PHY215-02: Ideal Gas Law

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1 How to derive the Ideal Gas Law?

The ideal gas law, $PV = nRT$, can be derived from a combination of experimental laws and theoretical considerations. Here is a step-by-step derivation:

1.1 Based on Experimental Laws: Macroscopic picture

From the 17th to the 18th century, physicists began to study the thermal properties of gases from a macroscopic perspective. The discovery of gas laws provided a macroscopic basis for understanding the behavior of atoms and molecules.

- **Boyle's Law:** For a given amount of gas at a constant temperature, the pressure P and volume V of the gas are inversely proportional. Mathematically, it can be expressed as $P \propto \frac{1}{V}$ or $PV = k_1$ (where k_1 is a constant depending on the amount of gas and the temperature).

- **Charles's Law:** At a constant pressure, the volume V of a given amount of gas is directly proportional to its absolute temperature T. That is $V \propto T$ or $V = k_2T$ (where k_2 is a constant depending on the amount of gas and the pressure).

- **Gay-Lussac's Law:** For a given mass of an ideal gas, at a constant volume, the pressure of the gas is directly proportional to its absolute temperature. That is $P \propto T$ or $P = k_3T$ (where k_3 is a constant depending on the amount of gas and the volume).

- **Avogadro's Law:** At the same temperature and pressure, equal volumes of all gases contain an equal number of molecules. Mathematically, for a gas, $V \propto n$ (where n is the number of moles of the gas), or $V = k_4 n$ (where k_4 is a constant depending on the temperature and pressure).

Combining these three laws, we can say that $V \propto \frac{nT}{P}$, or $PV = nR'T$, where R' is a proportionality constant. For convenience, we usually write R' as R, and then we get the Ideal Gas Law

$PV = nRT,$

where R is the universal gas constant, which is determined experimentally to be $R = 8.314 J/(molK)$. again, the temperature must be in Kelvins (K).

1.2 Based on Kinetic Theory of Gases: Microscopic picture

- Consider a gas composed of N molecules in a cubical container of side L. The volume of the container $V = L^3$.

- A molecule with velocity $\vec{v} = (v_x, v_y, v_z)$ collides elastically with the wall of the container perpendicular to the x-axis. The change in momentum of the molecule due to a collision with the wall is

$\Delta p = mv_x - (-mv_x) = 2mv_x,$

where m is the mass of the molecule.

- The time between successive collisions of the molecule with the

same wall is
$\Delta t = \frac{2L}{v_x}$.
So the average force exerted by the molecule on the wall is
$F = \frac{\Delta p}{\Delta t} = \frac{mv_x^2}{L}$.

- The total force exerted by all N molecules on the wall is
$F_{total} = \sum_{i=1}^{N} \frac{mv_{ix}^2}{L}$.
The pressure
$P = \frac{F_{total}}{A} = \frac{F_{total}}{L^2} = \frac{m}{L^3} \sum_{i=1}^{N} v_{ix}^2 = \frac{m}{V} \sum_{i=1}^{N} v_{ix}^2$.
- The average kinetic energy of a molecule is
$\frac{1}{2}m\overline{v^2}$, which is equal to $\frac{3}{2}kT$, according to the Equipartition Theorem.
Here, k is the Boltzmann constant and $k = 1.38 \times 10^{-23} J/K$.
Since $\overline{v^2} = v_x^2 + v_y^2 + v_z^2$, so $\overline{v_x^2} = \frac{1}{3}\overline{v^2}$. Hence, we have
$\overline{v_x^2} = \frac{kT}{m}$.
- The total number of molecules $N = nN_A$, where n is the number of moles and N_A is Avogadro's number (which is 6.022×10^{23}.)
- The pressure $P = \frac{N}{V}m\overline{v_x^2} = \frac{nN_A}{V}m \times \frac{kT}{m} = \frac{nN_AkT}{V}$, or
$PV = nN_AkT$.
- Defining $R = N_Ak$,
we get $PV = nRT$,
where R is the molar gas constant and $R = 8.314 J/(K \cdot mol)$.

1.3 A side remark

The ideal gas law, also called the general gas equation, is the equation of state of a hypothetical ideal gas. In thermodynamics, Ideal gas law is a well-defined approximation of the behavior of many gases under diverse conditions. Ideal Gas Equation is the combination of empirical laws like Charle's law, Boyle's law, Gay-Lussac's law, and Avogadro's law.

2 History of atoms and molecules

Here is an overview of the development of the understanding of atoms and molecules in chemistry and physics.

2.1 Ancient Greek Concepts

- The ancient Greeks were among the first to propose the idea of atoms. Philosophers such as Democritus suggested that matter was composed of tiny, indivisible particles called "atomos." However, these were more of philosophical speculations rather than scientific theories based on experimental evidence.

2.2 Dalton's Atomic Theory

- In the early 19th century, John Dalton proposed the modern atomic theory. He postulated that all matter is composed of tiny, indivisible atoms; atoms of the same element are identical in mass and properties, while atoms of different elements have different masses and properties; and chemical reactions involve the rearrangement of atoms. This theory provided a framework for understanding chemical reactions and the law of definite proportions.

2.3 Mendeleev's Periodic Table

- In 1869, Mendeleev published the periodic table which arranges elements in order of increasing atomic number. Elements with similar chemical and physical properties are grouped together in columns (groups) and rows (periods). This supported the idea that the properties of elements were related to their atomic structure. Mendeleev was even able to predict the existence and properties of several undiscovered elements based on the gaps in his table, which was a remarkable validation of the periodic law and atomic theory.

2.4 Avogadro's Hypothesis; Molecular Theory

- In 1811, Amedeo Avogadro put forward the hypothesis that, at the same temperature and pressure, equal volumes of any gas contain an equal number of molecules, laying the foundation for determining the relationship between atoms and molecules. This was crucial in understanding the relationships between the amounts of substances in chemical reactions.

Before Avogadro's Hypothesis, the concepts of atoms and molecules were often confused. Avogadro clearly proposed the distinction between atoms and molecules. He hypothesized that gases are composed of molecules and molecules are composed of atoms. This laid the foundation for clarifying the microscopic composition of substances and established the basic framework of molecular theory.

2.5 Development of Atomic Models

- Niels Bohr proposed the Bohr model in 1913, which described electrons orbiting the nucleus in specific energy levels or shells. This model could explain the spectral lines of hydrogen and provided a better understanding of atomic energy levels.

- The development of quantum mechanics in the 1920s led to the quantum mechanical model of the atom. This model described electrons not as particles in fixed orbits but as probability clouds or orbitals, based on the principles of wave-particle duality and the Schrödinger equation.

- With the development of modern atomic theory, especially the understanding of the atomic number and the structure of the atom (including the arrangement of electrons in shells and orbitals), the periodic table was further refined. The modern periodic table is arranged by atomic number, which is based on the number of protons in the nucleus of an atom. This arrangement more accurately reflects the underlying atomic structure and the trends in chemical and physical properties of the elements. The periodic table thus became a visual representation of the principles of atomic theory, showing how the properties of elements are determined by their atomic structure.

3 The Equipartition Theorem

The equipartition theorem in the case of an ideal gas is a fundamental concept in statistical mechanics. Here is a detailed explanation:

3.1 Definition and Statement

The equipartition theorem states that for a system of classical particles in thermal equilibrium, the average energy associated with each degree of freedom is $\frac{1}{2}kT$, where k is the Boltzmann constant and T is the absolute temperature (in Kelvin units).

3.2 Degrees of Freedom in an Ideal Gas

3.2.1 Monatomic Gas:

- An ideal monatomic gas consists of single atoms. Each atom has three degrees of freedom corresponding to its translational motion in the three spatial directions (x, y, and z). According to the equipartition theorem, the average kinetic energy per atom is $\frac{3}{2}kT$, and the total internal energy U of N atoms is $U = \frac{3}{2}NkT$. In terms of moles, since $N = nN_A$ (where n is the number of moles and N_A is Avogadro's number), and $R = N_Ak$ (where R is the universal gas constant), the internal energy can be written as $U = \frac{3}{2}nRT$.

- Monatomic substances are those composed of single atoms not chemically bonded to other atoms. Examples include Noble gases, such as Helium (He), Neon (Ne) and Argon (Ar), etc.

3.2.2 Diatomic Gas:

-A diatomic gas molecule has additional degrees of freedom compared to a monatomic gas. In addition to the three translational degrees of freedom, it has two rotational degrees of freedom (rotation about two axes perpendicular to the molecular axis) and, at high temperatures, two vibrational degrees of freedom (vibration along the molecular axis, which includes both kinetic and potential energy contributions). At moderate temperatures, where vibrational degrees of freedom are not fully excited, the average energy per molecule is $\frac{5}{2}kT$ (3 translational + 2 rotational), and the internal energy of N molecules is $U = \frac{5}{2}NkT$ or $U = \frac{5}{2}nRT$ in terms of moles. At high temperatures when vibrational degrees of freedom are fully active, each molecule has an additional $2 \times \frac{1}{2}kT$ (for kinetic and potential energy of vibration) for a total of $\frac{7}{2}kT$ per molecule, and $U = \frac{7}{2}nRT$.

- Examples include Hydrogen gas (H_2), Nitrogen gas (N_2), and Oxygen gas (O_2), etc.

3.2.3 The degrees of freedom of a polyatomic molecule like H_2O

- H_2O molecule is a V-shaped polyatomic molecule with a nonlinear geometry. The two O-H bonds are not in a straight line but form an

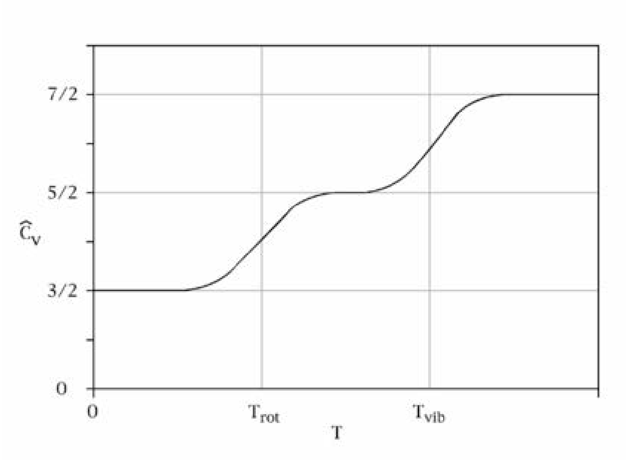


Figure 1: Constant-volume specific heat capacity of a diatomic gas (idealised), as a function of temperature.

angle, to be approximately 104 degrees. It has 9 degrees of freedom in total. They are distributed as 3 translational, 3 rotational, and 3 vibrational degrees of freedom. The detailed analysis is as follows:

- **Translational Degrees of Freedom:**

- A molecule can freely move in three independent directions in space, namely along the x, y, and z axes. This movement is known as translational motion, and thus, there are 3 translational degrees of freedom.

- **Rotational Degrees of Freedom:**

- For a non-linear molecule like H_2O, it can rotate around three mutually perpendicular axes. H_2O, being a bent molecule, can rotate about two axes perpendicular to the plane of the molecule and an axis along the line connecting the two hydrogen atoms, resulting in

3 rotational degrees of freedom.

- **Vibrational Degrees of Freedom:**

- The formula to calculate the number of vibrational degrees of freedom (f_v) for a non-linear molecule is $f_v = 3N - 3 - 3$, where N is the number of atoms in the molecule. (It was derived from the total degrees of freedom and the constraints due to translational and rotational motions.) In the case of H_2O, with $N = 3$, we get $f_v = 3 \times 3 - 6 = 3$. The three vibrational modes include one bending (or Scissoring) mode and two stretching modes, one symmetric and one asymmetric.

3.2.4 The degrees of freedom of a polyatomic molecule like CO_2

- CO_2 molecule is a linear polyatomic molecule. The two C-O bonds are in a straight line. The number of rotation and vibration modes can be determined by considering its degrees of freedom and the specific symmetry and geometry of the molecule. The analysis is as follows:

- **Total Degrees of Freedom:**

A molecule with N atoms has a total of $3N$ degrees of freedom. This is because each atom can move independently in three dimensions (x, y, and z directions). For CO_2, which has $N = 3$ atoms, the total degrees of freedom is $3 \times 3 = 9$.

- **Translation Degrees of Freedom:**

Translation refers to the overall motion of the molecule through space. A linear molecule has 3 translation degrees of freedom because it can move in the x, y, and z directions.

- **Rotation Degrees of Freedom:**

Rotation of a linear molecule is considered around two axes perpendicular to the axis of the molecule. Rotation about the axis of the molecule itself does not lead to a different orientation of the molecule in space and is not counted as a distinct rotational mode. So, a linear polyatomic molecule like CO_2 has 2 rotation degrees of freedom.

- **Vibration Degrees of Freedom:**

The number of vibration degrees of freedom F_v can be calculated by subtracting the translation and rotation degrees of freedom from the total degrees of freedom. For a linear molecule, the formula is $F_v = 3N - 5$. For CO_2, $N = 3$, so $F_v = 3 \times 3 - 5 = 4$. CO_2 has 4 vibration modes, which include two bending modes (in the plane and out of the plane) that are degenerate (have the same energy) and two stretching modes, one symmetric and one asymmetric.

3.3 Application: To predict the Specific Heat Capacity of ideal gas

- The equipartition theorem is used to predict the specific heat capacities of ideal gases. For example, the molar specific heat at constant volume C_V for a monatomic gas is $\frac{3}{2}R$, for a diatomic gas it is $\frac{5}{2}R$ at moderate temperatures and $\frac{7}{2}R$ at high temperatures, which agrees well with experimental values for many gases under appropriate conditions.

3.3.1 Specific Heat at Constant Volume C_V

- The internal energy U of an ideal gas is a function of temperature T only, and for an ideal gas, it is given by
$U = \frac{f}{2}nRT$,
where n is the number of moles, R is the universal gas constant, and f is the number of degree of freedom. For a monoatomic gas, such as the helium He gas, $f = 3$, having 3 translational degrees of freedom. In case that the temperature T is not too high, $f = 5$ for a diatomic molecule gas (such as Hydrogen H_2 gas, for having 3 translational and 2 rotational degrees of freedom), and $f = 6$ for some polyatomic molecule gas (such as methane CH_4, for having 3 translational and 3 rotational degrees of freedom).

- The specific heat at constant volume C_V is defined as the rate of change of internal energy with respect to temperature at constant

volume, i.e., $C_V = \left(\frac{\partial U}{\partial T}\right)_V$
- We know from the first law of thermodynamics that $dU = dQ - dW$. If the heat is added at constant volume, then $dW = pdV = 0$ and $dQ = nC_V dT$.
- Hence, for the general case of an ideal gas, At constant volume, $dU = dQ = nC_V dT$, so
$C_V = \frac{1}{n}\left(\frac{\partial Q}{\partial T}\right)_V = \frac{1}{n}\left(\frac{\partial U}{\partial T}\right)$.
- For a monoatomic ideal gas, differentiating $U = \frac{3}{2}nRT$ with respect to T gives $C_V = \frac{3}{2}R$. For a diatomic ideal gas, considering translational and rotational degrees of freedom, $U = \frac{5}{2}nRT$ and $C_V = \frac{5}{2}R$.

3.3.2 Specific Heat at Constant Pressure C_p

- We know from the first law of thermodynamics that $dU = dQ - dW$. At constant pressure, $dW = pdV$ and $dQ = nC_p dT$. Namely, $C_p = \frac{1}{n}\left(\frac{\partial Q}{\partial T}\right)_p$.
- As shown above, the change in internal energy $dU = nC_V dT$.
- So, the first law yields
$nC_V dT = nC_p dT - pdV$.
- From the ideal gas law $pV = nRT$, we have, at constant pressure, $pdV = nRdT$, so that
$nC_V dT = nC_p dT - nRdT$.
- Rearranging gives

$C_p - C_V = R$, so $C_p = C_V + R$.

3.3.3 Specific Heat Ratio γ

- The specific heat ratio γ is defined as $\gamma = \frac{C_p}{C_V}$.
- From $C_p = C_V + R$, we can express C_p in terms of C_V and substitute into the definition of γ to get $\gamma = \frac{C_V + R}{C_V} = 1 + \frac{R}{C_V}$.
- For example, for a monoatomic ideal gas with $C_V = \frac{3}{2}R$, $\gamma = \frac{5}{3}$. For a diatomic ideal gas with $C_V = \frac{5}{2}R$, $\gamma = \frac{7}{5}$.

3.4 Ideal Gas Law and normal gases

The equipartition theorem was developed within the framework of classical statistical mechanics. The theorem assumes that the motion of particles can be described by classical Newtonian mechanics. It uses the principles of classical statistical mechanics, which assume that the states of a system can be described by continuous variables and that the probability distribution of these states follows the Boltzmann distribution. In classical physics, the phase space (a space that describes the positions and momenta of all particles in a system) is considered to be continuous, and the equipartition theorem is derived by averaging over all possible states in this continuous phase space.

However, it should be noted that the equipartition theorem has limitations when it comes to quantum systems. In quantum mechanics, the energy levels of a system are quantized, and the concept of continuous degrees of freedom as assumed in classical physics may not hold. At very low temperatures or for systems with very small energy levels, quantum effects become significant, and the equipartition theorem may not accurately describe the behavior of the system.

3.4.1 When to be applied to normal gases?

The ideal gas law, expressed as $PV = nRT$ (where P is pressure, V is volume, n is the amount of substance in moles, R is the ideal gas constant, and T is temperature in Kelvin), can be applied to normal gases under the following conditions:

- **High Temperature:**

At high temperatures, the kinetic energy of gas molecules is large. This causes the molecules to move more freely and interact less with each other through intermolecular forces. The higher the temperature, the more the behavior of the gas approximates that of an ideal gas, where intermolecular forces are assumed to be negligible. For many common gases, when the temperature is well above their boiling points, they tend to follow the ideal gas law more closely. For example, nitrogen gas (N_2) at temperatures above 77°K or -196°C (its boiling point) starts to approach ideal gas behavior more closely as the temperature rises.

- **Low Pressure:**

At low pressures, the gas molecules are relatively far apart from each other. The volume occupied by the gas molecules themselves is negligible compared to the total volume of the gas. Also, the frequency of intermolecular collisions and interactions is reduced. As a result, the gas behaves more like an ideal gas. Typically, when the pressure is less than a few atmospheres, many gases show fairly good agreement with the ideal gas law. For instance, at 1 atmosphere or lower, gases like oxygen (O_2) and carbon dioxide (CO_2) often follow the ideal gas law reasonably well.

- **Non-Polar or Slightly Polar Gases:**

Non-polar gases, such as helium (He), neon (Ne), and nitrogen (N_2), and slightly polar gases tend to follow the ideal gas law more closely than highly polar gases. (Non-polar gases are gases composed of molecules that have no or very weak dipole moments.) This is because non-polar gases have weaker intermolecular forces. Highly polar gases or those that can form hydrogen bonds, like water vapor (H_2O) and ammonia (NH_3), have stronger intermolecular interactions and deviate more from ideal gas behavior. However, under high temperature and low pressure conditions, even these gases can approximate ideal gas behavior to some extent.

It's important to note that no real gas is truly an ideal gas, but under the appropriate conditions of high temperature, low pressure, and for gases with suitable molecular characteristics, the ideal gas law can be used to make reasonably accurate predictions and calculations about the behavior of normal gases.

4 The root-mean-square velocity of the Boltzmann distribution and the degree of freedom

4.1 The root-mean-square velocity of the Boltzmann distribution

The root-mean-square (rms) velocity of particles in an ideal gas, as described by the Boltzmann distribution, is related to the (linear) kinetic energy of the particles, but does not directly depend on the degrees of freedom of the gas. Instead, the rms velocity depends primarily on the temperature and mass of the gas particles.

The formula for the rms velocity (v_{rms}) of particles. in three space (x, y, z) dimensions, in an ideal gas is given by:

$$v_{\text{rms}} = \sqrt{\frac{3kT}{m}}$$

where:
- k is the Boltzmann constant,
- T is the absolute temperature of the gas,
- m is the mass of a single gas particle.

This equation shows that the rms velocity is determined by the temperature and the mass of the particles, but not by the total degrees of freedom (f) of the gas.

4.2 The total degrees of freedom and the internal energy of the gas

The degrees of freedom do play a role in the internal energy of the gas. For an ideal gas, the internal energy U is given by:

$$U = \frac{f}{2}NkT$$

where:
- f is the number of degrees of freedom,
- N is the number of particles,
- k is the Boltzmann constant,
- T is the absolute temperature (in kelvin).

The degrees of freedom affect how the energy is distributed among the translational, rotational, and vibrational modes, but do not change the rms velocity, which is specifically a measure of the translational kinetic energy of the particles.

5 To express 1 degree Kelvin (K) in terms of electron volts (eV)

To express 1 degree Kelvin (K) in terms of electron volts (eV) using the Boltzmann constant, we can use the following relationship based on the equipartition theorem and the definition of thermal energy.

The Boltzmann constant k has a value of approximately $k = 1.38 \times 10^{-23} J/K$

The relationship between the units of energy E and temperature T is given by $E = kT$

When $T = 1K$, the energy E is $E = k \times 1 = 1.38 \times 10^{-23} J$

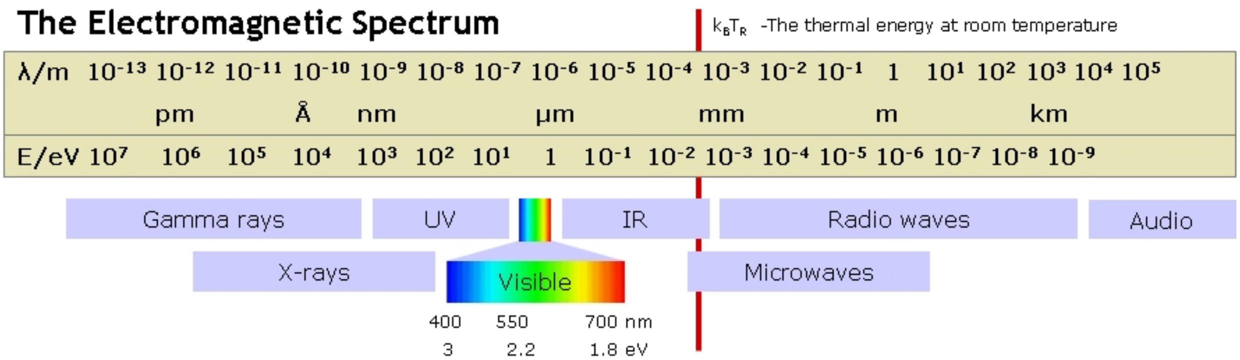
To convert from joules to electron volts, we use the conversion factor $1eV = 1.6 \times 10^{-19} J$ Let E in electron volts be E_{eV}, then

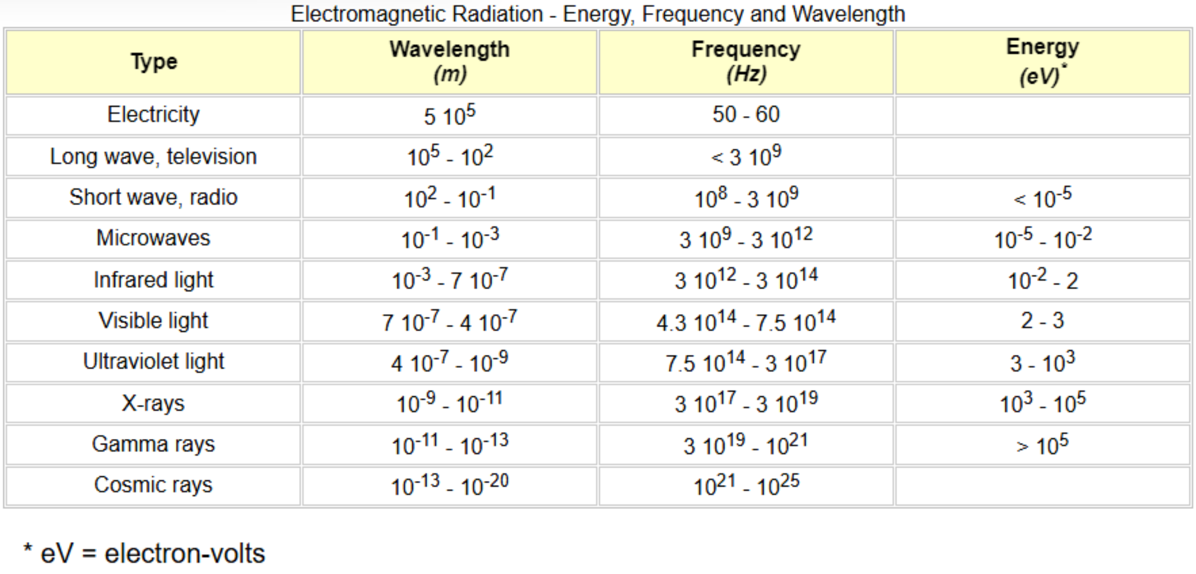
$$E_{eV} = \frac{E}{1.6 \times 10^{-19} J}$$

Substituting $E = 1.38 \times 10^{-23} J$ When $T = 1K$, the energy is $1.38 \times 10^{-23} J$, hence

$$1\ K = \frac{1.38 \times 10^{-23} J}{1.6 \times 10^{-19} J/eV} = 8.625 \times 10^{-5} eV.$$

So, 1 degree Kelvin is equivalent to $8.625 \times 10^{-5} eV \sim 10^{-4} eV$ in terms of energy using the Boltzmann constant.





Electromagnetic Radiation - Energy, Frequency and Wavelength

Type	Wavelength *(m)*	Frequency *(Hz)*	Energy *(eV)**
Electricity	$5\ 10^{5}$	50 - 60	
Long wave, television	10^{5} - 10^{2}	< $3\ 10^{9}$	
Short wave, radio	10^{2} - 10^{-1}	10^{8} - $3\ 10^{9}$	< 10^{-5}
Microwaves	10^{-1} - 10^{-3}	$3\ 10^{9}$ - $3\ 10^{12}$	10^{-5} - 10^{-2}
Infrared light	10^{-3} - $7\ 10^{-7}$	$3\ 10^{12}$ - $3\ 10^{14}$	10^{-2} - 2
Visible light	$7\ 10^{-7}$ - $4\ 10^{-7}$	$4.3\ 10^{14}$ - $7.5\ 10^{14}$	2 - 3
Ultraviolet light	$4\ 10^{-7}$ - 10^{-9}	$7.5\ 10^{14}$ - $3\ 10^{17}$	3 - 10^{3}
X-rays	10^{-9} - 10^{-11}	$3\ 10^{17}$ - $3\ 10^{19}$	10^{3} - 10^{5}
Gamma rays	10^{-11} - 10^{-13}	$3\ 10^{19}$ - 10^{21}	> 10^{5}
Cosmic rays	10^{-13} - 10^{-20}	10^{21} - 10^{25}	

* eV = electron-volts

Figure 2: The electromagnetic spectrum, which is the range of all possible electromagnetic radiation. Note that $1K = 8.625 \times 10^{-5} eV \sim 10^{-4} eV$. Also, nearly all objects in the universe emit, reflect or transmit some light. The distribution of this light along the electromagnetic spectrum (called the spectrum of the object) is determined by what the object is made of.

6 The energy and temperature requirements for exciting rotational and vibrational modes in diatomic molecules like H_2

The energy and temperature requirements for exciting rotational and vibrational modes in molecules like H_2 are determined by the molecular structure and the principles of quantum mechanics and thermodynamics. These excitations play crucial roles in various spectroscopic and chemical processes.

- **Rotational excitation:**

Molecules can also rotate around their axes. The energy levels of rotational motion are given by $E_J = \frac{h^2}{8\pi^2 I} J(J+1)$, where h is Planck's constant ($6.626 \times 10^{-34}\ Js$), E_J is the rotational energy, I is the moment of inertia of the molecule, and J is the rotational quantum number. The energy differences between rotational states are generally smaller than those for vibrational states. For H_2, the energy required to excite the first rotational mode is typically on the order of $10^{-23}\ J \sim 10^{-4}\ eV$, which corresponds to about $1\ K$. The rotational excitation becomes significant at temperatures around 10 - 50 K. At these temperatures, the thermal energy is sufficient to populate the lower rotational energy levels according to the Boltzmann distribution.

- **Vibrational excitation:**

Molecules vibrate due to the stretching and bending of chemical bonds. The energy required to excite a molecule from one vibrational state to another is given by the equation $\Delta E = h\nu$, where ΔE is the energy difference, h is Planck's constant ($6.626 \times 10^{-34}\ Js$), and ν is the frequency of the vibration. This energy is quantized, meaning that only specific discrete amounts of energy can be absorbed or emitted to cause a transition between vibrational states. For example, in the case of the H_2 molecule, the energy needed to excite the first vibrational mode is on the order of $10^{-20}\ J \sim 0.1\ eV$, which corresponds to about $1000\ K$. Hence, only when $T > 1000\ K$, a significant fraction of H_2 molecules may be in excited vibrational states.

- **Translational modes:**

In a thermal environment, the hydrogen molecules will have a distribution of translational energies according to the Maxwell-Boltzmann distribution. The average translational energy $\langle E \rangle$ is given by $\langle E \rangle = \frac{3}{2}kT$, where k is the Boltzmann constant ($1.38 \times 10^{-23}\ J/K$) and T is the temperature in Kelvin. However, this is a classical statistical average, and in the quantum mechanical picture, the actual energies are quantized, but the distribution of molecules among the different quantum states is still related to the temperature through the Boltzmann factor $e^{-\frac{E}{kT}}$. Hence, generally, temperatures above a few Kelvin ($\sim 10^{-4}\ eV$) are sufficient to induce a noticeable translational motion in H_2 molecules.