

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

**Carlo Caccamo, Jean-Pierre
Hansen, George Stell**



Mcquarrie Problem 7:

This book delves into Mcquarrie Problem 7. Mcquarrie Problem 7 is a vital topic that must be grasped by everyone, from students and scholars to the general public. This book will furnish comprehensive and in-depth insights into Mcquarrie Problem 7, encompassing both the fundamentals and more intricate discussions.

1. The book is structured into several chapters, namely:

- Chapter 1: Introduction to Mcquarrie Problem 7
- Chapter 2: Essential Elements of Mcquarrie Problem 7
- Chapter 3: Mcquarrie Problem 7 in Everyday Life
- Chapter 4: Mcquarrie Problem 7 in Specific Contexts
- Chapter 5: Conclusion

2. In chapter 1, the author will provide an overview of Mcquarrie Problem 7. The first chapter will explore what Mcquarrie Problem 7 is, why Mcquarrie Problem 7 is vital, and how to effectively learn about Mcquarrie Problem 7.

3. In chapter 2, the author will delve into the foundational concepts of Mcquarrie Problem 7. The second chapter will elucidate the essential principles that need to be understood to grasp Mcquarrie Problem 7 in its entirety.

4. In chapter 3, the author will examine the practical applications of Mcquarrie Problem 7 in daily life. The third chapter will showcase real-world examples of how Mcquarrie Problem 7 can be effectively utilized in everyday scenarios.

5. In chapter 4, this book will scrutinize the relevance of Mcquarrie Problem 7 in specific contexts. The fourth chapter will explore how Mcquarrie Problem 7 is applied in specialized fields, such as education, business, and technology.

6. In chapter 5, the author will draw a conclusion about Mcquarrie Problem 7. This chapter will summarize the key points that have been discussed throughout the book.

This book is crafted in an easy-to-understand language and is complemented by engaging illustrations. It is highly recommended for anyone seeking to gain a comprehensive understanding of Mcquarrie Problem 7.

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