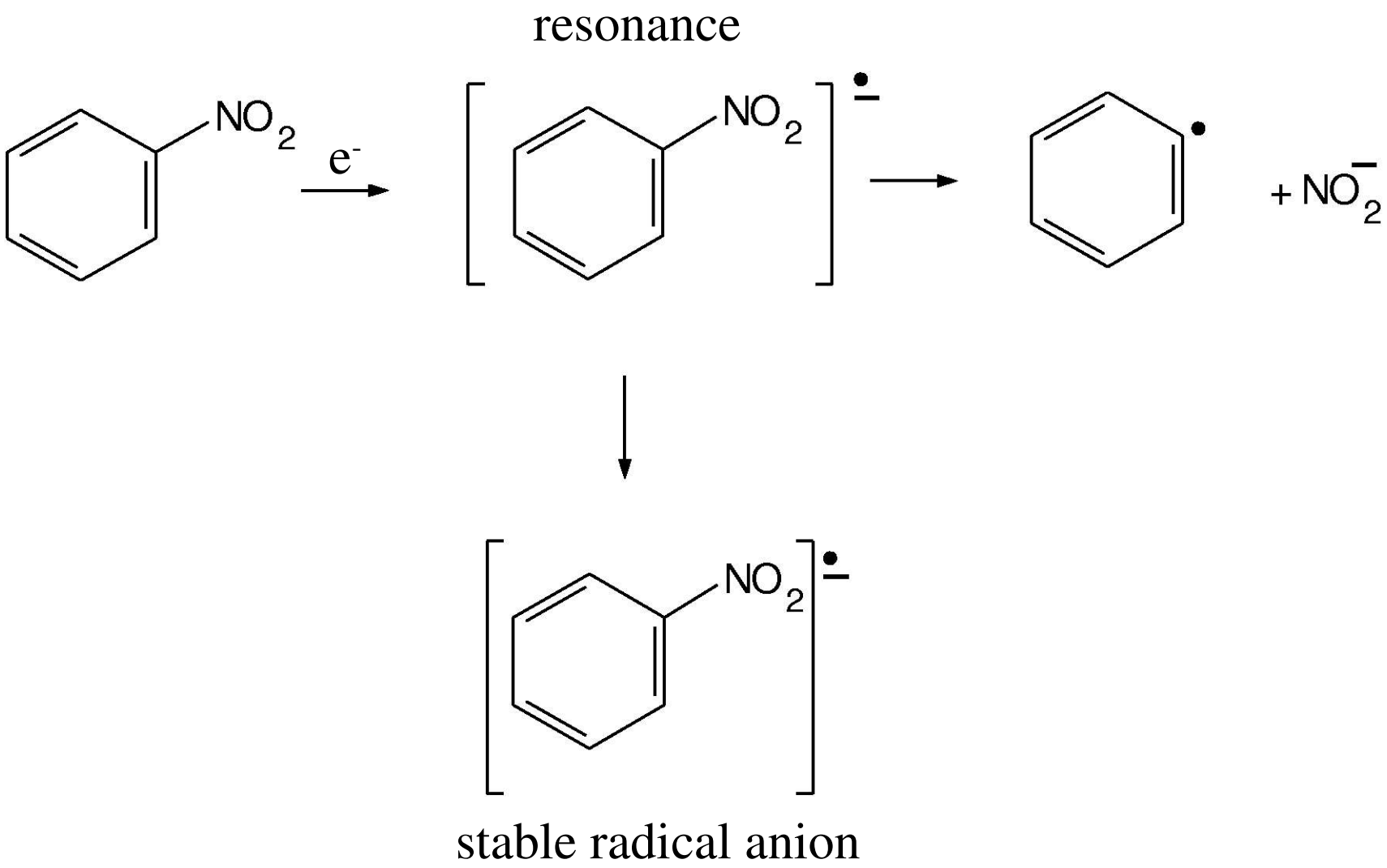
Hammond, LA

Doorway mechanism for Dissociative Electron attachment

Outline

- Dissociative Electron attachment
- Doorway mechanism for electron capture
- Electron-induced Water-loss from Fructose

Dissociative electron attachment

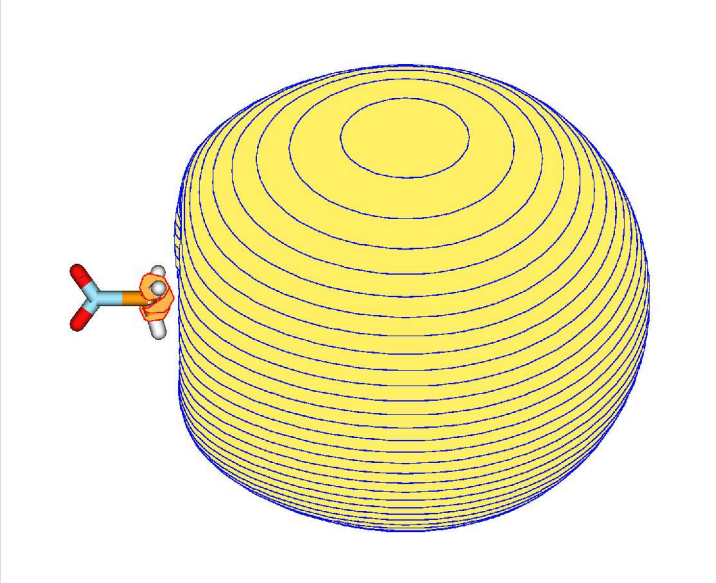


Doorway mechanism

Dipole-bound state

EA ≈ 100 meV

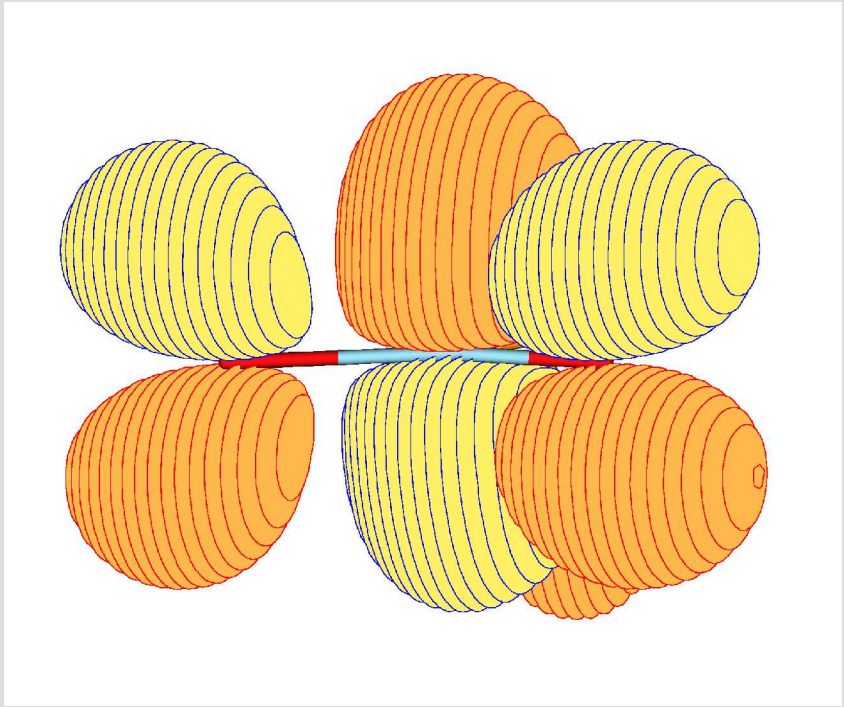
non-bonding



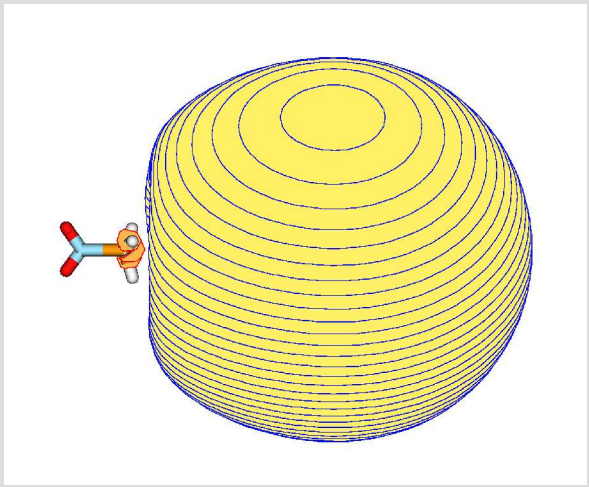
Valence state

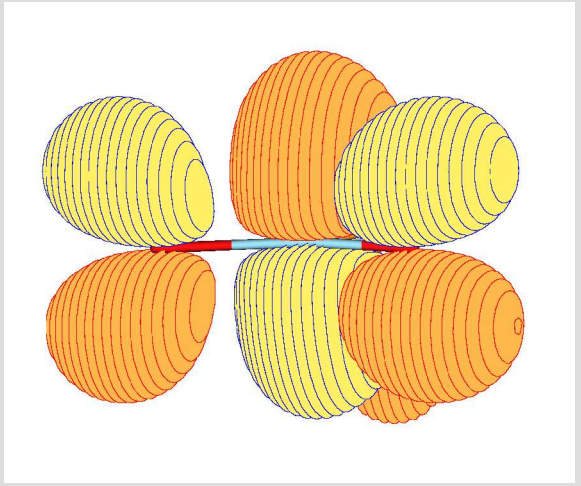
resonance E_r ≈ 1-3 eV

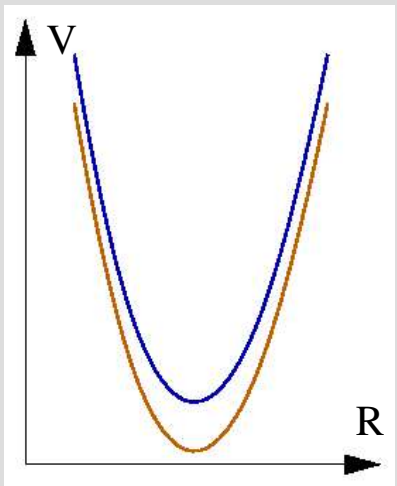
anti-bonding

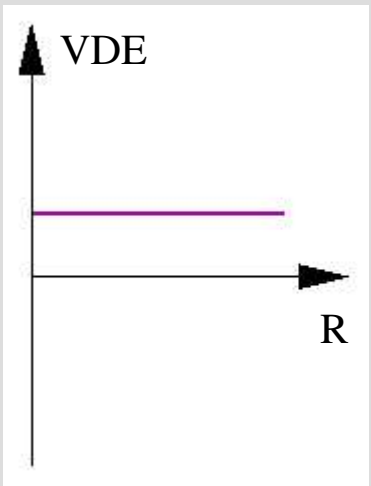


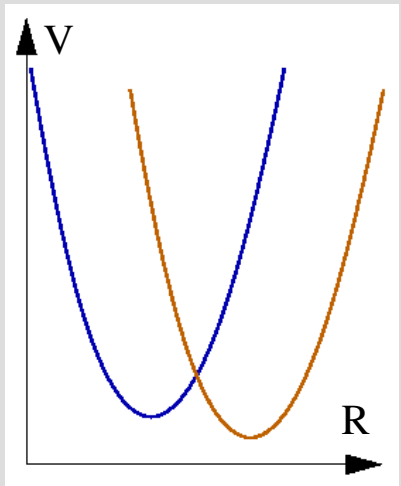
Dipole-bound vs Valence States

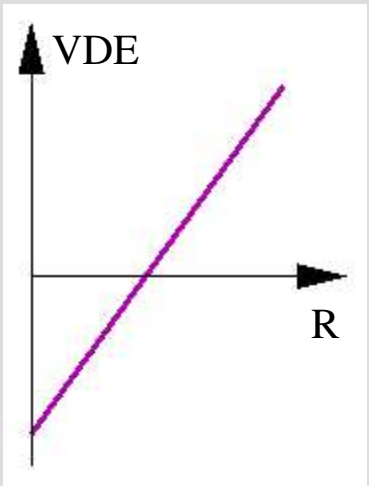












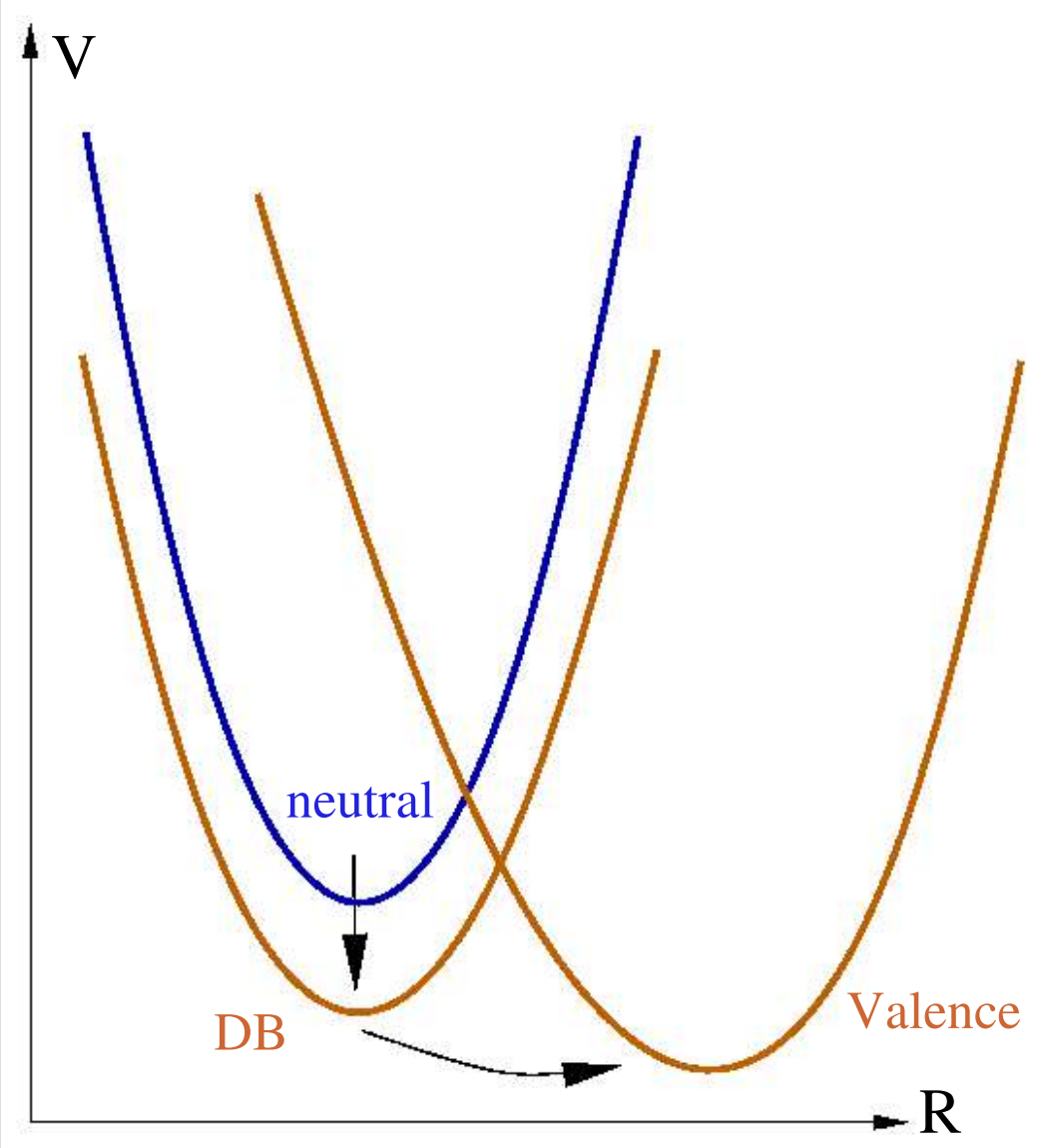
Doorway mechanism

Step #1

Electron attachment
into dipole-bound state

Step #2

Electron transfer
to the valence state



Doorway mechanism

On the binding of electrons to nitromethane: Dipole and valence bound anions

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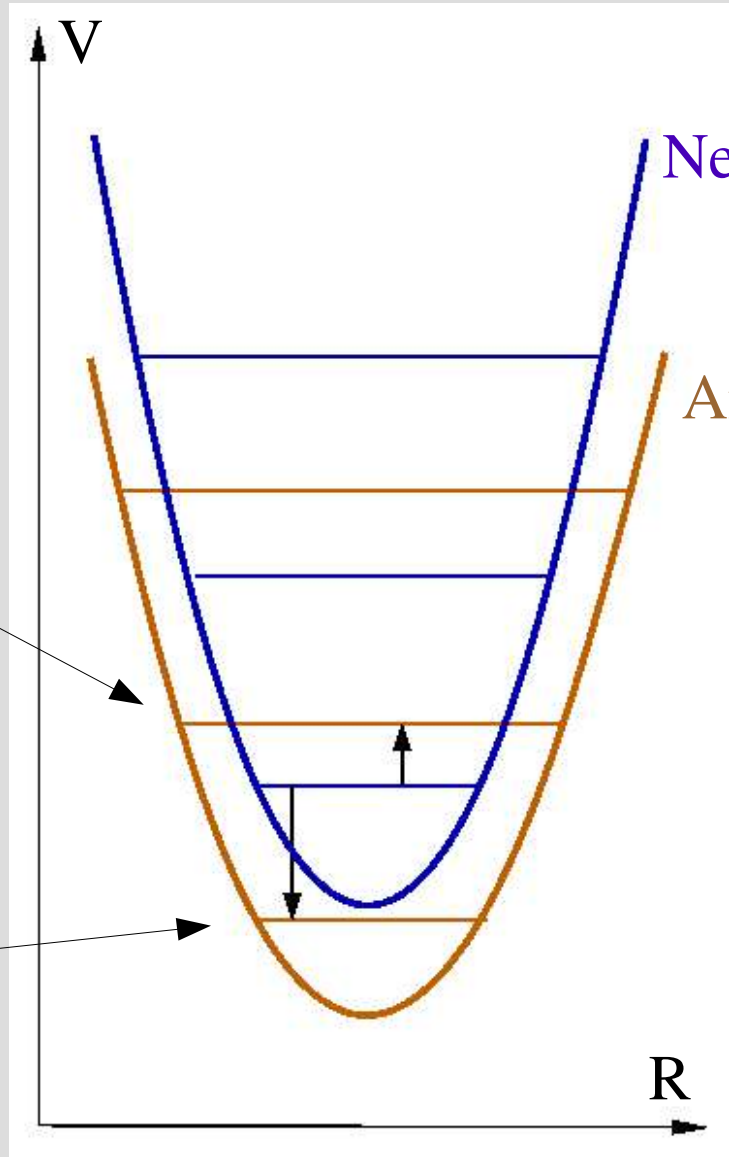
(Received 28 December 1995; accepted 9 May 1996)

J. Chem. Phys. **105**, 3472 (1996)

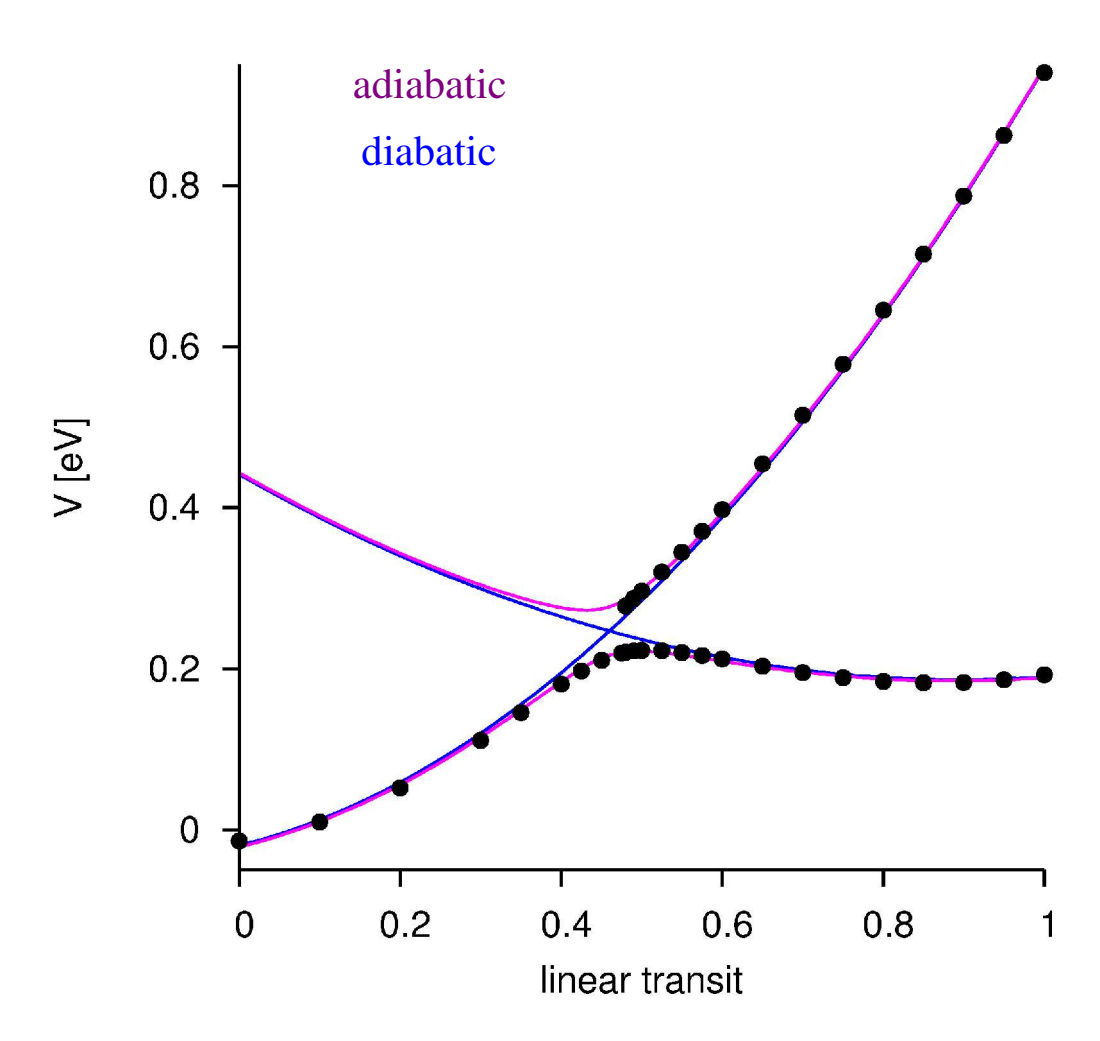
Doorway Step #1
Capture into a dipole-bound state

Free electron attachment
close to threshold
→ vibrational Feshbach resonance



Rydberg electron transfer
→ stable anion

Doorway Step #2
Coupling with a valence state



Ab initio:

- Two states
- Balance
- Metastable region

$$\hat{V} = \begin{pmatrix} V_{DB} & W \\ W & V_{val} \end{pmatrix}$$

W ≈ 20 – 30 meV

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Dissociative electron attachment to furan, tetrahydrofuran, and fructose

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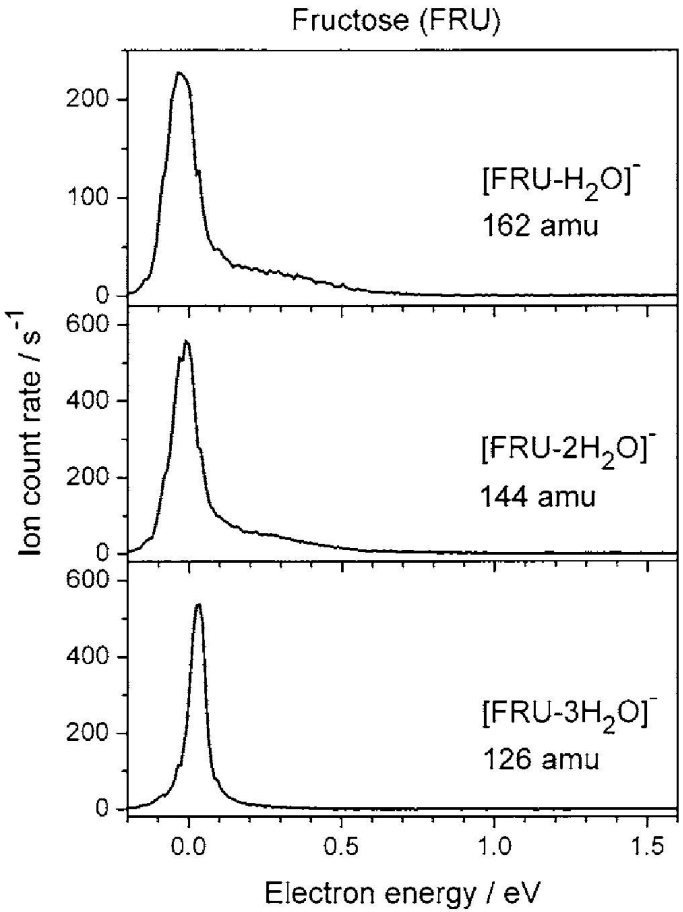
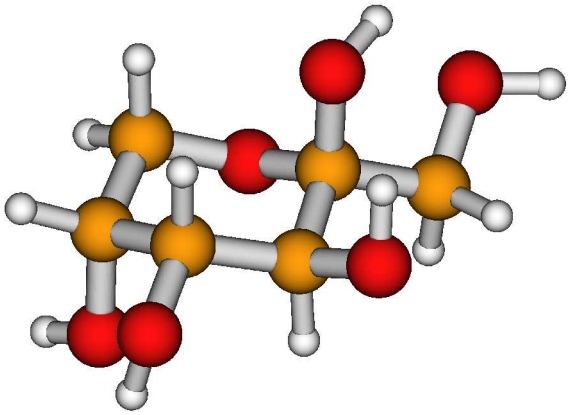


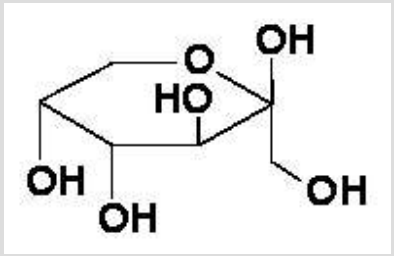


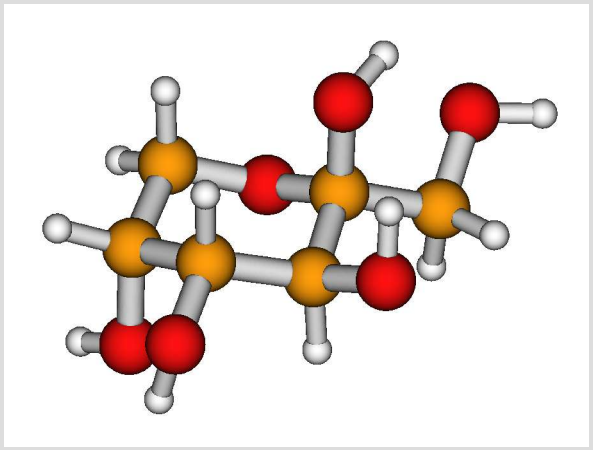
+ e$^-$ (0 eV)

H_2O + ?$^-$

Fructose Primer

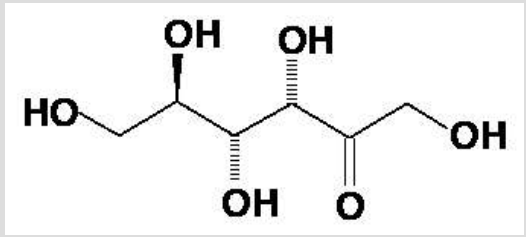
Pyranose

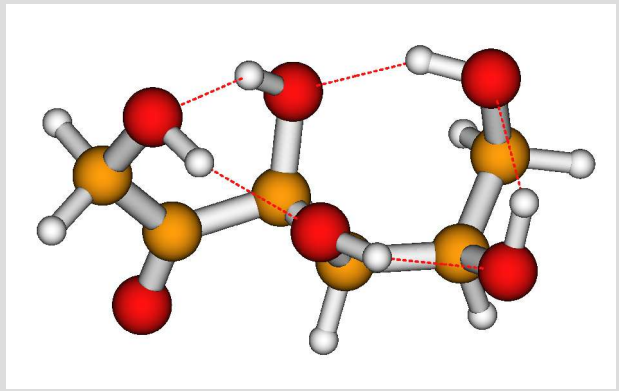




0 kcal/mol

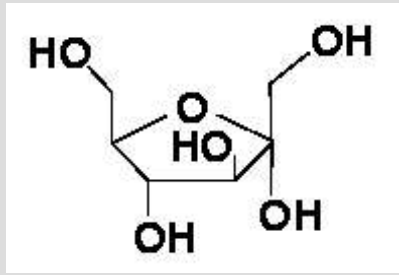
Chain

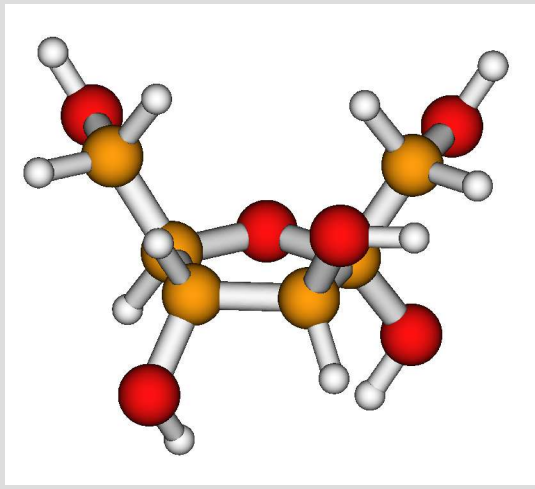




7 kcal/mol

Furanose





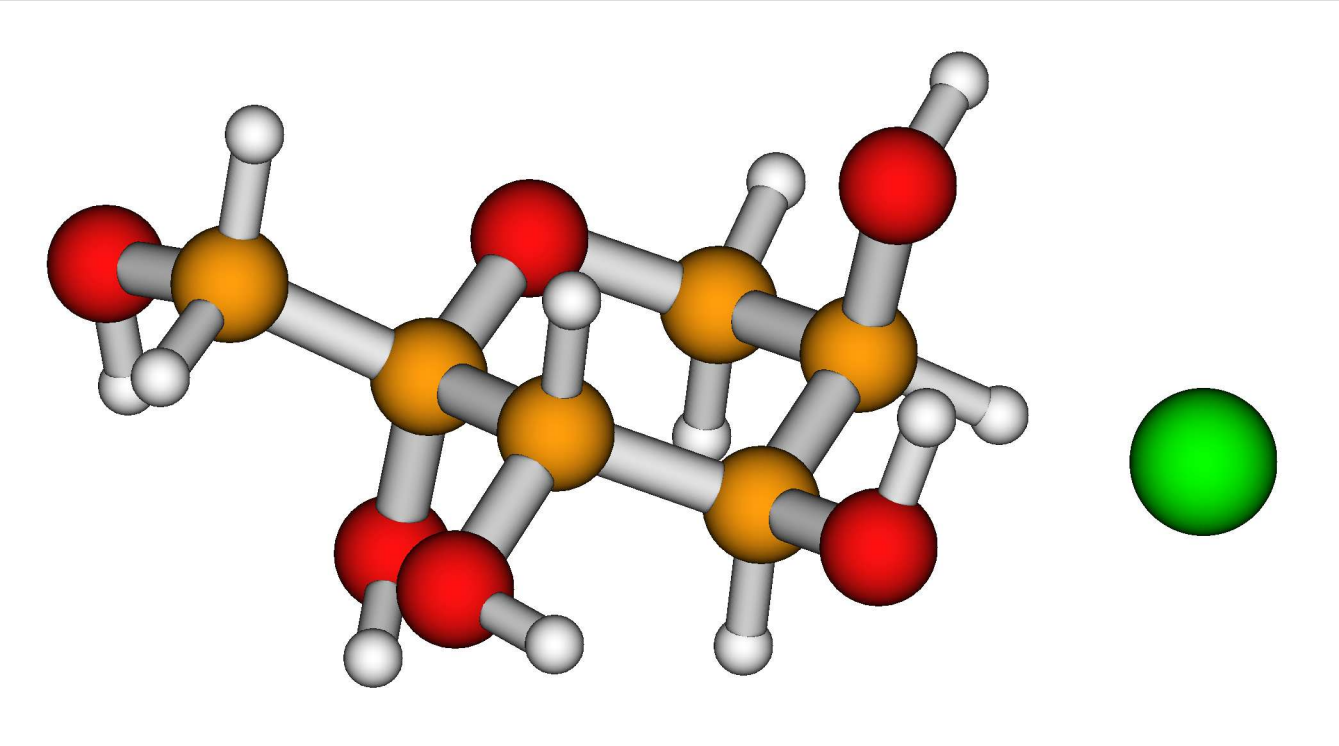
3 kcal/mol

Doorway DEA to Fructose?

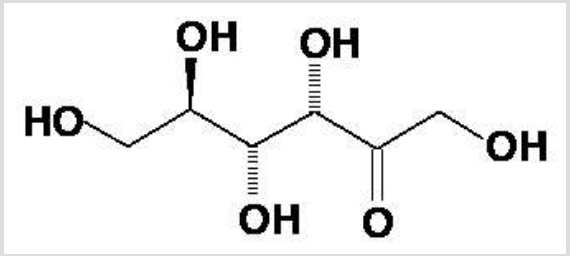
- Dipole-bound state
- Valence state below the neutral
- Coupling
- Water loss from the valence anion

Dipole-bound states

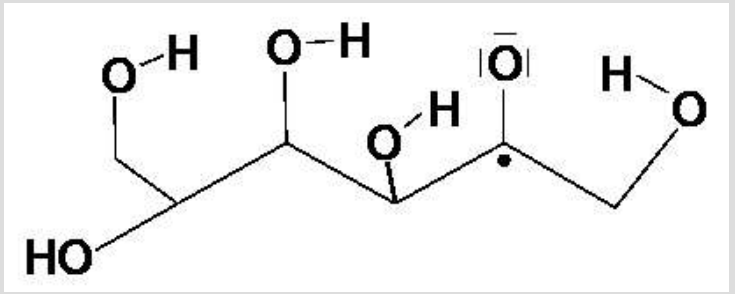
Dipole moment: 4 D
Electron binding energy: 5 meV



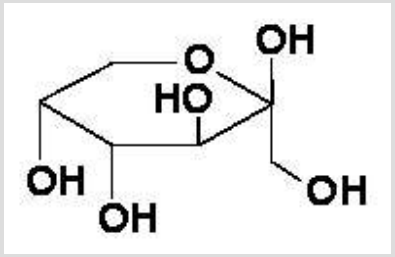
Valence attachment to Fructose

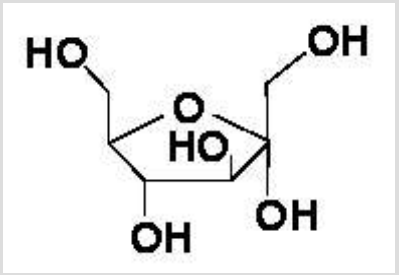


+ e^-



VDE = 1.71 eV
ADE = 0.36 eV





+ e^-

H-loss several eV uphill

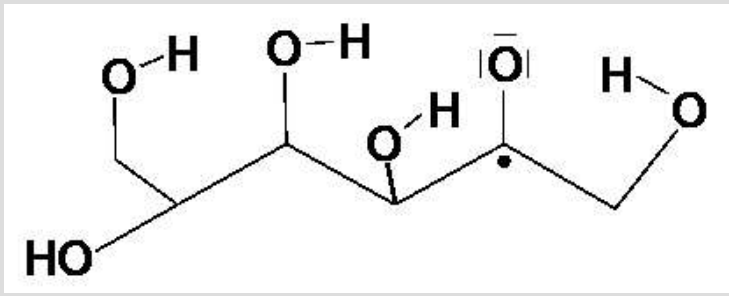
Doorway DEA to Fructose

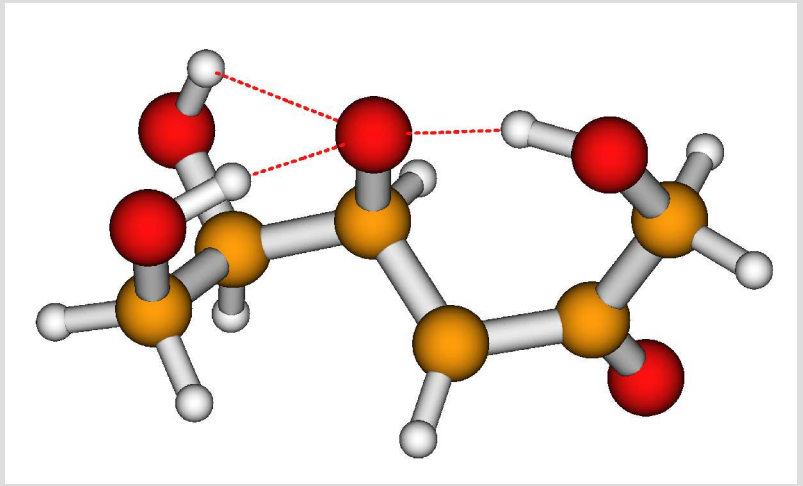
Pyranose
Furanose
Chain

→

Dipole
bound
state

?





- From Pyranose the reaction energy is -4.5 kcal/mol
- The water elimination step from the chain anion is endothermic (2.5 kcal/mol)