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Basic Properties of Quantum Chemistry

1.1 Introduction

Physics can be divided into two realms: classical and quantum. In classical physics, the properties of a system in a given moment can be represented geometrically as a point in a phase space with a number of dimensions related to the number of degrees of freedom of the system [1]. For example, if one considers a spring–mass system – i.e., an object of mass \( m \) coupled to a fixed string and constrained to move along one direction, the so-called one-dimensional (1-D) harmonic oscillator – its state can be represented as a point in a 2-D plane. If a coordinate system is constructed to make a correspondence between each point to a pair of numbers, \((q, p)\), the first number can be the distance of the object to the position at which the string is relaxed \((x)\), while the second number can be the product of the mass of the object by \(\frac{dx}{dt}\) (the object velocity). In other words, the second number is the linear momentum of the object along \(x, p = mx/\dot{t}\).

The dynamics of the system is represented, in the phase space, as a curve whose points are states successively occupied by the system as the time goes on. In terms of coordinates, we have a trajectory given by the time-dependent state vector \(S = [x(t), p(t)]\). The temporal evolution of \(S\) can be obtained by considering the Hamiltonian function \(H(S)\):

\[ H(S) = \frac{p^2}{2m} + V(x). \]  

Here, \(p^2/2m\) is the kinetic energy of the object and \(V(x)\) its potential energy, which in the case of the spring–mass system is given by \(V(x) = kx^2/2\), where \(k\) is the elastic constant of the spring. The time evolution of the state is found by solving Hamilton equations:

\[ \frac{dx}{dt} = \frac{\partial H}{\partial p}, \]  

(1.2)
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\[-\frac{dp}{dt} = \frac{\partial H}{\partial x},\]  

(1.3)

or, considering the state vector \( S \),

\[\frac{dS}{dt} = \{S, H\},\]  

(1.4)

where \( \{A, B\} \) is the Poisson bracket,

\[\{A, B\} = \left( \frac{\partial A}{\partial x} \frac{\partial B}{\partial p} - \frac{\partial B}{\partial x} \frac{\partial A}{\partial p} \right).\]  

(1.5)

Thus, the Hamiltonian rules the evolution of the classical state \( S \) in time.

As a matter of fact, this method can be extended to systems much more complex than the spring–mass system. If the system has \( N \) particles, with independent spatial coordinates \( (q_1, q_2, \ldots, q_N) \) and respective conjugated momenta \( (p_1, p_2, \ldots, p_N) \), the Hamiltonian is a function of the state:

\[S = (q_1, q_2, \ldots, q_N, p_1, p_2, \ldots, p_N),\]  

(1.6)

which evolves in time according to the Eq. (1.4) provided we redefine the Poisson bracket as

\[\{A, B\} = \sum_{i=1}^{N} \left( \frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial q_i} \frac{\partial A}{\partial p_i} \right).\]  

(1.7)

At every moment, the classical system is completely described by the classical state \( S \), and one can always in principle solve Hamilton equations to evaluate its past and future states. Classical physics is completely deterministic: knowing \( S \) at some time \( t_0 \) and the form of its Hamiltonian function, it is possible to disclose the whereabouts of the system at any given time \( t \). This picture, however, is radically changed in quantum mechanics.

In a quantum system, the physical state is described not by a position-momentum vector \( S \) but by a unit complex vector \( \lvert \Psi \rangle \) in an abstract geometric space called Hilbert space. The \( x \) and \( p \) coordinates of our spring-mass oscillator must be replaced by Hermitian operators \( \hat{x} \) and \( \hat{p} \), whose eigenstates correspond, respectively, to states with well-defined values of the position \( x \) and the momentum \( p \).

Unfortunately, these eigenstates do not belong to Hilbert space, and, therefore, one cannot find the spring–mass system with well-defined position or momentum! Besides, the eigenstates of \( \hat{x} \) and \( \hat{p} \) always “point” along different directions in such a way that a well-defined value of the position coordinate is physically described as a somewhat homogeneous superposition of infinitely many momentum eigenstates and vice versa. This leads directly to the Heisenberg uncertainty principle, which affirms the impossibility of measuring accurately the position and the momentum of a quantum particle at the same time.
1.2 The Schrödinger Equation

The time evolution of the complex vector $|\Psi_t\rangle$, however, is governed by the Hamiltonian operator $\hat{H}$ (obtained from the classical Hamiltonian by replacing $x$ and $p$ with the operators $\hat{x}$ and $\hat{p}$, respectively), according to

$$\hat{H} |\Psi_t\rangle = i\hbar \frac{\partial}{\partial t} |\Psi_t\rangle,$$

which, projected along an arbitrary eigenstate of the position operator $\hat{x}$, leads to the differential equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x) \Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t}$$

(1.9)

if one uses the classical Newtonian form given by Eq. (1.1).

Equation (1.9) is the time-dependent one-dimensional Schrödinger equation. The function $\Psi(x,t)$ is the wave function of the spring–mass oscillator, and it contains all the information about its physical state. Unfortunately, however, one cannot evaluate from it the exact position and momentum of the 1-D harmonic oscillator at a given moment, as already explained. The wave function $\Psi(x,t)$ allows one only to find the probability of observing the oscillator in a given region of space at a given moment $t$. Such probability is given by

$$P(a \leq x \leq b) = \int_a^b \Psi^*(x,t) \Psi(x,t) dx = \int_a^b |\Psi(x,t)|^2 dx.$$  (1.10)

As the complex vector $|\Psi\rangle$ is unitary, the wave function is normalized to the unity,

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = 1,$$  (1.11)

which means that the probability of finding the oscillator at some place is one.

For a given classic dynamical variable $A(x,p,t)$, one assigns the Hermitian operator $\hat{A}(\hat{x}, \hat{p}, t)$. This Hermitian operator, together with the wave function $\Psi(x,t)$, allows the evaluation of the average value of $A$ at instant $t$ according to

$$\langle A \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t) \hat{A}(\hat{x}, \hat{p}, t) \Psi(x,t) dx.$$  (1.12)

In the representation of the position operator $\hat{x}$ eigenstates, the two operators $\hat{x}$ and $\hat{p}$ are $\hat{x} = x$ and $\hat{p} = -i\hbar \partial/\partial x$. If the complex vector $|\Psi\rangle$ is expanded in the eigenstates of the Hermitian operator $\hat{A}$, the absolute square of the inner product $\langle a | \Psi \rangle$ gives the probability (probability density) of finding the system in the


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eigenstate $|a\rangle$ if the eigenvalue $a$ is discrete (continous). Therefore, in quantum mechanics, one introduces a statistical element that is intrinsic to the theory. Before performing a measurement on the physical system, its quantum state evolves deterministically obeying Schrödinger’s equation, but when a measurement is carried out, all one can do is to evaluate the probability of obtaining a particular outcome. The quantum state collapses to a single eigenstate of the operator representing the measurement being performed, and its time evolution proceeds deterministically from this eigenstate until another measurement is done.

For a quantum system consisting of a single particle of mass $m$ moving in 3-D space, the wave function becomes a function of three spatial coordinates and time, $\Psi(r,t)$, where $\mathbf{r} = (q_1, q_2, q_3)$ is a three-coordinate vector. In Cartesian coordinates, $\mathbf{r} = (x, y, z)$. The quantity $|\Psi(r,t)|^2 d\mathbf{r}$ is the probability of finding the system within the infinitesimal volume $d\mathbf{r}$. Schrödinger’s equation then becomes

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi(r,t) + V(r) \Psi(r,t) = i\hbar \frac{\partial \Psi(r,t)}{\partial t},$$

(1.13)

where $V(r)$ is the 3-D potential in which it moves, and $\nabla^2$ the Laplacian operator. Equation (1.13) can be solved by separating the space and time coordinates according to

$$\Psi(r,t) = \psi(r) \varphi(t),$$

(1.14)

which leads to two differential equations – one for $\varphi(t)$ and another for $\psi(r)$, namely

$$i\hbar \frac{d\varphi(t)}{dt} = E \varphi(t),$$

(1.15)

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(r) + V(r) \psi(r) = E \psi(r).$$

(1.16)

Equation (1.15) has a simple solution,

$$\varphi(t) = \exp \left( -\frac{iEt}{\hbar} \right),$$

(1.17)

while Eq. (1.16) is the time-independent Schrödinger equation. The integration constant $E$ is the energy of the particle. It is an eigenenergy equation for the energy eigenfunctions $\psi(r)$ – i.e., $\hat{H} \psi(r) = E \psi(r)$. If the energy spectrum of the system is discrete, one can label the eigenenergies $E$ using a vector with integer components $\mathbf{n}$, $E$ becoming $E_n$. The time-independent solutions can be written as $\psi_n(r)$, while the time-dependent solutions are

$$\Psi_n(r,t) = \psi_n(r) \exp \left( -\frac{iE_n t}{\hbar} \right).$$

(1.18)
1.2 The Schrödinger Equation

The probability density assigned to \( \Psi_n(r, t) \) does not depend on time, so the \( \Psi_n(r, t) \) are labeled stationary states. The general solution of Eq. (1.13) is a superposition of stationary states:

\[
\Psi(r, t) = \sum_n c_n \Psi_n(r, t),
\]

(1.19)

where \( |c_n|^2 \) gives the probability of finding the system with energy \( E_n \) at instant \( t \).

If the eigenenergies of Eq. (1.16) are continuous, one can label the eigenfunctions using a vector with continuous components \( k \). In this case, one finds the general solution:

\[
\Psi(r, t) = \int \limits_{V_k} c(k) \Psi_k(r, t) dk.
\]

(1.20)

Here, \( |c(k)|^2 dk \) is the probability of finding the system with energy \( E(k) \) within the volume \( V_k \).

Lastly, if the eigenenergies have a mixed spectrum, the general solution of the time-dependent Schrödinger equation is a combination of Eqs. (1.19) and (1.20).

1.2.1 The Born-Oppenheimer Approximation

In a molecule or crystal, we have mutual interactions between electrons and nuclei. In this case, one can write the following interaction potentials to describe the system:

\[
V_{nn}(R_i, R_j) = \frac{kZ_iZ_je^2}{|R_i - R_j|}, \quad (1.21)
\]

\[
V_{en}(r_i, R_j) = -\frac{kZ_je^2}{|r_i - R_j|}, \quad (1.22)
\]

\[
V_{ee}(r_i, r_j) = \frac{ke^2}{|r_i - r_j|}. \quad (1.23)
\]

Here, \( V_{nn}(R_i, R_j) \) is the Coulomb potential between two nuclei \( i \) and \( j \) at the positions \( R_i \) and \( R_j \) with atomic numbers \( Z_i \) and \( Z_j \), respectively; \( V_{en}(r_i, R_j) \) is the Coulomb potential between the \( i \)th electron at the position \( r_i \) and the atomic nuclei at \( R_j \) with atomic number \( Z_j \); and \( V_{ee}(r_i, r_j) \) is the Coulomb potential between the \( i \)th and \( j \)th electron at positions \( r_i \) and \( r_j \).

The wave function for this system is \( \psi(r_1, r_2, \ldots, r_N, R_1, R_2, \ldots, R_N, t) \) or, put more simply, \( \Psi(r, R, t) \), where \( r \) and \( R \) stand for the electron and nuclei
coordinates, respectively. The time-dependent Schrödinger equation for a system with $N_e$ electrons and $N_n$ nuclei is
\[
\left[ T_e + T_n + V_{nn}(\mathbf{R}) + V_{en}(\mathbf{r}, \mathbf{R}) + V_{ee}(\mathbf{r}) \right] \psi(\mathbf{r}, \mathbf{R}, t) = i\hbar \frac{\partial \psi(\mathbf{r}, \mathbf{R}, t)}{\partial t}.
\] (1.24)
Here, we identify the electron and nuclei kinetic energy terms, $T_e$ and $T_n$, the total interaction energy between the nuclei $V_{nn}(\mathbf{R})$, the total interaction energy between the electrons and the nuclei $V_{en}(\mathbf{r}, \mathbf{R})$, and the total interaction energy between the electrons $V_{ee}(\mathbf{r})$.

If we separate the spatial and time-dependent parts,
\[
\psi(\mathbf{r}, \mathbf{R}, t) = \Phi(\mathbf{r}, \mathbf{R}) \phi(t),
\] (1.25)
we obtain the time-independent Schrödinger equation:
\[
\left[ T_e + T_n + V_{nn}(\mathbf{R}) + V_{en}(\mathbf{r}, \mathbf{R}) + V_{ee}(\mathbf{r}) \right] \Phi(\mathbf{r}, \mathbf{R}) = E_T \Phi(\mathbf{r}, \mathbf{R}),
\] (1.26)
where $E_T$ is the total energy of the system.

We now decouple the kinetic nuclear energy according to
\[
\Phi(\mathbf{r}, \mathbf{R}) = \Phi_e(\mathbf{r}; \mathbf{R}) \Phi_n(\mathbf{R}).
\] (1.27)

Putting Eq. (1.27) into Eq. (1.26), we have
\[
\frac{\left[ T_e + V_{nn}(\mathbf{R}) + V_{en}(\mathbf{r}, \mathbf{R}) + V_{ee}(\mathbf{r}) \right] \Phi_e(\mathbf{r}; \mathbf{R})}{\Phi_e(\mathbf{r}; \mathbf{R})} + \frac{T_n \Phi_n(\mathbf{R})}{\Phi_n(\mathbf{R})} = E_T.
\] (1.28)

Making the assumption that the nuclear coordinates change much more slowly than the electron coordinates due to the large difference between the masses of electrons and nuclei, $\{\mathbf{R}\}$ becomes a set of constant parameters for the motion of the electrons. This is known as the Born-Oppenheimer approximation. It allows us to convert Eq. (1.28) into two independent equations, namely
\[
\left[ T_e + V_{nn}(\mathbf{R}) + V_{en}(\mathbf{r}, \mathbf{R}) + V_{ee}(\mathbf{r}) \right] \Phi_e(\mathbf{r}; \mathbf{R}) = E_e(\mathbf{R}) \Phi_e(\mathbf{r}; \mathbf{R}),
\] (1.29)
\[
T_n \Phi_n(\mathbf{R}) = \left[ E_T - E_e(\mathbf{R}) \right] \Phi_n(\mathbf{R}.
\] (1.30)

From Eq. (1.29), for a given configuration of nuclear coordinates $\{\mathbf{R}\}$, one obtains a set of electron eigenstates $\{\Phi_{e,v}(\mathbf{r}; \mathbf{R})\}$ with eigenenergies $E_{e,v}(\mathbf{R})$. Of particular interest is the lowest-energy eigenstate, $\Phi_{e,0}(\mathbf{r}; \mathbf{R})$, with eigenenergy $E_{e,0}(\mathbf{R})$ (assuming a non-degenerate case). This ground state defines, as we change $\mathbf{R}$ slowly, a potential energy hypersurface (or adiabatic surface) for the nuclear motion, which allows one to minimize the total energy of the electron–nuclei system (geometry optimization procedure).
1.2 The Schrödinger Equation

1.2.2 Slater Determinant

Let us consider now what happens when one has a system formed by \( N \) identical particles interacting with each other in a fixed external potential \( V(\mathbf{r}) \). The interaction potential between the particles \( i \) and \( j \) is \( v(\mathbf{r}_i, \mathbf{r}_j) \), while the kinetic energy operator of the \( i \)th particle is \( -(\hbar^2/2m)\nabla_i^2 \). The wave function of the system depends on the coordinates \( \{\mathbf{r}_i\} \) and can be written as \( \Psi = \Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t) \). Hence, the time-dependent Schrödinger equation for this system is

\[
\left[ \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m} \nabla_i^2 + V(\mathbf{r}_i) + \sum_{j=1}^{N} v(\mathbf{r}_i, \mathbf{r}_j) \right) \right] \Psi = i\hbar \frac{\partial \Psi}{\partial t}. \tag{1.31}
\]

One can perform a separation between space and time coordinates, \( \Psi = \Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t) = \psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)\varphi(t) \), to obtain stationary states with well-defined energy \( E \), yielding

\[
\left[ \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m} \nabla_i^2 + V(\mathbf{r}_i) + \sum_{j=1}^{N} v(\mathbf{r}_i, \mathbf{r}_j) \right) \right] \psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = E\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N). \tag{1.32}
\]

which is the time-independent Schrödinger equation for the system with \( N \) identical particles.

As each vector \( \mathbf{r}_i \) has three components, one has a partial differential equation with \( 3N \) independent variables without analytical solution in most cases. However, one can move forward from Eq. (1.32) in the case of non-interacting particles, in which \( v(\mathbf{r}_i, \mathbf{r}_j) = 0 \). For such situation, one obtains

\[
\left[ \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m} \nabla_i^2 + V(\mathbf{r}_i) \right) \right] \psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = E\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N). \tag{1.33}
\]

Here, a separation of variables is feasible:

\[
\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = u_1(\mathbf{r}_1)u_2(\mathbf{r}_2)\ldots u_N(\mathbf{r}_N), \tag{1.34}
\]

which leads to a set of \( N \) equations of the form:

\[
\left[ -\frac{\hbar^2}{2m} \nabla_i^2 + V(\mathbf{r}_i) \right] u_i(\mathbf{r}_i) = E_iu_i(\mathbf{r}_i). \tag{1.35}
\]

The normalized eigenstates \( u_i \) can have a discrete, continuous, or mixed eigenenergy spectrum. We will assume the first case and write the eigenstates as \( u_{m(i)}(\mathbf{r}_i) \) and the eigenenergies as \( E_{m(i)} \). Then one finds

\[
\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = u_{m(1)}(\mathbf{r}_1)u_{m(2)}(\mathbf{r}_2)\ldots u_{m(N)}(\mathbf{r}_N), \tag{1.36}
\]
with energy

\[ E = E_{n(1)} + E_{n(2)} + \cdots + E_{n(N)}. \]  

(1.37)

Note that an eigenfunction with exactly the same energy can be obtained if the coordinates of the \( i \)th and \( j \)th particles are permuted in Eq. (1.36). As a matter of fact, identical quantum particles are indistinguishable, so the permutation of spatial coordinates does not change the probability density obtained from \( \psi(r_1, r_2, \ldots, r_N) \). This leads to

\[ \hat{P}_{ij} \psi(r_1, r_2, \ldots, r_N) = \pm \psi(r_1, r_2, \ldots, r_N), \]  

(1.38)

where \( \hat{P}_{ij} \) is the operator that permutes the coordinates \( r_i \) and \( r_j \) in the wave function. Also, \( \psi(r_1, r_2, \ldots, r_N) \) is an eigenfunction of \( \hat{P}_{ij} \) with only two eigenvalues, +1 and −1. In the former, the identical particles are called bosons, and in the latter, they are called fermions. Some examples of two-particle bosonic solutions are

\[ \psi(r_1, r_2) = u_{n(1)}(r_1)u_{n(2)}(r_2), \]  

(1.39)

\[ \psi(r_1, r_2) = (1/\sqrt{2})\left[u_{n(1)}(r_1)u_{n(2)}(r_2) + u_{n(1)}(r_2)u_{n(2)}(r_1)\right]. \]  

(1.40)

From Eqs. (1.39) and (1.40), one can see that bosons can occupy the same quantum states. Indeed, statistically they prefer this kind of configuration. For fermions, however, the opposite is true. In the case of a two-particle fermionic state, we have

\[ \psi(r_1, r_2) = (1/\sqrt{2})\left[u_{n(1)}(r_1)u_{n(2)}(r_2) - u_{n(1)}(r_2)u_{n(2)}(r_1)\right]. \]  

(1.41)

If the states are the same — i.e., \( n(1) = n(2) \) — then the wave function vanishes! So it is impossible for two fermions to occupy the same quantum state at the same time (Pauli’s exclusion principle). Because of this, the quantum state occupation statistics for fermions is different from the statistics for bosons.

In general, the normalized wave function for \( N \) indistinguishable non-interacting fermions is given by the Slater determinant:

\[ \psi(r_1, r_2, \ldots, r_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} u_{n(1)}(r_1) & u_{n(1)}(r_2) & \cdots & u_{n(1)}(r_N) \\ u_{n(2)}(r_1) & u_{n(2)}(r_2) & \cdots & u_{n(2)}(r_N) \\ \vdots & \vdots & \ddots & \vdots \\ u_{n(N)}(r_1) & u_{n(N)}(r_2) & \cdots & u_{n(N)}(r_N) \end{vmatrix}. \]  

(1.42)

If \( n(i) = n(j) \) for \( i \neq j \), two lines of the determinant are equal, and it becomes zero, ensuring that two identical one-particle quantum states cannot be occupied.
1.3 Chemical Bonds

When atoms interact, they change their electronic structures in such a way that an effective attraction takes place between them, forming a chemical bond [2]. This attraction can be either very strong, creating a new stable chemical compound (a molecule), or less strong, forming unstable structures that can be dismantled with relatively small amounts of energy. The nature of the interaction depends on the electronic structure of the atoms involved. The stable atomic arrangements have a constant characteristic nuclear geometry, making it possible to obtain different configurations with the same set of atoms (isomers).

This fact was already known at the beginning of the nineteenth century, as the atomic theory of J. Dalton was being embraced by chemists. After the discovery of the electron and the beginnings of quantum mechanics, the American physical chemist G. N. Lewis proposed, in 1916, an electronic theory to explain the chemical bonds between atoms in molecules. According to him, two atoms can form a bond by transferring one electron to another (the electron-pair model); by sharing two electrons, one from each atom (his covalent bond model); or by one atom sharing two electrons with another.

With the progress of quantum mechanics, however, it became clear that Lewis’s original idea could not reflect accurately the reality of the interatomic forces in molecules, as the electrons are truly indistinguishable and delocalized, meaning that one cannot point out them and say which electrons in particular effectively are involved in a chemical bond.

However, there are ways to establish a correspondence between the original concepts of Lewis and the quantum mechanics postulates. It can be done by analyzing the nuclear geometry, which allows the definition of a concept of nuclear vicinities, and the definition of space domains, where there is a large probability of finding two electrons with opposite spins. One can also consider an evaluation of the differential electron density, meaning the difference between the electron density of the compound and the superposition of electron densities from the isolated atoms, to see which regions are electronically populated or depopulated when a molecule is formed.

1.3.1 The Ionic Bond

The electron affinity of an atom is essential to determine the character of a chemical bond. If two elements, one with high electronegativity and the other with low electronegativity, approach each other, one or more electrons of the latter can be effectively transferred to the first. This electron migration ionizes each original atom, and the resulting ionic compound forms a strong electric dipole (see Figure 1.1).
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Ionic bond

![Figure 1.1 Pictorial view of the ionic bond.](image1)

![Figure 1.2 Pictorial view of the covalent bond.](image2)

The potential energy between the ions can be approximated by a superposition of the attractive Coulomb potential with a repulsive term due to the exchange quantum interaction:

\[ V(r) = -\frac{k e^2}{r} + \frac{\alpha}{r^s}, \quad (1.43) \]

where \(\alpha\) and \(s\) are constant dependent on the elements involved.

The ionic bond is the strongest of all chemical bonds, with binding energies per bond between 150 and 1,000 kcal/mol.

1.3.2 The Covalent Bond

The covalent bond occurs between two atoms with similar electronegativities, which prevents the transfer of electrons from one atom to the other. Instead, both atoms reach a compromise and share pairs of electrons (see Figure 1.2), leading to binding energies between 50 (the weakest single covalent bond) and 250 kcal/mol (the strongest triple covalent bond).

An approximate description of these bonds can be given using quantum mechanics: molecular orbitals are formed from the linear combination of original atomic...