北京高等教育精品教材

BEIJING GAODENG JIAOYU JINGPIN JIAOCAI

应用化学专业英语

第二版

万有志　王幸宜　主编

纪红兵　主审

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《应用化学专业英语》第二版是北京高等教育精品教材，是根据大学英语教学大纲（理工科本科用）的专业阅读部分的要求，受“全国部分高校化工类及相关专业大学英语专业阅读教材编审委员会”委托而编写的，旨在为应用化学专业师生提供一本较系统的专业英语教学用书。

本教材具有以下特点：一、内容选自近年来国外英文原版高等院校化学和化工类教学用书及化学专著，能体现当代专业英语的篇章结构特点和词汇特点；二、题材新颖，文体各异；三、围绕本专业若干重点内容精选阅读材料，覆盖本专业主要研究领域及发展历史、发展趋势；四、内容丰富，共包括五部分 24 个单元，每单元含精读课文、专业词汇（附音标）、课文注释、多种形式的练习和泛读课文。

本教材供已通过大学英语四级的应用化学专业学生及相关专业学生、同等英语水平和相关专业的科技人员使用。

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前　言

《应用化学专业英语》自出版以来，承蒙广大读者厚爱已重印8次。本教材第二版已经获得“北京高等教育精品教材”建设项目立项。笔者在教学过程中不断地探索、总结，多方收集用书教师和学生的意见和建议。为了适应不断变化的教学要求，紧跟科技发展的步伐，同时也弥补初版时的疏漏之处，笔者对初版教材进行了修订，现作为第二版出版发行。修改主要在以下几个方面。

1. 保持原版的编写体例和风格，对素材进行了更新。

2. 增加了化学专业类文章，删减了诺贝尔化学奖颁奖致辞及类似体裁的内容。部分章节的内容进行了修订。考虑到近年来学生英语水平的提高，也删除了一些难度较低的文章。

3. 课后练习中增加了英文原版教材中的练习题，旨在使学生尝试以英文思维方式解决化学问题，加强语感训练。

4. 修订了原版中的部分错漏。

5. 几位教师为本书编写了配套的教师手册（非出版物），供使用该教材的教师参考。内含课文注释相关材料、参考译文、习题参考答案和试题库。用书教师可直接和本书责任编辑（010-64519157）或笔者（yzhwan@mail. buct. edu. cn）联系。

第二版第1～11单元由万有志修订，12～15单元由张丽娟修订，16～24单元由王幸宜修订，全书由万有志统稿，纪红兵主审。

本书的修订得到同仁及化学工业出版社的鼎力支持，北京化工大学王探宇、史汝金、栗婷婷等参与了部分工作，特此致谢。虽然笔者倾力而为，但囿于水平，错漏之处在所难免，敬请广大读者批评指正。

万有志

2008年4月

第一版前言

组织编审出版系列的专业英语教材，是许多院校多年来共同的愿望。在高等教育面向21世纪的改革中，学生的基本素质和实际工作能力的培养受到了空前重视。对非英语专业的学生而言，英语水平和能力的培养不仅是文化素质的重要部分，在很大程度上也是能力的补充和延伸。在此背景下，教育部（原国家教委）几次组织会议研究加强外语教学问题，制定有关规范，使外语教学更加受到重视。教材是教学的基本要素之一，与基础英语相比，专业英语教学的教材问题此时显得尤为突出。

国家主管部门的重视和广大院校的呼吁引起了化学工业出版社的关注，他们及时向原化工部教育主管部门和全国化工类专业教学指导委员会请示后，组织全国十余所院校成立了大学英语专业阅读教材编委会。在经过必要的调研后，根据学校需求，编委会优先从各院校教学（交流）讲义中确定选题，同时组织力量开展编审工作。本套教材涉及的专业主要包括化学工程与工艺、石油化工、机械工程、信息工程、生产过程自动化、应用化学及精细化工、生化工程、环境工程、制药工程、材料科学与工程、化工商贸等。

高等学校理工科本科《大学英语教学大纲》规定，高等学校理工科本科生在完成《大学英语教学大纲》所规定的大学英语基础阶段学习后，从第五学期起要开设必修的专业阅读课。基础英语是专业英语的基础，但专业英语在词汇、语法、句法及文风等诸方面又都带有各自专业的特色。为了使学生毕业后能够更快和更有效地应用英语这一工具为自己的专业工作服务，在授完基础英语之后，再开设相应的专业英语课程是非常必要的。认真总结多年从事专业英语教学的经验，结合本专业的特点，编写出针对性强、质量较高的教材，以提高这门课程的教学质量和教学效率，是当前专业英语教学中亟待解决的问题之一。

本书旨在为应用化学专业提供一本比较系统的专业英语教学用书。在选编课文时，从纵、横两个方面覆盖本专业的相关内容（本专业的发展历史和发展趋势、本专业的知识面和研究领域），体裁包括一般专业论文、著作的前言、鸣谢、颁奖会致辞等。通过阅读该教材，可以对本专业概貌有一个相对全面的了解，包括专业内容和文章体裁。

每单元包括精读课文、词汇表（附音标）、课文注释、练习、阅读材料等。其中精读课文和阅读材料选自近年来国外原版的化学化工类和相关专业的教学用书及专著，内容准确，具有一定概括性，文字流畅，难度适中，能体现现代专业英语的篇章结构特点和词汇特点，使学生在学完本教程之后能顺利阅读应用化学专业的英语资料。

本教材分五部分，共25个单元，内容涉及化学发展史，无机化学（元素及周期表、命名、络合物等），有机化学（有机合成、命名等），物理化学（热力学、动力学、结构化学），专业基础（结晶、蒸馏、物料衡算）等，并附有专业词缀和总词汇表等。内容既注重对专业知识面的覆盖，又照顾专业的历史发展资料，并反映当前最新发展状况和若干重要科技领域（如能源、环保等）。目的是为学生提供阅读素材，通过大量阅读，提高学生阅读英语资料的能力。

高等学校理工科本科《大学英语教学大纲》规定，专业英语阅读阶段的主要任务是：“指导学生阅读有关专业的英文书刊和文选，进一步提高阅读英语资料的能力，并能以英语

为工具，获取专业所需要的信息。”因此，本书以阅读为中心，以获取课文提供的信息为目的，注重对内容理解的准确性。

本书第1～6单元、8～15单元由万有志（北京化工大学）编写，第7单元由张丽娟（北京化工大学）编写，第16～25单元由王幸宜、荣国斌（华东理工大学）编写。全书由万有志统稿，钟理（华南理工大学）主审。

本书在编写过程中，许多同志提出了宝贵建议，并得到他们的鼎力支持和热情帮助，华东理工大学王秀环同志参与了第16～25单元的材料收集、编排以及练习、注释的编写等工作，特此表示真挚的谢意。

本教材获“北京化工大学化新教材建设基金”资助。

虽经多次补充和完善，但限于编者水平，书中谬误、不足之处在所难免，恳请广大读者指正。

编　者

2000年2月

CONTENTS

PART ONE
CHEMISTRY AND SOCIETY

Unit 1 The Roots of Chemistry

Chemistry can be broadly defined as the science of molecules and their transformations. In contrast to mathematics, chemistry is older than people. The appearance of life and people on our planet (Earth) is most probably the end result of specific chemical processes. Chemical processes have been present in the lives of people from the dawn of history until the present time. Initially, these processes were not under our control, for instance, the fermentation of fruit juice, the rotting of meat and fish, and the burning of wood. Later on we learned to control chemical processes and to use them to prepare a variety of different products such as food, metals, ceramics and leather. In the development of chemistry, four periods may be distinguished: prehistoric chemistry, Greek chemistry, alchemy, and scientific chemistry.

The early beginnings of chemistry were clearly motivated by the practical needs of people. The discovery of fire offered the first opportunity to prehistoric people to carry our controlled chemical processes. They learned to prepare objects made of copper, bronze and other materials that were readily available. Since the use of chemical processes by these early people predates writing there are no written records about their chemical skills. One can judge their chemical abilities only from the archeological discoveries of various artifacts. What has been found indicates clearly that practical needs influenced the early development of chemistry, as was the case for the early development of mathematics. But chemistry and mathematics at this stage probably did not interact. If they did, there is no record to establish this.

Greek chemistry was based mainly on speculation rather than on experiment. This was a common trait of all Greek science in antiquity. The Greek scientist of antiquity was in fact the Greek philosopher, and so it is not surprising that the Greeks were much more interested in contemplating than in experimenting. Actually they seldom performed experiments outside of the thought experiment. This was a good approach for mathematics but hardly one to recommend itself for the physical, chemical or biological sciences. Nevertheless, because the Greeks thought a lot about the nature and structure of matter, they can be considered as the creators of the first chemical theories.

The Greeks introduced the concept of the element and proposed in all four elements. Thales (625—547 BC) of Miletus thought that all things were formed from one elementary substance, namely water. Anaximenes (ca 585—ca 528 BC), also from Miletus, accepted the idea of element, but he believed that the single element from which all things are made is air. Heraclitus (ca 540—480 BC) of Ephesus, who considered that the fundamental characteristic of the universe is continuous change, regarded fire as the element that embodied perpetual change. Empedocles (ca 490—ca430 BC), from the Greek city of Akragas in Sicily, abandoned the idea of a single element and introduced the principle of four elements: water, air, fire and earth, and the two forces of attraction and repulsion that operate between them. Empedocles is also known for his experimental proof that air is a material body.

The term "element" was first used by Plato (428—347 BC) who assumed that the particles of each element have a specific shape, even though such particle are too small to be seen. Thus, the smallest particle of fire had the shape of a regular tetrahedron; of air a regular octahedron; of water a regular icosahedron, and of earth a cube (or regular hexahedron).[2] The regular tetrahedron, the regular octahedron, the regular icosahedron and the cube are examples of regular polyhedra, and there are in all five of them; the fifth is the regular dodecahedron. In regular polyhedra the surfaces are bounded by congruent regular polygons and the vertices are symmetrically equivalent to one another.

Fire was thought to be the smallest, most pointed and lightest among the elements because it can easily attack and destroy. It seemed a natural choice that the regular tetrahedron (which consists of four regular triangles) be taken as the shape of fire, since it is the smallest and most pointed among the regular polyhedra. Water was the largest, smoothest and heaviest, because it always flows smoothly into the valleys of the Earth. Therefore, it appeared a natural choice that the regular icosahedron, composed of twenty regular triangles, was taken as its shape. Air is between fire and water and so it appeared natural to assign the regular octahedron (which consists of eight regular triangles) to air. The regular octahedron has the same faces, viz. the regular triangles, as the regular tetrahedron and the regular octahedron. Its numbers of faces is between the numbers of faces of those two. From the fact that the tetrahedron, octahedron and icosahedron could be decomposed into regular triangles which could be reassembled to form the other polyhedra, Plato concluded that fire, air and water could also be mutually transformed, that is, water could be transformed by fire into air, whereas when air loses fire in the upper atmosphere it becomes water in the form of rain or snow. The last element was earth which is heavy and stable, and this was assumed to take the shape of a cube, composed of six squares. Since it was not possible to reduce the cube into regular triangles, but only into squares, Plato concluded that earth could not be transformed into fire, air or water. This is discussed in Plato's dialogue *Timaeus*. In the dodecahedron, because, of all the regular polyhedra, its volume most nearly approaches that of the sphere, Plato saw the outer shape of the universe. The *Timaeus* also contains discussion on the composition of organic and inorganic bodies and may be considered as a rudimentary treatise on chemistry. At this point it should be perhaps emphasized that Plato taught that the idea, the form, was the truly fundamental pattern behind phenomena, that is to say, ideas are more fundamental than objects.

Plato's description of the shapes of the four elements was perhaps the first mathematical model used in chemistry, since regular polyhedra are mathematical objects. The regularity that exists between the numbers of vertices $\boldsymbol{V}$, edges $\boldsymbol{E}$ and faces $\boldsymbol{F}$, was discovered by Euler (1707—1783) and is thus called the Euler theorem.

This states that:

$$\boldsymbol{V}+\boldsymbol{F}-\boldsymbol{E}=2$$

Which is considered by some to be the second most beautiful mathematical theorem? It is of interest to speculate why the Greeks did not discover Euler's theorem. Perhaps the simplest explanation is that Greek mathematics was two thousand years away from topology.

Topology ("rubber sheet geometry") is the part of mathematics that deals with the way objects are connected, without regard to "straightness" and metric.

A generalization of the above ideas on elements was put forward by Aristotle (384—322 BC). He accepted the idea of four elements, but introduced the concept of transmutation of elements. Aristotle thought that the elements could be obtained by combining the pairs of opposing fundamental properties of matter. These properties were hotness, coldness, moistness and dryness. The combination of hotness and moistness produced air. Moistness and coldness gave water and, similarly, coldness and dryness produced earth. Aristotle added the fifth element or quintessence, ether. The sky and heavenly bodies were supposedly made up of this fifth element. Aristotle defined an element as simple body that other bodies can be decomposed into but one that is not itself capable of being divided into simpler bodies.[3] He classified several chemical processes, first mentioned mercury and was familiar with the technique of distillation.[4] Aristotle's ideas dominated science for almost two thousand years.

There was another theory on the structure of matter put forward by Greek thinkers. This was concerned with the divisibility of matter. The first Greek philosopher to think about this problem appears to have been Leucippus (ca 470—420 BC) from Miletus. He came up with the proposition that matter cannot be divided endlessly, for in the process of dividing matter one will sooner or later come to a piece not divisible into smaller parts. His pupil Democritus (ca 460—ca 370 BC), from Abdera, continued to develop the ideas of Leucippus. He named these ultimately small pieces of matter *ατομοσ* (atomos), meaning indivisible. This is the origin of our term atom. The concept of the atom is the basis of the atomic theory of the structure of matter and the philosophy of materialism. Most Greek philosophers, and particularly Aristotle, did not accept the atomistic teachings of Leucippus and Democritus. Atomism, however, did not die out because Epicurus (ca 342—270 BC) made atomism part of his philosophy, and Epicureanism won many followers over the next few centuries. One of these was the Roman poet and philosopher Lucretius (ca 96—55 BC), who wrote a fine didactic poem entitled *De Rerum Natura* (On the Nature of Things) in which he expounded the atomistic teachings of Democritus and Epicurus. Most of the works by Democritus and Epicurus are lost, but Lucretius's poem has survived intact and has served to convey the atomistic teachings of the Greeks to modern times. The splitting of the atom and the advent of the atomic bomb have surely confirmed what an excellent model of reality atomistic theory was.

The philosophy of idealism and the philosophy of materialism were opposed throughout history. From a chemical point of view the philosophy of materialism affords a basis for an understanding of the structure of compounds. However, the collective properties of compounds such as their smell or color or taste can also be interpreted in terms of Plato's ideas, which are particularly well suited for studying the mathematical properties of chemical structures. If we link the philosophy of materialism with experimental work in chemistry and likewise the philosophy of idealism with theoretical work, it is clear that both philosophies as well as both experiment and theory are needed to advance chemistry. This is of course also true for other sciences.

Alchemy is a type of chemistry that existed from about 300 BC until the second half of the seventeenth century. This constitutes a less interesting period for our purposes, since alchemists were practical people who did not care much for theories and mathematics. The alchemists had two main objectives: (ⅰ) to turn base metals into gold and (ⅱ) to discover the elixir of life. The origins of alchemy can be traced back to the ancient Egyptians.

There was a lot of magic involved in the work of alchemists and their symbols were difficult to decipher. However, the coding systems used by various alchemists are really cryptograms and as such possess a mathematical basis.

It is important to stress that chemistry as a science started only in the second half of the seventeenth century when alchemy gradually transformed itself into the science now known as chemistry following the appearance of the book *The Sceptical Chymist* (London, 1661) by Boyle (1627—1691).[5] The transition period from alchemy to chemistry lasted more than a century. It started with Boyle's book and ended with the book *Traité Élémentaire de Chimie* (Elementary Treatise on Chemistry, Paris, 1789) by Lavoisier (1742—1794). During this period appeared the first unifying chemical theory, namely, the phlogiston theory. The term phlogiston is derived from the Greek word φλογιστοσ, which means flammable.

Now, most dictionaries define chemistry as ***the science that deals with the composition, structure, and properties of substances and the reactions by which one substance is converted into another***. Knowing the definition of chemistry, however, is not the same as understanding what it means. In essence, ***chemistry is an experimental science***. Experiment serves two important roles. It forms the basis of observations that define the problems that theories must explain, and it provides a way of checking the validity of new theories. This text emphasizes an experimental approach to chemistry. As often as possible, it presents the experimental basis of chemistry before the theoretical explanations of these observations.

From *Concepts in Chemistry by N. Trinajstic*
and *Chemistry: Structure and Dynamics by James N. Spencer*

New Words and Expressions

fermentation [ˌfəːmen'teiʃən] *n.* 发酵
ceramics [si'ræmiks] *n.* 制陶术，陶瓷学，陶瓷制品
leather ['leðə] *n.* 皮革，皮革制品
alchemy ['ælkimi] *n.* 炼金术，炼丹术
bronze [brɔnz] *n.* 青铜（一种铜锡合金），青铜制品
archeological [ˌɑːkiə'lɔdʒikəl] *a.* 考古学的
artifact ['ɑːtifækt] *n.* 人工制品
speculation [ˌspekju'leiʃən] *n.* 思索，推测
antiquity [æn'tikwiti] *n.* 古代，古人，古迹
Thales ['θeiliːz] *n.* 泰利斯（古希腊哲学家，数学家，天文学家）
tetrahedron ['tetrə'hedrən] *n.* 四面体
octahedron [ˌɔktə'hedrən] *n.* 八面体
icosahedron [ˌaikəusə'hedrən] *n.* 二十面体
hexahedron [ˌheksə'hedrən] *n.* 六面体
polyhedra [ˌpɔli'hiːdrə] (polyhedron的复数形式) *n.* 多面体
theorem ['θiərəm] *n.* 定理，原则
topology [tə'pɔlədʒi] *n.* 拓扑学，拓扑
Aristotle ['æristɔtl] *n.* 亚里士多德（古希腊哲学家）
elixir [i'liksə] *n.* 长生药，万能药
decipher [di'saifə] *v.* 解开（疑团），破译（密码）
cryptogram ['kriptəugræm] *n.* 密码，暗记，暗号

flammable [ˈflæməbl] *n.* 易燃物 *a.* 易燃的，可燃的
phlogiston [flɔˈdʒistən] *n.* 燃素

Notes

1. as作关系代词时可代替整个主句或一件事（上文或下文所说的事），并在从句中作主语、宾语或表语。as引出的定语从句为非限制性定语从句。本句在从句中作主语。参考译文：已有事实清楚地表明：正如早期数学的发展一样，实际需要影响着化学的发展。

2. of air与a regular octahedron之间、of water与a regular icosahedron之间、and of earth与a cube之间均省略had the shape of。参考译文：所以，火的最小微粒具有正四面体形状，气的最小微粒具有正二十面体的形状，土的最小微粒具有立方体（或正六面体）形状。

3. 参考译文：亚里士多德把元素定义成一个简单的物体，其他的物体能被分解成元素，而元素本身不能被分解成更简单的物体。

4. 句中classified，mentioned，was familiar with为并列成分，主语均为He。参考译文：他对数种化学过程进行了分类，第一个论及汞，并通晓蒸馏技术。

5. 参考译文：化学是在17世纪后半叶才开始被称为一门科学的，强调这一点很重要。因为当时炼金术才逐渐将其本身转变为科学，随着Boyle（1627—1691）所著的书*The Sceptical Chymist*（1661年，伦敦）的出现。这种科学被看作是化学。

Exercises

Ⅰ. Comprehension

1. It can be inferred from this article which one of the following items is not mainly based on practical use ____.

A. prehistoric chemistry and alchemy B. alchemy and chemistry
C. Greek chemistry D. Greek chemistry and chemistry

2. It was ____ who first introduced the idea that all things are not formed from just one element.

A. Aristotle B. Empedocles C. Theatetos D. Theodoros

3. In the development of Greek chemistry, ____ was the first one definiting the ultimately constituents of matter?

A. Plato B. Aristotle C. Leucippus D. Democritus

4. According to Plato, there are ____ "elements" whose faces are constituted by regular polygons.

A. 3 B. 4 C. 5 D. 6

5. In the last paragraph, authors think that experiment ____.

A. can examine whether the assumption is right
B. can be used to check the new theories
C. can be carried out by the chemist
D. can deal with the reactions by which one substance is converted into another

Ⅱ. Make a sentence out of each item by rearranging the words in brackets

1. The purification (is usually/a matter of considerable difficulty, /often/of an organic compound/for this purpose/to employ various methods/it is/necessary/and).

2. Science is (is generated/and systematized knowledge/an ever-increasing body of accumulated/and is also an activity/by which knowledge).

3. Life, after all, is (in fact, /a small example of chemistry/observed on a single, /only chemistry, /mundane planet).

4. People (some of the molecules/are made of molecules; /in people are rather simple/are/highly complex/whereas others).

5. Chemistry is (from birth to death/ever present in our lives/there is neither life nor death/because without chemistry).

6. Mathematics appears (and also permeates/to be almost as humankind/all aspects of human life, /are not fully/although many of us/aware of this).

Ⅲ. Translation

1. (a) 化学过程；(b) 自然科学；(c) 蒸馏技术。
2. 正是原子构成了铁、水、氧等。
3. 化学具有悠久的历史，事实上，人类的化学活动可追溯到无记录时代以前。
4. 根据水的蒸发现象，人们认识到液体在一定条件下可以变成气体。
5. 在你使用这种材料之前，你必须弄清它的各种性质。

Ⅳ. Translation

Chemistry is one of three fundamental natural sciences, the other two being physics and biology. Chemical processes have continually unfolded since the Big Bang and are probably responsible for the appearance of life on the planet Earth. One might consider that life is the end result of an evolutionary process in three steps, the first step being very fast and the other two rather slow. These steps are (ⅰ) physical evolution (the formation of chemical elements); (ⅱ) chemical evolution (the formation of molecules and biomolecules); and (ⅲ) biological evolution (the formation and development of organisms).

Ⅴ. Problem

(1) The absolute mass of a ^{1}H atom is 1.6735×10^{-24} grams, whereas the absolute mass of a ^{12}C atom is 1.9926×10^{-23} grams. Calculate the ratio of the mass of a ^{1}H atom to that of a ^{12}C atom when the masses are measured in units of grams. Use this ratio to calculate the mass of a ^{1}H atom in units of amu if the mass of a ^{12}C atom is exactly 12 amu.

(2) A bone taken from a garbage pile found buried deep under a Turkish hillside had a $^{14}C/^{12}C$ ratio 0.477 times the ratio in a living plant or animal. What was the date of the prehistoric village in which the bone was discovered?

Reading Material

What is Modern Molecular Structure About

One of the more fundamental issues chemistry addresses is molecular structure, which means how the molecule's atoms are linked together by bonds and what the interatomic distances and angles are.[1] Another component of structure analysis relates to what the electrons are doing in the molecule; that is, how the molecule's orbitals are occupied and in which electronic state the molecule exists. For example, in the arginine molecule shown in Fig. 1.1, a HOOC— carboxylic acid group is linked to an adjacent carbon atom which itself is bonded to an $—NH_2$ amino group. Also connected to the α-carbon atom are a chain of three methylene $—CH_2—$ groups, an —NH— group, then a carbon atom attached both by a double bond to an imine —NH group and to an amino $—NH_2$ group.

The connectivity among the atoms in arginine is dictated by the well-known valence preferences displayed by H, C, O and N atoms. The internal bond angles are, to a large

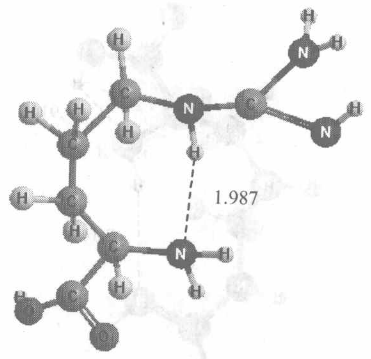

Fig. 1. 1 the arginine molecule in its non-zwitterion form with dotted hydrogen bond

extent, also determined by the valences of the constituent atoms (i. e. , the sp^3 or sp^2 nature of the bonding orbitals). However, there are other interactions among the several functional groups in arginine that also contribute to its ultimate structure. In particular, the hydrogen bond linking the α-amino group's nitrogen atom to the —NH— group's hydrogen atom causes this molecule to fold into a less extended structure than it otherwise might.

What does theory have to do with issues of molecular structure and why is knowledge of structure so important? It is important because the structure of a molecule has a very important role in determining the kinds of reactions that molecule will undergo, what kind of radiation it will absorb and emit, and to what "active sites" in neighboring molecules or nearby materials it will bind. A molecule's shape (e. g. , rod-like, flat, globular, etc.) is one of the first things a chemist thinks of when trying to predict where, at another molecule or on a surface or a cell, the molecule will "fit" and be able to bind and perhaps react. The presence of lone pairs of electrons (which act as Lewis base sites), of π orbitals (which can act as electron donor and electron accepter sites), and of highly polar or ionic groups guide the chemist further in determining where on the molecule's framework various reactant species (e. g. , electrophilic or nucleophilic or radical) will be most strongly attracted. Clearly, molecular structure is a crucial aspect of the chemists' toolbox.

How does theory relate to molecular structure? As we discussed in the Background Material, the Born-Oppenheimer approximation leads us to use quantum mechanics to predict the energy E of a molecule for any positions ({R(a)}) of its nuclei given the number of electrons N_e in the molecule (or ion). This means, for example, that the energy of the arginine molecule in its lowest electronic state (i. e. , with the electrons occupying the lowest energy orbitals) can be determined for any location of the nuclei if the Schrödinger equation governing the movements of the electrons can be solved.

It often turns out that a molecule has more than one stable structure (isomer) for a given electronic state. Moreover, the geometries that pertain to stable structures of excited electronic states are different than those obtained for the ground state (because the orbital occupancy and thus the nature of the bonding is different). [2] Again using arginine as an example, its ground electronic state also has the structure shown in Fig. 1. 2 as a stable isomer. Notice that this isomer and that shown earlier have the atoms linked together in identical manners, but in the second structure the α-amino group is involved in two hydrogen bonds while it is involved in only one in the former. In principle, the relative energies of these two geometrical isomers can be determined by solving the electronic Schrödinger equation while placing the constituent nuclei in the locations described in the two figures.

If the arginine molecule is excited to another electronic state, for example, by promo-

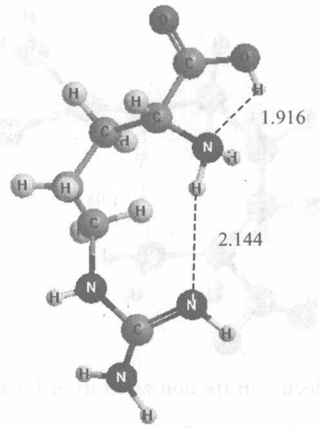

Fig. 1. 2 another stable structure for the arginine molecule

ting a non-bonding electron on its C═O oxygen atom into the neighboring C—O π* orbital, its stable structures will not be the same as in the ground electronic state. In particular, the corresponding C—O distance will be longer than in the ground state, but other internal geometrical parameters may also be modified (albeit probably less so than the C—O distance). Moreover, the chemical reactivity of this excited state of arginine will be different than that of the ground state because the two states have different orbitals available to react with attacking reagents.

In summary, by solving the electronic Schrödinger equation at a variety of geometries and searching for geometries where the gradient vanishes and the Hessian matrix has all positive eigenvalues, one can find stable structures of molecules (and ions). [3]The Schrödinger equation is a necessary aspect of this process because the movement of the electrons is governed by this equation rather than by Newtonian classical equations. The information gained after carrying out such a geometry optimization process includes (ⅰ) all of the interatomic distances and internal angles needed to specify the equilibrium geometry and (ⅱ) the total electronic energy E at this particular geometry.

From *An Introduction to Theoretical Chemistry by Jack, Simons*

New Words and Expressions

arginine [ˈɑːdʒiniː(ː)n] *n.* 精氨酸
carboxylic [ˌkɑːbɔkˈsilik] *a.* 羧基的
adjacent [əˈdʒeisənt] *a.* 邻近的，接近的
methylene [ˈmeθiliːn, -lin] *n.* 亚甲基
imine [ˈimiːn, -in; iˈmiːn] *n.* 亚胺
amino [ˈæminəu] *a.* 氨基的
zwitterions [ˈtsvitəraiən] *n.* 两性离子
electrophilic [iˌlektrəuˈfilik] *a.* 亲电（子）的
nucleophilic [ˌnjuːkliəuˈfilik] *a.* 亲核的，亲质子的
isomer [ˈaisəumə] *n.* 异构体
gradient [ˈgreidiənt] *n.* 梯度，倾斜度
vanish [ˈvæniʃ] *vi.* 消失，变成零
matrix [ˈmeitriks] *n.* 矩阵

eigenvalue [ˈaigənˌvælju:] *n.* 特征值
Newtonian [nju:ˈtəunjən, -niən] *a.* 牛顿的，牛顿学说的

Notes

1. 这是一个名词性从句，which 引导的句子用来说明 molecular structure。参考译文：很多化学文章讨论的基本论点之一就是分子结构，也就是说，分子中原子是怎样通过化学键、分子间距和键角连接在一起的。

2. 参考译文：然而，用于描述电子激发态稳定结构的几何学与那些用于描述基态几何学是不相同的（因为占据轨道与成键的性质是不同的）。

3. solving 和 searching 是并列成分。参考译文：总体上说，通过对不同几何构型的电子薛定谔方程求解，寻找梯度变为零和赫赛函数矩阵均具有正特征值的几何构型，可以找出分子（和离子）的稳定结构。