

The curve in Figure 16.11 of the text shows how the vibrational heat capacity depends on temperature. Note that even when the temperature is only slightly above the vibrational temperature, the heat capacity is close to its equipartition value.

The total heat capacity of a molecular substance is the sum of each contribution (Figure 16.12 of the text). When equipartition is valid (when the temperature is well above the characteristic temperature of the mode  $T \gg \theta_M$ ) we can estimate the heat capacity by counting the numbers of modes that are active. In gases, all three translational modes are always active and contribute  $\frac{3}{2}R$  to the molar heat capacity. If we denote the number of active rotational modes by  $\nu_R^\ddagger$  (so for most molecules at normal temperatures  $\nu_R^\ddagger = 2$  for linear molecules, and 3 for non-linear molecules), then

the total heat capacity is given by  $C_{V,m} = \frac{3}{2}R + \frac{\nu_R^\ddagger}{2}R + \frac{\nu_V}{2}R$ , where  $\nu_V$  is the number of active vibrational modes. In the equipartition limit  $\nu_V = 3N - 5$  for linear molecules and  $\nu_V = 3N - 6$  for non-linear molecules, where  $N$  is the number of atoms in the molecule.

$$C_{V,m} = \frac{3}{2}R + \frac{\nu_R^\ddagger}{2}R + \frac{\nu_V}{2}R$$

The equipartition value of  $C_{V,m}$  is the value that the heat capacity approaches as  $T \rightarrow \infty$ . The value of  $C_{V,m}$  at a given temperature is given by the sum of the equipartition value and the contribution of the vibrational modes that are not yet active. The number of active vibrational modes is given by  $\nu_V = 3N - 5$  for linear molecules and  $\nu_V = 3N - 6$  for non-linear molecules. The number of active vibrational modes is given by  $\nu_V = 3N - 5$  for linear molecules and  $\nu_V = 3N - 6$  for non-linear molecules. The number of active vibrational modes is given by  $\nu_V = 3N - 5$  for linear molecules and  $\nu_V = 3N - 6$  for non-linear molecules.

### Solutions to exercises

The thermal energy is given by  $U = \frac{1}{2}k_B T$  per degree of freedom. When equipartition is valid, the thermal energy is given by  $U = \frac{1}{2}k_B T$  per degree of freedom.

$$U = \frac{1}{2}k_B T$$

At 298 K, the thermal energy is given by  $U = \frac{1}{2}k_B T$ .

$$U = \frac{1}{2}k_B T = \frac{1}{2}(1.38 \times 10^{-23} \text{ J K}^{-1})(298 \text{ K}) = 2.05 \times 10^{-21} \text{ J}$$

At 1000 K, the thermal energy is given by  $U = \frac{1}{2}k_B T$ .

$$U = \frac{1}{2}k_B T = \frac{1}{2}(1.38 \times 10^{-23} \text{ J K}^{-1})(1000 \text{ K}) = 6.90 \times 10^{-21} \text{ J}$$

$$C_{V,m} = \frac{3}{2}R + \frac{\nu_R^\ddagger}{2}R + \frac{\nu_V}{2}R$$

At 298 K, the thermal energy is given by  $U = \frac{1}{2}k_B T$ .

# Physical Chemistry 9th Solution Manual

**WJ Hussar**



## Physical Chemistry 9th Solution Manual:

*Instructor's Solutions Manual to Accompany Atkins' Physical Chemistry, Ninth Edition* C. A. Trapp, M. P. Cady, Carmen Giunta, 2010 The Instructor's solutions manual to accompany Atkins Physical Chemistry provides detailed solutions to the exercises and the even numbered discussion questions and problems that feature in the ninth edition of Atkins Physical Chemistry The manual is intended for instructors and consists of material that is not available to undergraduates The manual is free to all adopters of the main text Solutions Manual to Accompany Elements of Physical Chemistry David Smith, 2013-05-30 The Solutions Manual to accompany Elements of Physical Chemistry 6th edition contains full worked solutions to all end of chapter discussion questions and exercises featured in the book The manual provides helpful comments and friendly advice to aid understanding It is also a valuable resource for any lecturer who wishes to use the extensive selection of exercises featured in the text to support either formative or summative assessment and wants labour saving ready access to the full solutions to these questions *Solutions Manual for Principles of Physical Chemistry, 3rd Edition, Solutions Manual* Hans Kuhn, David H. Waldeck, Horst-Dieter Försterling, 2024-10-25 This is a Solutions Manual to Accompany with solutions to the exercises in the main volume of Principles of Physical Chemistry Third Edition This book provides a unique approach to introduce undergraduate students to the concepts and methods of physical chemistry which are the foundational principles of Chemistry The book introduces the student to the principles underlying the essential sub fields of quantum mechanics atomic and molecular structure atomic and molecular spectroscopy statistical thermodynamics classical thermodynamics solutions and equilibria electrochemistry kinetics and reaction dynamics macromolecules and organized molecular assemblies Importantly the book develops and applies these principles to supramolecular assemblies and supramolecular machines with many examples from biology and nanoscience In this way the book helps the student to see the frontier of modern physical chemistry developments The book begins with a discussion of wave particle duality and proceeds systematically to more complex chemical systems in order to relate the story of physical chemistry in an intellectually coherent manner The topics are organized to correspond with those typically given in each of a two course semester sequence The first 13 chapters present quantum mechanics and spectroscopy to describe and predict the structure of matter atoms molecules and solids Chapters 14 to 29 present statistical thermodynamics and kinetics and applies their principles to understanding equilibria chemical transformations macromolecular properties and supramolecular machines Each chapter of the book begins with a simplified view of a topic and evolves to more rigorous description in order to provide the student and instructor flexibility to choose the level of rigor and detail that suits them best The textbook treats important new directions in physical chemistry research including chapters on macromolecules principles of interfaces and films for organizing matter and supramolecular machines as well as including discussions of modern nanoscience spectroscopy and reaction dynamics throughout the text Solutions Manual for Principles of Physical Chemistry, 3rd Edition Hans

Kuhn, David H. Waldeck, Horst-Dieter Försterling, 2024-10-29 This is a Solutions Manual to Accompany with solutions to the exercises in the main volume of Principles of Physical Chemistry Third Edition This book provides a unique approach to introduce undergraduate students to the concepts and methods of physical chemistry which are the foundational principles of Chemistry The book introduces the student to the principles underlying the essential sub fields of quantum mechanics atomic and molecular structure atomic and molecular spectroscopy statistical thermodynamics classical thermodynamics solutions and equilibria electrochemistry kinetics and reaction dynamics macromolecules and organized molecular assemblies Importantly the book develops and applies these principles to supramolecular assemblies and supramolecular machines with many examples from biology and nanoscience In this way the book helps the student to see the frontier of modern physical chemistry developments The book begins with a discussion of wave particle duality and proceeds systematically to more complex chemical systems in order to relate the story of physical chemistry in an intellectually coherent manner The topics are organized to correspond with those typically given in each of a two course semester sequence The first 13 chapters present quantum mechanics and spectroscopy to describe and predict the structure of matter atoms molecules and solids Chapters 14 to 29 present statistical thermodynamics and kinetics and applies their principles to understanding equilibria chemical transformations macromolecular properties and supramolecular machines Each chapter of the book begins with a simplified view of a topic and evolves to more rigorous description in order to provide the student and instructor flexibility to choose the level of rigor and detail that suits them best The textbook treats important new directions in physical chemistry research including chapters on macromolecules principles of interfaces and films for organizing matter and supramolecular machines as well as including discussions of modern nanoscience spectroscopy and reaction dynamics throughout the text

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