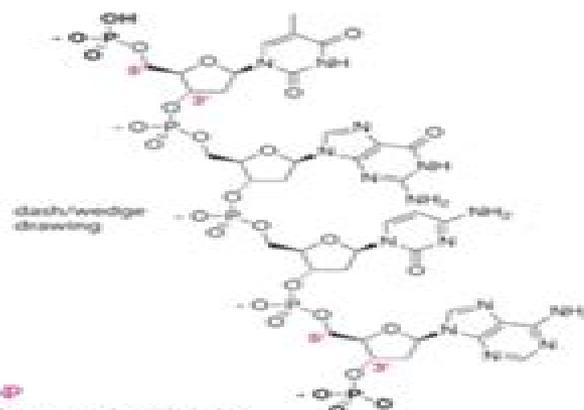


Answers to Chapter 3 (in-text & asterisked problems)

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.

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



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

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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Marye Anne Fox, James K. Whitesell



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