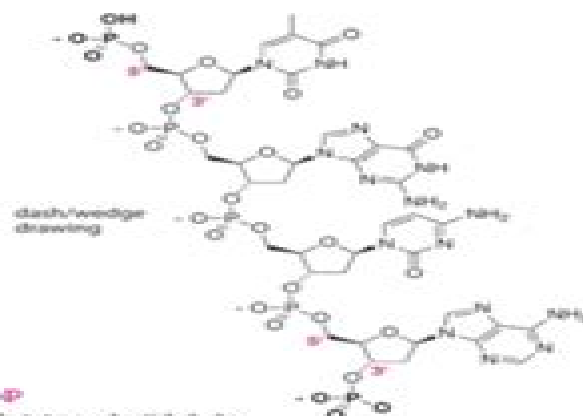


Answers to Chapter 3 (in-text & asterisked problems)

Answer 3.1



The labor of drawing a simple tetranucleotide helps one to appreciate why we use a combination of one-letter code and atom-numbering to discuss DNA.

Answer 3.2

In the gas phase, the charge separation costs 83 kcal mol⁻¹, which is much more costly than the maximum benefit of aromaticity (35 kcal mol⁻¹). However, in water, where the dielectric constant is about 78, charge separation costs only 1.1 kcal mol⁻¹, which is a small compared with the energetic benefits conferred by aromaticity.

$$\begin{aligned}
 \text{Energy} &= k_e \frac{q_1 \cdot q_2}{r \cdot \text{distance}} \\
 &= \frac{9.0 \times 10^9 \cdot (1.6 \times 10^{-19}) \cdot (1.6 \times 10^{-19})}{1 \cdot 4.0 \times 10^{-10}} \\
 &= 5.8 \times 10^{-13} \text{ J} \cdot \frac{1 \text{ kJ}}{1000 \text{ J}} \cdot \frac{6.0 \times 10^{23}}{\text{mol}} \\
 &= 35 \text{ kJ mol}^{-1} \\
 &\text{or } 83 \text{ kcal mol}^{-1} \quad (1 \text{ cal} = 4.18 \text{ J}) \quad \text{in gas phase } (\epsilon = 1)
 \end{aligned}$$



$$\text{Energy} = 1.1 \text{ kcal mol}^{-1} \quad \text{in water at } 25^\circ\text{C } (\epsilon = 78)$$

It is important to recognize that the positive charge on nitrogen and negative charge on oxygen is a Lewis structure formalism. In fact, the nitrogen atom has a partial negative charge and most of the positive charge is distributed on the various hydrogen atoms. Surprisingly, ab initio calculations HF/STO-3G predict a dipole moment of 4.8 Debye units, not too different from the dipole moment predicted from a +1 charge and -1 charge separate by 4.0 Å (4.0 Debye units).

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Table of Contents Mastering Chemistry Chapter 3 Answer Key

1. Understanding the eBook Mastering Chemistry Chapter 3 Answer Key
 - The Rise of Digital Reading Mastering Chemistry Chapter 3 Answer Key
 - Advantages of eBooks Over Traditional Books
2. Identifying Mastering Chemistry Chapter 3 Answer Key
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Mastering Chemistry Chapter 3 Answer Key
 - User-Friendly Interface
4. Exploring eBook Recommendations from Mastering Chemistry Chapter 3 Answer Key
 - Personalized Recommendations
 - Mastering Chemistry Chapter 3 Answer Key User Reviews and Ratings
 - Mastering Chemistry Chapter 3 Answer Key and Bestseller Lists
5. Accessing Mastering Chemistry Chapter 3 Answer Key Free and Paid eBooks
 - Mastering Chemistry Chapter 3 Answer Key Public Domain eBooks
 - Mastering Chemistry Chapter 3 Answer Key eBook Subscription Services
 - Mastering Chemistry Chapter 3 Answer Key Budget-Friendly Options
6. Navigating Mastering Chemistry Chapter 3 Answer Key eBook Formats

- ePub, PDF, MOBI, and More
 - Mastering Chemistry Chapter 3 Answer Key Compatibility with Devices
 - Mastering Chemistry Chapter 3 Answer Key Enhanced eBook Features
7. Enhancing Your Reading Experience
- Adjustable Fonts and Text Sizes of Mastering Chemistry Chapter 3 Answer Key
 - Highlighting and Note-Taking Mastering Chemistry Chapter 3 Answer Key
 - Interactive Elements Mastering Chemistry Chapter 3 Answer Key
8. Staying Engaged with Mastering Chemistry Chapter 3 Answer Key
- Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Mastering Chemistry Chapter 3 Answer Key
9. Balancing eBooks and Physical Books Mastering Chemistry Chapter 3 Answer Key
- Benefits of a Digital Library
 - Creating a Diverse Reading Collection Mastering Chemistry Chapter 3 Answer Key
10. Overcoming Reading Challenges
- Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
11. Cultivating a Reading Routine Mastering Chemistry Chapter 3 Answer Key
- Setting Reading Goals Mastering Chemistry Chapter 3 Answer Key
 - Carving Out Dedicated Reading Time
12. Sourcing Reliable Information of Mastering Chemistry Chapter 3 Answer Key
- Fact-Checking eBook Content of Mastering Chemistry Chapter 3 Answer Key
 - Distinguishing Credible Sources
13. Promoting Lifelong Learning
- Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
14. Embracing eBook Trends
- Integration of Multimedia Elements
 - Interactive and Gamified eBooks

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