Review: Chapter 14 More Polyatomic Molecules and Hydrocarbons

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1   Synopsis

The theoretical approach used in Chapter 13 to model polyatomic molecular ions and molecules has been used in Chapter 14 to model other polyatomic molecules and hydrocarbon molecules. As in Chapter 13, bond energies, bond lengths and bond angles are treated within a common theoretical framework to yield simple closed form solutions containing fundamental constants only. In all, 17 species are considered: CO_2, NO_2, CH_3CH_3, CH_2CH_2, $CHCH$, C_6H_6, C_3H_8, C_4H_{10}, C_5H_{12}, C_6H_{14}, C_7H_{16}, C_8H_{18}, C_9H_{20}, $C_{10}H_{22}$, $C_{11}H_{24}$, $C_{12}H_{26}$, $C_{18}H_{36}$. Parameters for the first six compounds, that is, carbon dioxide through benzene, are determined on an individual basis. The last eleven compounds (propane, butane,… octadecane) are alkanes with the general chemical formula C_nH_{2n+2}. After determining bond angles, vibration characteristics, and energies for the various sub-structures of the alkanes, a general equation for the total bond dissociation energy of C_nH_{2n+2}, denoted by $E_D(C_nH_{2n+2})$, is developed. The calculated results for the various molecular parameters for all 17 compounds are compared with available experimental data in Table 14.1. The agreement is excellent. For a total of 41 comparisons between the theoretically-calculated and experimental parameters, more than 60% of these differed by less than 0.2%. The distribution of the differences is detailed more completely in Fig. 1 below. Note that all of the 41 parameters differed from the measured value by less than 3%.
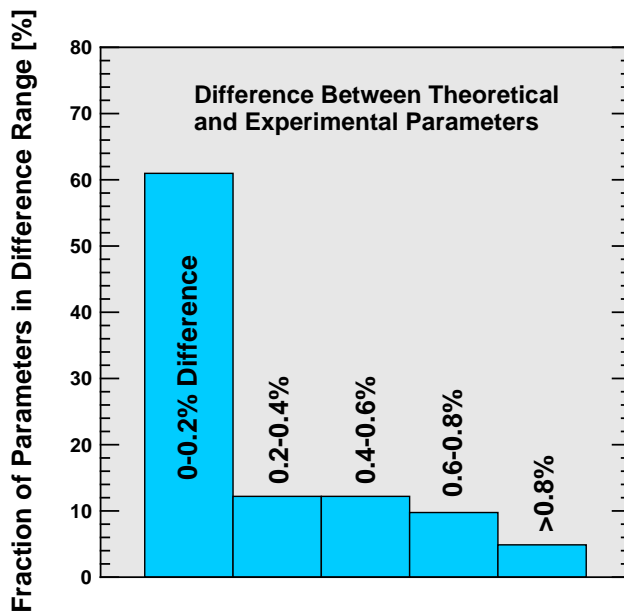

Figure 1. Comparison of theoretically-calculated and experimental parameters.

2   Equation verification

A total of 665 equations form the basis of the theoretical presentation in Chapter 14. These equations are generally presented in a coherent and logical sequence. Many of the

equations are related to equations of similar type in Chapter 13. In these cases the reference to the corresponding or parent equation in Chapter 13 was verified. In other cases reference is made to equations or values which reside outside of Chapters 13 and 14. The origin of these external equations or values was not considered.

The equations in Chapter 14 were checked for internal (internal to Chapters 13 and 14) algebraic consistency, numerical accuracy, and clarity of presentation. Most of the equations were verified by hand calculation, a few of the more lengthy equations and those of transcendental type were checked with the aid of a spreadsheet, and some were checked by both methods. In this way the validation is relatively independent of the original method used to generate the data (spreadsheet). The following set of numerical constants was used in the verification process:

$$h = 6.62608 \times 10^{-34} \text{ J-s}$$
$$\hbar = 1.05457 \times 10^{-34} \text{ J-s}$$
$$m_e = 9.10939 \times 10^{-31} \text{ kg}$$
$$\varepsilon_0 = 8.85419 \times 10^{-12} \text{ C}^2/\text{N-m}^2$$
$$\mu_0 = 4\pi \times 10^{-7} \text{ N/A}^2$$
$$e = 1.6022 \times 10^{-19} \text{ C}$$
$$c = 2.998 \times 10^8 \text{ m/s}$$
$$a_0 = 5.29177 \times 10^{-11} \text{ m}$$
$$m_p = 1.67262 \times 10^{-27} \text{ kg}$$