

Problem #7, 10 points, McQuarrie and Simon: Chapter 12, Problem 28 + Extra.

Given the four symmetry orbitals of butadiene:

$$\phi_1 = \frac{1}{\sqrt{2}}(\psi_1 - \psi_4)$$

$$\phi_2 = \frac{1}{\sqrt{2}}(\psi_2 - \psi_3)$$

$$\phi_3 = \frac{1}{\sqrt{2}}(\psi_1 + \psi_4)$$

$$\phi_4 = \frac{1}{\sqrt{2}}(\psi_2 + \psi_3)$$

Derive the Hückel theory secular determinant

$$\begin{vmatrix} \alpha - E & \beta & 0 & 0 \\ \beta & \alpha - \beta - E & 0 & 0 \\ 0 & 0 & \alpha - E & \beta \\ 0 & 0 & \beta & \alpha + \beta - E \end{vmatrix} = 0$$

Which, given the substitution $x = \frac{\alpha - E}{\beta}$, reduces to

$$(x^2 - x - 1)(x^2 + x - 1) = 0.$$

Use this expression to solve for the four values of x , which yield four values of E . Specify these values, and plot them on an energy diagram.

Mcquarrie Problem 7

M Walker



Mcquarrie Problem 7:

Enjoying the Song of Appearance: An Psychological Symphony within **Mcquarrie Problem 7**

In a global taken by screens and the ceaseless chatter of fast communication, the melodic elegance and mental symphony produced by the published word frequently disappear in to the background, eclipsed by the persistent noise and disturbances that permeate our lives. Nevertheless, nestled within the pages of **Mcquarrie Problem 7** a stunning fictional prize brimming with organic feelings, lies an immersive symphony waiting to be embraced. Crafted by a wonderful composer of language, this fascinating masterpiece conducts visitors on a psychological trip, skillfully unraveling the hidden songs and profound influence resonating within each cautiously constructed phrase. Within the depths with this moving evaluation, we can examine the book is key harmonies, analyze its enthralling publishing style, and submit ourselves to the profound resonance that echoes in the depths of readers souls.

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