Doorway mechanism for Dissociative Electron attachment

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Outline

• Dissociative Electron attachment

• Doorway mechanism for electron capture

• Electron-induced Water-loss from Fructose
Dissociative electron attachment

\[ \text{resonance} \]

stable radical anion
Doorway mechanism

Dipole-bound state
EA ≈ 100 meV
non-bonding

Valence state
resonance $E_r \approx 1$-$3$ 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
On the binding of electrons to nitromethane: Dipole and valence bound anions

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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

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

\[W \approx 20 - 30 \text{ meV}\]
Dissociative electron attachment to furan, tetrahydrofuran, and fructose

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Fructose Primer

Pyranose

Chain

Furanose

0 kcal/mol

7 kcal/mol

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

$\text{VDE} = 1.71 \text{ eV}$
$\text{ADE} = 0.36 \text{ eV}$

H-loss several eV uphill
Doorway DEA to Fructose

Pyranose → 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)