

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

**Peter Neijens, Theo Araujo, Judith
Möller, Claes Vreese**



Mcquarrie Problem 7:

Unveiling the Magic of Words: A Review of "**Mcquarrie Problem 7**"

In some sort of defined by information and interconnectivity, the enchanting power of words has acquired unparalleled significance. Their ability to kindle emotions, provoke contemplation, and ignite transformative change is really awe-inspiring. Enter the realm of "**Mcquarrie Problem 7**," a mesmerizing literary masterpiece penned by way of a distinguished author, guiding readers on a profound journey to unravel the secrets and potential hidden within every word. In this critique, we shall delve in to the book is central themes, examine its distinctive writing style, and assess its profound affect the souls of its readers.

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