1
Structure and Properties

A general opinion of chemists adopted by textbooks is that in chemistry, structure[1] is a central concept: the key to everything. Properties[2] of a given substance depend on the number and nature of its constituting atoms and their mode of connection (*connectedness*). It is less obvious but quite important that looking at structural formula, a well-versed chemist should be able to deduce many properties of a substance. In order to exploit this possibility, in this chapter, we are going to define some basic principles associated with structure and properties. After having defined the concept of structure, we will proceed to discuss correlations of structure and properties, with special emphasis on the spatial features of structure and properties derived from changes thereof. First of all, we will discuss properties derived from the spatial structure of typical organic compounds; but for the sake of completeness, the stereochemical features of inorganic compounds will be dealt briefly as well.

1.1
The Covalent Bond and the Octet Rule

The covalent nature of the chemical bond, assuming a shared pair of electrons, was first proposed by G. N. Lewis in 1916 [1]. According to this concept, by sharing two electrons, two hydrogen atoms can establish a stable bond by forming a closed shell of electrons similar to that of the noble gas helium (Figure 1.1).

In the ***Lewis* structures,** electrons are symbolized by dots. The amount of energy required to dissociate a hydrogen molecule to two hydrogen atoms is called the bond dissociation (or bond) energy. In the case of H_2, this is quite high: 435 kJ mol^{-1}.

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1) Under *structure*, chemists often understand a single state of a single molecule; therefore, at this level, structure is a *microscopic* concept (to be discussed in more detail later).

2) *Properties* of a material are generally defined not on the basis of a given state of a single molecular structure but on an assembly of a large number of molecules, on a timescale relatively long compared to the timescale of molecular events, and therefore these properties are generally *macroscopic* concepts.

Stereochemistry and Stereoselective Synthesis: An Introduction, First Edition.
László Poppe and Mihály Nógrádi.

Companion Website: www.wiley.com/go/poppe/stereochemistry

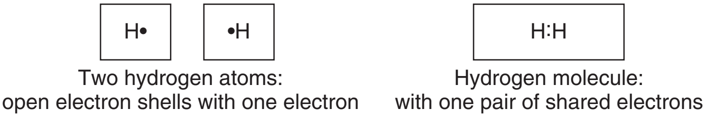

Figure 1.1 Formation of the covalent bond of the hydrogen molecule.

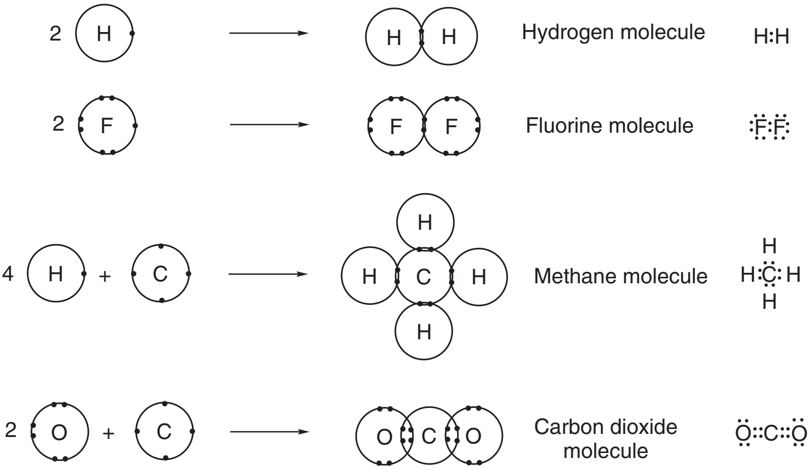

Figure 1.2 Covalent bonds in some simple molecules (*Lewis* representation).

While with hydrogen molecule the number of electrons present in the valence forming shell is limited to two, in the *Lewis* model, molecules composed from elements of the second row (Li, Be, B, C, N. O, F, and Ne) in the valence shells contain eight (shared and unshared) electrons. Most organic compounds follow the octet rule: on formation of their compounds, electrons are taken up, and elements are shared or removed in a way that they should assume a stable structure involving eight valence electrons. When in compounds of carbon, nitrogen, oxygen, and fluorine, the octet rule is valid, their electron configuration is analogous to that of the noble gas neon. *Lewis* representation of some simple molecules is shown in Figure 1.2.

Such structures showing the distribution of electrons (*Lewis* structures) are useful aids for understanding covalent bond formation, but it is simpler to use the s.c. ***Kekulé* formulas**.[3] The latter are derived from *Lewis* formulas by replacing a shared pair of electrons with a line connecting the corresponding atomic symbols. Nonbonding electrons are shown by dots. Examples for **structural formulas** drawn according to this principle are shown in Table 1.1. As a further

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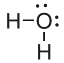
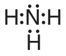
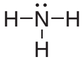
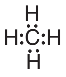
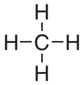
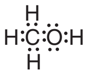
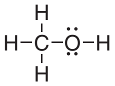
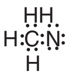
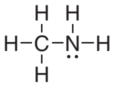
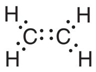
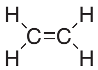
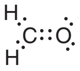
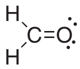
[3] Based on the work of A. M. Butlerov, A. Couper, and F. A. Kekulé but at variance with their original formulas, bonds between elements are shown by lines (Kekulé formulas).

Table 1.1 Lewis and Kekulé formulas of some simple molecules.

Name	Molecular formula	*Lewis* formula	*Kekulé* formula
Water	H_2O		
Ammonia	H_3N		
Methane	CH_4		
Methanol	CH_4O		
Methylamine	CH_5N		
Ethene	C_2H_4		
Formaldehyde	CH_2O		
Acetylene	C_2H_2	H:C⁝⁝C H	$H-C\equiv C-H$
Hydrogen cyanide	CHN	H:N⁝⁝C	$H-C\equiv N:$

simplification of *Kekulé* formulas, nonbonding electrons are not shown since these can be readily calculated following the octet rule.

As illustrated in Table 1.1 by ethene, formaldehyde, acetylene, and hydrogen cyanide, atoms may share more than one pair of electrons forming in this way **multiple bonds**. Compounds of boron, such as BH_3 or BF_3, are exceptional in a way that the valence shell of boron is not filled up with electrons as would be required by the octet rule. Accordingly, these compounds have a high affinity to electrons and are very reactive.

Valence is the number of those valence electrons, which must be taken up or shed that the valence shell should attain the octet state (Table 1.2). In their covalent compounds, the number of bonds adjoined to an atom is equal to the valence of the given atom. Valences listed in Table 1.2 are typical of atoms common in organic compounds.

Table 1.2 Valence states of selected elements common in organic compounds.

Atom	H	C	N	O	F	Cl	Br	I
Valence	1	4	3	2	1	1	1	1

1.2
Representation of Chemical Structures

For the representation of simpler compounds, condensed *Kekulé* formulas are suitable; but this is a cumbersome way to represent more complex compounds. Thus, cyclic compounds are best represented by further simplified, s.c. **linear formulas**. Application of linear formulas is exemplified by formulas for cycloalkanes (Figure 1.3).

Linear formulas are also convenient to depict open chain compounds (Figure 1.4).

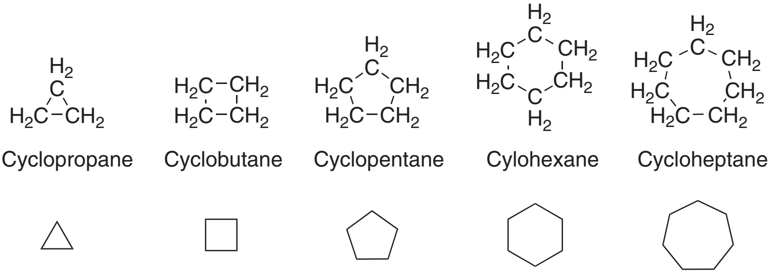


Figure 1.3 Representation of cycloalkanes by linear formulas.

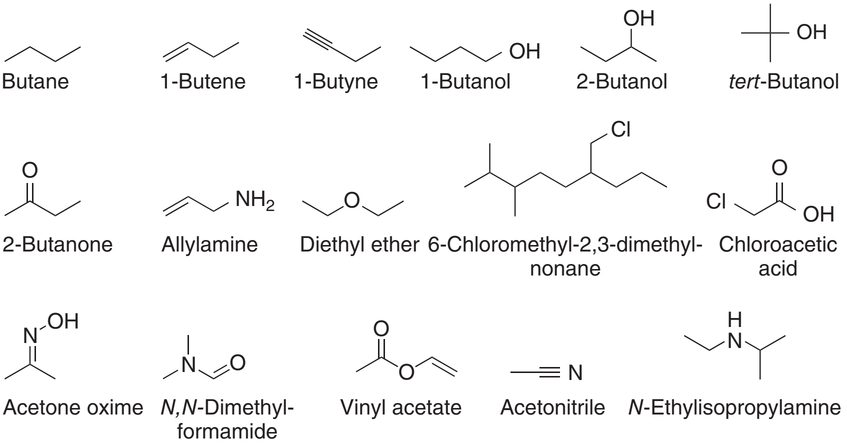


Figure 1.4 Representation of open-chain compounds with linear formulas.

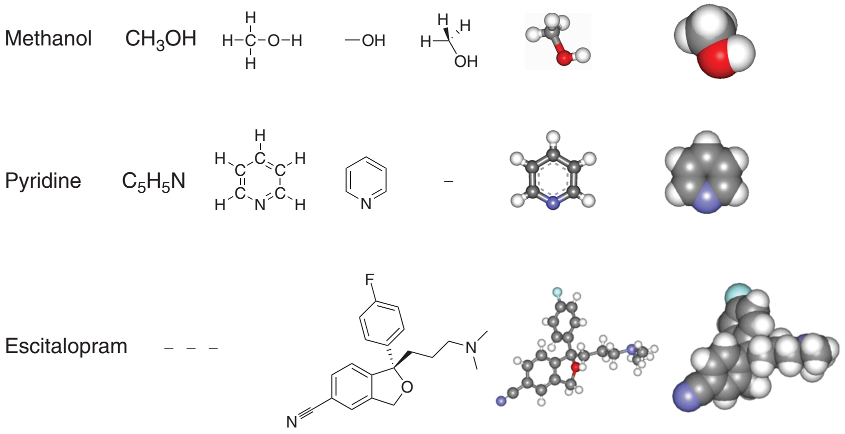


Figure 1.5 Various modes of representation for methanol, pyridine, and the antidepressant escitalopram.

When drawing linear formulas, for simplicity, symbols of carbon atoms, the pairs of electrons, and hydrogen atoms attached to carbons are omitted. Accordingly, all end points, breaking points, and points of branching represent a carbon atom. Multiple bonds are shown by an appropriate number of parallel lines. Heavy atoms other than carbon are shown by their atomic symbols together with the hydrogen atoms attached.

Additional ways of representation are shown in Figure 1.5 by the example of methanol, pyridine, and the antidepressant escitalopram. Representations include the following:

- **A**: Name (trivial or systematic)
- **B**: Condensed formulas (generally suitable for printing in a single line)
- **C**: *Kekulé* formulas (showing all the atoms and bonds)
- **D**: Linear formulas (hydrogens omitted, breaking, branching, and end points represent carbon atoms; heavy atoms are shown with the hydrogen attached)
- **E**: **Stereoformulas**[4] (depicting the spatial orientation of bonds)
- **F**: Ball and stick model (often used to depict X-ray structures or computed models)
- **G**: Space-filling model (approaches the electron distribution).

Figure 1.5 well demonstrates that for smaller open-chain organic compounds (e.g., methanol), it is the condensed or *Kekulé* formula that is the most appropriate for the demonstration of the two-dimensional features of the structure. In case of smaller cyclic compounds (e.g., pyridine), the linear formulas are most often used. To depict more complex structures (e.g., escitalopram), condensed

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[4] The details of the use of stereo formulas are exactly defined by IUPAC recommendations [2]. Easily perceptible stereo formulas have only become generally used in the second half of the twentieth century. Earlier, various other representations were used.

or *Kekulé* representations are practically useless, and therefore a combination of linear and stereo representation is recommended. The complete stereostructure of molecules can be best depicted by a simplified representation of 3D structures. In Figure 1.5, two possible modes of representation of molecular models that is, ball and stick and space-filling models are shown.5) As can be seen with more complex molecules, space-filling models refer to their overall shape, while the details of the structure are less apparent.

1.3
Description of Chemical Structure

Chapters of the rules of International Union of Pure and Applied Chemistry (IUPAC) for naming compounds [3] do not give a precise definition of what should be understood under "chemical structure." Therefore, we define in a general way as **chemical structure** as it is understood by crystallographers: chemical structure is an accurate description of the spatial arrangement of the constituting atoms (atomic nuclei) in space.

The exact spatial arrangement of atoms can be described, for instance, by their **Cartesian coordinates**.6) From a structural point of view, however, it is not the absolute position and orientation of the molecule that is decisive; therefore, it is often more useful to describe the relative position of atoms by s.c. **internal coordinates**7) (Figure 1.6). Internal coordinates for the description of molecules are the bond lengths (r), the bond angles (α), and the torsion angles (ω).8)

For the description of molecules containing two atoms (**I**), besides defining the type of atoms (A, B), it is sufficient to give the bond length as a single internal coordinate. In organic molecules, the value of **bond lengths** varies in a relatively narrow range (Table 1.3).

The structure of a triatomic molecule (**II**) is characterized by the type of atoms (A, B, and C), two bond lengths (r_1 and r_2), and one **bond angle** (α).9) In real triatomic molecules, bond lengths and bond angles depend on the type of constituting atoms, their hybridization state, and the order of the bonds (Figure 1.7).

It is apparent from Figure 1.7 that in triatomic molecules, bond angles vary in a wide range. The molecules of hydrogen sulfide and water form an angular

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5) Computer programs suitable to visualize chemical structures offer further possibilities (e.g., wire models, ball and stick models, covering surfaces according to various properties and combinations thereof).

6) A molecule containing n atoms can have a maximum of $3n - 6$ internal degrees of freedom and can be described by $3n - 6$ Cartesian coordinates. Use of Cartesian coordinates also defines its absolute position, and therefore their use is uncomfortable.

7) A molecule containing n atoms can have a maximum of $3n - 6$ internal degrees of freedom and can be described by $3n - 6$ internal coordinates. Internal coordinates reflect to local bonds and symmetries; they can be composed by linear combinations of Cartesian coordinates.

8) Bond angles are often denoted by the symbol Θ. In polymer chemistry, it is usual to denote bond angles as τ, while the symbol Θ is for torsion angles.

9) Bond angles are sometimes called valence angles.

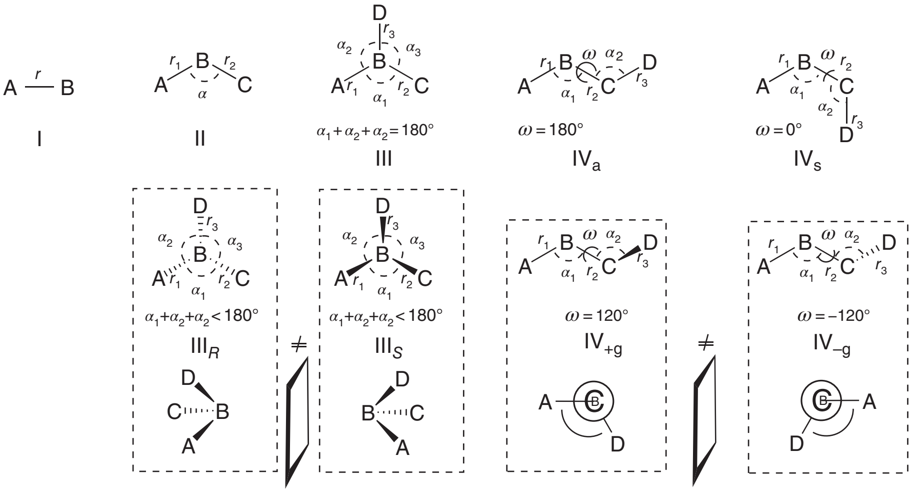

Figure 1.6 Characterization of molecules consisting of two, three, and four atoms with internal coordinates.

Table 1.3 Characteristic values of bond lengths commonly occurring in organic compounds.

	C–C	C=C	C≡C	C–H	C–O	C=O	C–N	C–S	C–F	C–Cl	C–Br	C–I
pm	154	133	120	109	143	122	147	182	135	176	192	212
Å	1.54	1.33	1.20	1.09	1.43	1.22	1.47	1.82	1.35	1.76	1.92	2.12

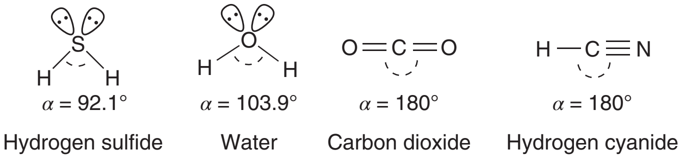

Figure 1.7 Bond angles in selected triatomic molecules.

structure owing to the presence of two nonbonding pairs of electrons in an approximately tetrahedral arrangement. (The difference in the bond angles is caused by the different strengths of repulsion between the pairs of electrons.) On the other hand, hydrogen cyanide and carbon dioxide are linear due to the *sp* hybridization state of the central atom. In bond angles between atoms of given types, the value of bond angles varies in a narrow range and therefore when discussing structures, organic chemists take them as constant.

Molecules consisting of four atoms (A, B, C, and D) present a new situation (Figure 1.6). If the fourth atom (D) is attached to the central atom (B) of the chain formed by the other three, we are dealing with a branched structure (Figure 1.6, **III**, **III**$_R$, and **III**$_S$). When the four atoms (A, B, C, and D) are coplanar (the sum of the three bond angles α_1, α_2, and α_3 is 180°), the structure is planar (**III**). When, however, the sum of the three bond angles α_1, α_2, and α_3 is less than 180°, pyramidal structures (**III**$_R$ and **III**$_S$) are formed. It can be seen that while the internal coordinates of the two structures (α_1, α_2, and α_3) are identical, the structures themselves are nonidentical.

If the atoms in a molecule consisting of four atoms form a continuous chain, in addition to bond lengths (r_1, r_2, and r_3) and bond angles (α_1 and α_2), an additional type of internal coordinate, the **torsion angle** (ω),[10] has to be taken into consideration (Figure 1.6). With the variation of torsion angles, a further multiplication of structural alternatives arises (Figure 1.6, **IV**$_S$, **IV**$_R$, **IV**$_{+g}$, and **IV**$_{-g}$). While in organic molecules, as discussed before, the values of bond lengths ($r_1 \cdots r_n$) and bond angles ($\alpha_1 \cdots \alpha_n$) are relatively constant, torsion angles (ω) for single bonds can take up any value between 0° and 180°. Coplanarity of the four atoms is possible in two different ways: $\omega = 0°$ (**IV**$_s$) or $\omega = 180°$ (**IV**$_a$) (Figure 1.6). While in structures built up from the same kind of atoms, bond lengths and bond angles may be identical, it is apparent that owing to the difference of torsion angles, the two structures are different. Besides the two coplanar arrangements (**IV**$_s$ and **IV**$_a$), an infinite number of noncoplanar structures is possible with the alteration of torsion angles in the range of 0–180°. It can be seen that the arrangement of a chain of atoms A–B–C–D assuming a given torsion angle (e.g., $\omega = 120°$: **IV**$_{+g}$) and the corresponding arrangement characterized by an identical but negative torsion angle ($\omega = -120°$: **IV**$_{-g}$) are nonidentical mirror images.

1.4
Problems of Correlating Chemical Structure with Properties

For a representation of chemical structures **bonding matrices**, describing the order of attachment of atoms and bonds (connectedness) may be useful (Figure 1.8).

Figure 1.8 clearly demonstrates that while the chemical formula of ethanol and dimethyl ether (C_2H_5O) is identical, their bonding matrices are different. We can therefore reasonably assume that these molecules are in fact different, in other words **isomers**.[11]

While acetaldehyde and "vinyl alcohol" have the same chemical formula (C_2H_4O, Figure 1.9), both their structural formulas and their bonding matrices are apparently different.

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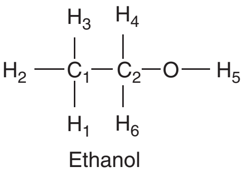
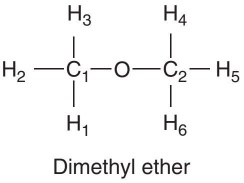
[10] A torsion or dihedral angle (ω) is defined in case of a consecutive nonlinear chain of atoms A, B, C, and D as the angle formed by the planes of atoms ABC and BCD. If the plane is seen along the line BC, the torsion angle is taken as positive if the bond AB ought to be moved clockwise (in an angle <180°) to superpose bond CD. If AB ought to be rotated counterclockwise, the torsion angle is taken as negative.

[11] According to their most common definition, **isomers** have the same molecular formula but are nevertheless different. This definition is inexact, since it lacks the definition of the circumstances (thermal energy level, environment, state, and time interval) under which the compounds are viable as stable entities (cf. Section 2.2.2).

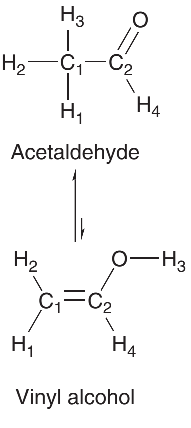


$$\begin{array}{c|ccccccccc} & C_1 & C_2 & O & H_1 & H_2 & H_3 & H_4 & H_5 & H_6 \\ \hline C_1 & \diagdown & 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ C_2 & 1 & \diagdown & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ O & 0 & 0 & \diagdown & 0 & 0 & 0 & 0 & 1 & 0 \\ H_1 & 1 & 0 & 0 & \diagdown & 0 & 0 & 0 & 0 & 0 \\ H_2 & 1 & 0 & 0 & 0 & \diagdown & 0 & 0 & 0 & 0 \\ H_3 & 1 & 0 & 0 & 0 & 0 & \diagdown & 0 & 0 & 0 \\ H_4 & 0 & 1 & 0 & 0 & 0 & 0 & \diagdown & 0 & 0 \\ H_5 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \diagdown & 0 \\ H_6 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \diagdown \end{array}$$



$$\begin{array}{c|ccccccccc} & C_1 & C_2 & O & H_1 & H_2 & H_3 & H_4 & H_5 & H_6 \\ \hline C_1 & \diagdown & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ C_2 & 0 & \diagdown & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ O & 1 & 1 & \diagdown & 0 & 0 & 0 & 0 & 0 & 0 \\ H_1 & 1 & 0 & 0 & \diagdown & 0 & 0 & 0 & 0 & 0 \\ H_2 & 1 & 0 & 0 & 0 & \diagdown & 0 & 0 & 0 & 0 \\ H_3 & 1 & 0 & 0 & 0 & 0 & \diagdown & 0 & 0 & 0 \\ H_4 & 0 & 1 & 0 & 0 & 0 & 0 & \diagdown & 0 & 0 \\ H_5 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & \diagdown & 0 \\ H_6 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \diagdown \end{array}$$

Figure 1.8 Kekulé formula and the bonding matrix of ethanol and dimethyl ether.



$$\begin{array}{c|ccccccc} & C_1 & C_2 & O & H_1 & H_2 & H_3 & H_4 \\ \hline C_1 & \diagdown & 1 & 0 & 1 & 1 & 1 & 0 \\ C_2 & 1 & \diagdown & 2 & 0 & 0 & 0 & 1 \\ O & 0 & 2 & \diagdown & 0 & 0 & 0 & 0 \\ H_1 & 1 & 0 & 0 & \diagdown & 0 & 0 & 0 \\ H_2 & 1 & 0 & 0 & 0 & \diagdown & 0 & 0 \\ H_3 & 1 & 0 & 0 & 0 & 0 & \diagdown & 0 \\ H_4 & 0 & 1 & 0 & 0 & 0 & 0 & \diagdown \end{array}$$

$$\begin{array}{c|ccccccc} & C_1 & C_2 & O & H_1 & H_2 & H_3 & H_4 \\ \hline C_1 & \diagdown & 2 & 0 & 1 & 1 & 0 & 0 \\ C_2 & 2 & \diagdown & 1 & 0 & 0 & 0 & 1 \\ O & 0 & 1 & \diagdown & 0 & 0 & 1 & 0 \\ H_1 & 1 & 0 & 0 & \diagdown & 0 & 0 & 0 \\ H_2 & 1 & 0 & 0 & 0 & \diagdown & 0 & 0 \\ H_3 & 0 & 0 & 1 & 0 & 0 & \diagdown & 0 \\ H_4 & 0 & 1 & 0 & 0 & 0 & 0 & \diagdown \end{array}$$

Figure 1.9 Kekulé formulas and the bond matrices of acetaldehyde and "vinyl alcohol."

Looking at the structures, we might assume that also in this case the compounds are isomers, but in reality, the two structures cannot be separated because they form a dynamic equilibrium mixture of **tautomers** (cf. Chapter 6).[12]

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[12] A relatively exact definition of **tautomers** may be that these are inseparable isomers in a dynamic equilibrium.

Examples in Figures 1.7–1.9 already demonstrate that without the examination of additional features, structures in themselves do not give information about the nature of differences of the entities in question. The inherent difficulty of correlating structure with properties is that structure is a concept at the molecular (*microscopic)* level, while properties are in general "*macroscopic*" manifestations. Difficulties of comparing the two levels can be attributed to two factors: the quantity of material and the time required for the determination of properties.

For the determination of the **amount of substance** (n, mol), it is necessary to know the number (N) of the units (generally atoms or molecules) constituting the substance (Figure 1.10). This can be determined based on the ***Avogadro* constant** (N_A) using the equation $N_A = N/n$. The best value of the experimentally determined value of the *Avogadro* constant is $6.022140857(74) \times 10^{23}$ units/mol [4]. This number is the link between microscopic (at the atomic or molecular level) and macroscopic level of observing natural phenomena.

In order to demonstrate the significance of **time**, it is useful to compare the timescale of molecular vibrations and rotations with the actual time needed to determine the properties of a given substance. On the molecular level, it is the former that characterizes and determines the dynamics of chemical bonds and reactions. The timescale of these motions is in the range of 10^{-10}–10^{-13} s. Femtosecond laser techniques are probably the fastest method of measurement.

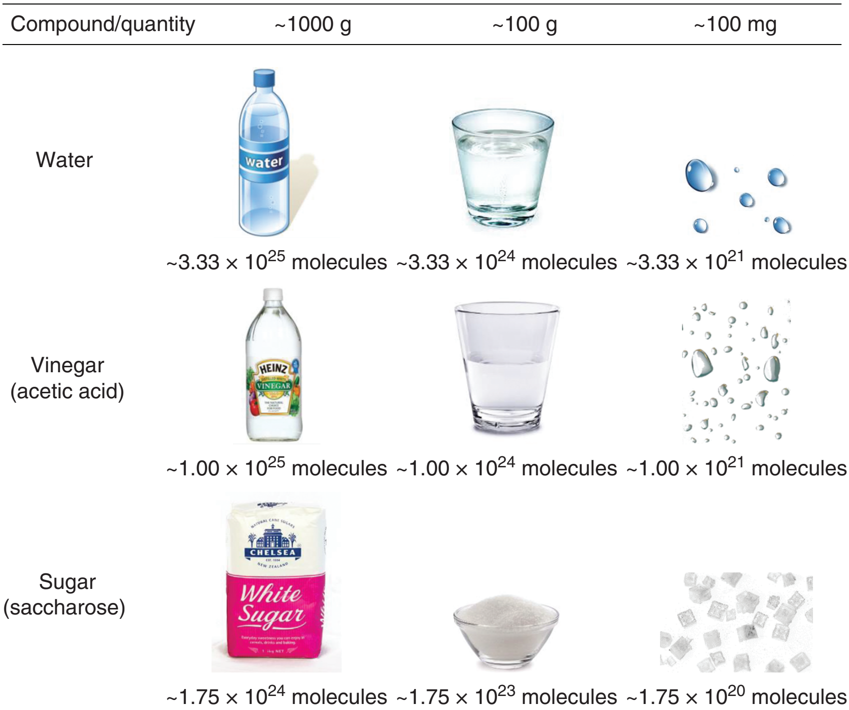

Figure 1.10 Number of molecules in a customary amount of various substances.

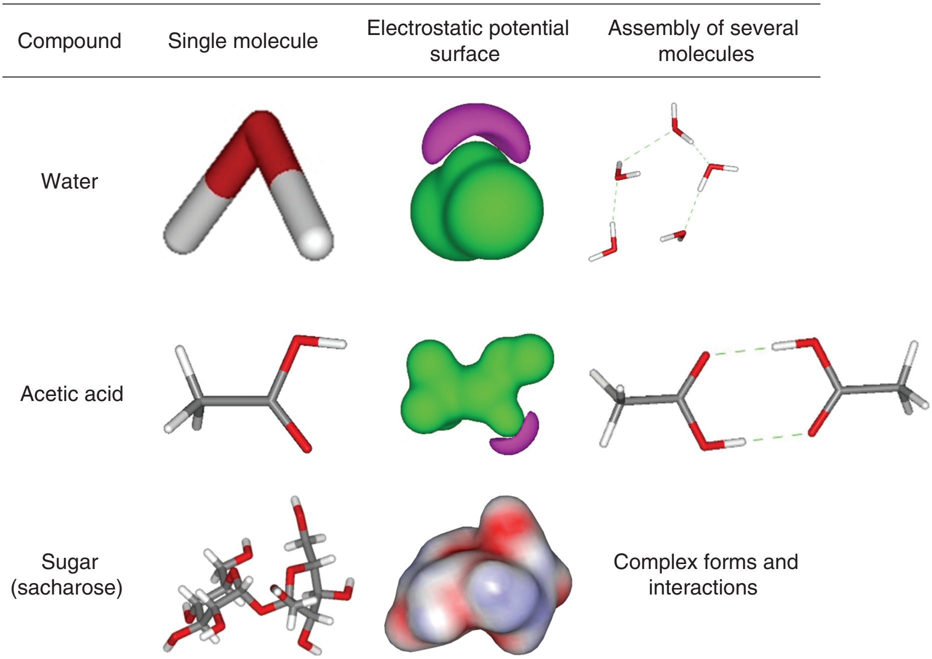

Figure 1.11 Properties of certain well-known compounds at the molecular level.

For elaborating a method capable to study the response of molecules brought into a coherent state of laser irradiation for a few femtoseconds,13) A. H. Zewail was awarded the Nobel Prize (1999).

For the determination of a property on the macroscopic scale (e.g., boiling point, melting point, dielectric constant, heat of combustion, optical rotation, infrared spectrum, and pK_a), usually at least 10 mg of material and 100 s of time are required. It is very enlightening to consider that these quantities and time mean dealing with an assembly of at least 10^{19} molecules and each of this vast number of individual entities undergoes, during the time of measurements, at least $10^{12}-10^{15}$ changes of rotational and vibrational states.

At the same time, when defining our concepts on the microscopic (molecular) level, most often we investigate the properties of a single isolated molecule (Figure 1.11, second column) in vacuum using the methods of quantum chemistry providing structural (energetic) properties, for example, electrostatic potential surfaces (Figure 1.11, third column).

When interpreting structure–property correlations, what sort of molecular assemblies should be considered as uniform is important from the point of view of properties. In general, molecules are taken as the smallest unit of a chemical entity. This interpretation assumes that molecules included in the assembly of

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13) $1\ \text{fs} = 10^{-15}\ \text{s}$.

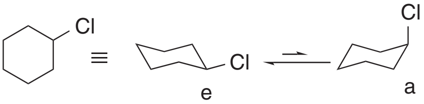

Figure 1.12 Structure of chlorocyclohexane.

a given material are identical/indistinguishable. This assumption is not fulfilled under all circumstances, as illustrated by the example of chlorocyclohexane [5] (Figure 1.12).

Under **normal conditions,**[14] we consider chlorocyclohexane as a single molecule. It is well known, however, that owing to conformational motions[15] chlorocyclohexane is a mixture of conformational states containing the chlorine atom either in an axial or in an equatorial disposition, respectively, as can be demonstrated by observing two different C–Cl bond vibration bands in the infrared spectrum.[16] Nevertheless, from most practical points of views – such as distillation, density, chromatographic behavior, and chemical reactions – chlorocyclohexane behaves as a homogeneous material. Some features of chlorocyclohexane are, however, temperature dependent. For example, at room temperature its ^{13}C NMR spectrum contains, as expected for a single molecule, four different signals, while at $-100\,°$C, eight signals, indicating the coexistence of the two conformations. At this temperature, chlorocyclohexane exists in two clearly discernable molecular states. Whether these molecular states can be distinguished is thus dependent on the temperature and the technique used for their differentiation (isolation, IR, or NMR spectroscopy). At low temperature, for example, $-150\,°$C, the two forms of chlorocyclohexane behave as isomers[17] and can be isolated [6, 7]. It was proposed [8, 9] that substances with interconvertible molecular states should be considered as uniform when the energy barrier separating them is less than kT,[18] while different when it exceeds kT.

An additional difficulty of interpreting structure–property correlations is that looking at individual molecular structures is often insufficient for the assessment of even fundamental macroscopic properties. Characteristics of materials may be significantly influenced by interactions of entities of the same structure and produce assemblies (Figure 1.11, fourth column) significantly differing from the properties of the isolated molecules (Figure 1.11, second column).

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[14] Under *normal conditions*, generally, room temperature and atmospheric pressure are understood. Conditions of observation may be, however, much influenced by latitude and height above sea level.

[15] For a more precise definition of conformation, see Section 2.2.1.

[16] The energy barrier separating the axial and equatorial conformations of chlorocyclohexane is relatively high (~45 kJ mol^{-1}).

[17] For a more precise definition of isomerism, see Section 2.2.2.

[18] In macroscopic systems, with large numbers of molecules, RT value is commonly used. Its SI units are joules per mole (J mol^{-1}): ($RT = kT \cdot N_A$). At room temperature 25 °C (298 K), kT is equivalent to 4.11×10^{-21} J; thus, $kT \cdot N_A = RT = 2.479$ kJ mol^{-1}.

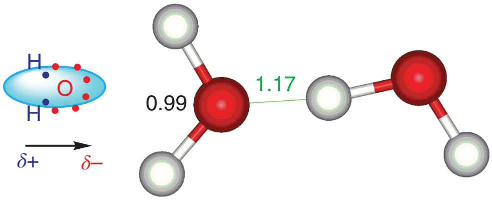

Figure 1.13 Dipolar character of water and the hydrogen bond.

The molecular mass of water ($M = 18$) is, for instance, much lower than that of molecular nitrogen ($M = 28$) or oxygen ($M = 32$), and on the basis of molecular mass, we might infer that at room temperature water is, like air, a gas. This assumption might be confirmed by the fact that hydrogen sulfide having a similar structure but a much higher molecular mass ($M = 34$) than water is under normal conditions a gas. A similar anomaly is encountered when regarding a single isolated molecule of acetic acid. Comparing its molecular mass ($M = 60$) with that of diethyl ether ($M = 74$), we may infer that acetic acid should be more volatile than diethyl ether (bp = 34.6 °C). Similarly, methoxyethane of the same molecular mass ($M = 60$) or n-butane with only a slightly lower molecular mass ($M = 58$) are both gases. Acetic acid ($M = 60$) is, however, a liquid with a rather high boiling point (118 °C) and a freezing point of 16.7 °C.

When instead of individual molecular structures (Figure 1.11, second column) we regard their assembly (Figure 1.11, fourth column), the importance of interactions between individual molecules becomes apparent. Water is namely a neutral molecule but with unevenly distributed positive and negative charges (Figure 1.13). As a consequence, a hydrogen bond19) is established between the oxygen atom with an excess of negative charge and the hydrogen atom of a second water molecule (Figure 1.13).

Formation of hydrogen bonds is possible between molecules in an intra- or an intermolecular way20) (Figure 1.11, fourth column). Formation of intermolecular hydrogen bonds explains the surprisingly high melting and boiling points relative to their low molecular mass of water and acetic acid. Intramolecular hydrogen bonds contribute significantly to the steric structure of peptides and proteins. For instance, a hydrogen atom attached to a nitrogen atom in a peptide bond often forms a hydrogen bond with the carbonyl oxygen of another peptide bond.

19) Among secondary chemical bonds, *hydrogen bond* (*hydrogen bridge*) is the strongest. Its energy is about a tenth of that of a primary chemical bond. For its formation, an element of small dimensions and displaying high electronegativity (first of all O and N) with a nonbonding pair of electrons and a directly attached hydrogen atom is necessary. The hydrogen bond is established between this hydrogen atom and the nonbonding electron pair on the aforementioned other atom.

20) A pragmatic definition of a chemical bond by Pauling [10] is as follows: "… there is a chemical bond between two or more atoms when forces acting between them are such that they result in the formation of aggregates which are sufficiently stable that chemists should deal with them as independent molecular entities."

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