Atomic Structures and Bonding

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INTRODUCTION

This Unit will tie together the way atoms bond chemically, using the three types of chemical bonds to form three-dimensional shapes. These three bonds are then arranged, defined and used to explain the formation of the seven different crystal systems, or three-dimensional patterns. These crystalline shapes are then placed into a unit cell and arranged to fit the space as compactly as possible. The atoms inside the unit cell are then dissected for percentage of particular atom inside (or outside) the unit cell box. These percentages are then used to determine the "coordination number" of the ions used to form the crystalline structure. This information is then used to determine the chemical formula of the particular compound selected. These seven different crystal systems will be drawn using the AutoCAD Program Release 12 so that the actual crystalline structure can be rotated to allow examination in detail from any angle or side.

The normal way of teaching this unit is to present the individual topics in a lecture format, draw the structures and bonds as two-dimensional representations, and then allow the students to build three-dimensional models from stick and ball sets (or using any material the student can find). The rotation of the angles and the sides of the three-dimensional model are expected to be supplied by the imagination of the student from the two-dimensional information provided by the instructor. This unit will point out the uses of the AutoCAD Program Release 12, now available commercially, which will accommodate this information in a three-dimensional display that can be rotated, inverted, manipulated, or shaped in any way to show any desired chemical bond, structure, crystal or unit cell model. This will present to visual or concrete learners a new way to actually see and comprehend the topics cited above. With this look into the structures, the average student will be able to visually rotate the structure into any configuration needed to explain the theory taught by the instructor. In addition gifted learners will be able to expand their understanding and extrapolate their simple ideas into the complex, with a visual representation to refer to while expanding their insight into the atomic structure they are studying.

Chemical bonding and structural analysis of compounds

The theoretical explanation of chemical bonding of a molecule or compound is usually taught by using the lecture format. The actual representation of the bond is often abstract, or as a representative two-dimensional stick and ball drawing, or a poor three-dimensional isometric picture on a blackboard. The student is expected to visualize the areas that can not be seen. The resulting lapses in their visualization of the abstract concept is a frustration for the average student. The typical bond can also be displayed as a dot diagram (or a pictograph) after the Lewis Electron Pair Model of bond formation, which again leads to lapses in visualization of the bonding concept. These models are not clear to the average student because of these two-dimensional pictographic structural limitations.

The transfer of the electrons form one atom to another is also represented as a dot or *e*- on the board. This dissociation of charge from its atom is then explained as the valence charge that is transferred in the typical chemical formulas that are written to balance chemical equations. To the average student this can again be more confusing than helpful when we attempt to show how models are limiting in the typical science class that uses the stick and ball models. The ability to visualize the structures that are arranged around the atoms due to these areas of charge is severely hampered in the two-dimensional drawn models. The ability to make and then see a three-dimensional model is often the concrete example that the average student needs. The available model kits manufactured commercially are never differentiated enough to accommodate the structure of the atom's *e*- configuration. These kits are three-dimensional but not representatively three-dimensional to the atomic theory we are currently teaching. The assignment of model building using Styrofoam balls is also not representative above the original molecule or compound because of the limited ability to hold the multiple balls and sticks rigid in spatial bonds and stabilize the large structures that the complex molecules and compounds would require.

The advent of computer graphics programs has freed the Chemistry instructor to look at the three-dimensional nature of molecules, compounds and various crystalline structures they make to explain the concepts being introduced. These computer models can then be rotated, inverted or turned inside out to reveal their internal and external morphology. This allows the instructor to rethink the theoretical concepts into true three-dimensional models with endless vistas of presentation and avenues of explanation for the various students taught.

The average student today understands the computer and its application. The ramifications of the programs and the matrices they produce will allow the mentally abstract visualizer to see on the screen the structures that the teacher is explaining. It also allows the average student, who is often a concrete learner, to see displayed a model that will allow the student (or teacher) to rotate the image created through the x,y,and/or z axis of rotation. If the learner wishes to hold one reference fixed, then the model can be rotated through 360 degrees in the x and y axis or the x and z axis. Thus is created a model free to rotate in two planes of rotation at the same time. This gives the student (teacher) a model that can be rotated through 720 degrees of rotation for any single observation of that image. Therefore a model can now be visualized in any orientation the theory requires and will allow all students to see the models theorized in the teachers lectures.

Several potential applications of the drawing software, AutoCAD, will be presented in this unit, including the construction of a three-dimensional Periodic Table, and the building of molecular and crystal structures.

The program will allow the learner to select the size, shape and color of each atom used in the program. The atoms can be arranged to allow the student to create a periodic chart that they can then manipulate to help them in their understanding of the elementary periodicity observed in nature. The student can then expand the periodic chart in three dimensions in such a way that it can capture the elements in any pattern the learner chooses to display them. In particular, they can be arranged in a particular manner to help explain or visualize the topic the teacher is addressing. For example, the valence electrons can be arranged in a configuration that demonstrates the bonding configurations in a particular compound under examination. This will help in the identification of the bonds in the compounds and molecules the student is studying.

From these visualized bonding studies, the beginning of crystallization of the atomic world can be taught. The ability to see into the patterns of the atoms as they continue to bond and form compounds and macromolecules is possible only in the computers of today. The ability to recognize the structure and pattern type of an individual crystal is beyond the scope of the two-dimensional drawings or stick and ball models of yesterday.

The ability to create the crystalline pattern to infinite dimensions is a simple command, called array, in the AutoCAD Program. This command allows the student to “grow” a three-dimensional drawing into any size desired instead of copying what was there endlessly. This command is different from the old “copy” in that it allows the student to grow a crystal in any dimension (x,y,z) or at any angle he selects.

The ability to then break down and examine the crystalline structure into its unit cells is a bonus of this program. This enables the instructor to demonstrate the chemical species’ inherent atomic structural pattern as a chemical formula. The bonds used in this chemical formula can then be isolated and examined to determine the type and structure of each bond that contributes to the compound or molecule. The individual bond (ionic, covalent, metallic, and Van der Waal) lengths can be preset in the program to help the students to identify the way their compound or molecule is bonded together. These preset lengths can also be used to determine a typical unit which can be used to determine the unit formula for the molecule or compound under studying. We can then place the molecule or compound within this unit cell and determine the chemical formula for any compound or molecule.

Demonstrating the unit cell inside a stick and ball model requires the use of many different models. The inability to slice a quarter or eighth of an atom to demonstrate the amount in a unit cell, and hence a chemical formula, was a deterrent to the average student. The average students were then unable to correctly determine the chemical formula for the compound or molecule under examination. The recognition of the compound NaCl as being cubic with one eight of a Na and one eighth of a Cl in alternating corners of the cubic model was not easily demonstrated or drawn by the instructor. The AutoCAD Program allows dissection of the individual atoms within the unit cell and thus calculation of the part they are contributing to the particular chemical formula under analysis. The average students never grasp this fundamental concept and this explains why the school district has dropped this requirement for their average students. Only the more advanced math student could usually visualize this concept and they are the only ones being offered this concept in their curriculum today. The computer makes the creation of the unit cell, and the partial atoms within, visible to the average student. This makes it possible for them to visualize the species and its subparts involved in the chemical bonds. Thus the average students can now once again study and comprehend this complicated concept.

The outcome of this unit will be to create a program that will show a chemistry instructor how to find and use new computer programs to show how atoms and bonds are used to create the world around us. These programs will be used to demonstrate the chemical world in a real time three-dimensional fashion that can give them immediate feed back from all their students in a visually useful way. The instructor will be able to explain through rotating three-dimensional models the bonding characteristics of different types of atoms and bonds within the crystalline structures needed to create the macroscopic world.

ACTIVITIES

The first day is the introductory lecture. This will review students over the historical trends of chemistry and the principles taught in Integrated Physics and Chemistry (Physical Science, in the past). This introduction should should only be included if the students have not demonstrated an understanding of the basic tenets of the Integrated Physics and Chemistry Course or if they never had the Integrated Physics and Chemistry Course. The topics mastered or reviewed should include the development of the Atomic Theory from the Greek Atomic Model of Democritus to the final Atomic Theory of John Dalton. The ten laws of atomic theory as taught by Dalton should be explained and eventually elaborated into the new theories of the quantified atomic theory.

The discovery of the quantum effect and the ideas of Max Planck should be explained in relationship to the new discoveries about to be made in the liberation of energy from the atom itself. The realization that the atom could be split into three parts and the attempted explanations given by Thomson, Rutherford, and Bohr to explain this division could or should be the culmination of the first day.

The second day should begin with a review, or introduction, of the Bohr Atomic Model. The development of this theory explains the way atoms bond according to their valence structures. These valence structures are the explanation of the octet rule. This octet rule explains the need to complete the electron configuration of the atoms by creating different types of chemical bonds. The ability to form a ionic, covalent or metallic bond is determined by the position of the atom in a particular group of atoms on the periodic chart. These atoms are arranged on the chart in A and B groups that make it easy to visualize how atoms must complete their octet of valence electrons. Thus the different types of bonds made by atoms make in this attempt to reduce or increase the number of valence electrons maybe introduced.

The third day the students will review writing and balancing the different types of chemical equations as part of a lecture and modeling of balancing techniques at the board. The different types of bonds formed in each type of reaction are then determined as either ionic, covalent, metallic, or Van der Waal in nature. The student can determine the bond strength and affinities for each type of bond, by reviewing the periodicity principle from the periodic chart. The students can then examine the different types of models possible to aid in this introduction or be required to draw the bonds using the Lewis Dot Model. The students can then create their own models from different student-acquired materials that represent the different types of bond and atomic structures they are required to make. The student can also log onto the Internet and discover elementary web sites that display this information.

On days four to seven, the students will perform different chemical experiments that allow the different types of reactions to occur and interpret the outcomes of each lab analytically. The students will identify any crystalline structure that forms in the precipitate and attempt to determine the correct formula. The student can use a magnifier or a stereoscope to examine the precipitation products of these reactions. The student can also attempt to simulate the crystals formed in the computer to compare them to the real models.

On the eighth day, the students will create models of these bonds and molecules using the stick and ball sets. The different bonds are then allowed to expand into different sized compounds and molecules. The students can also use an organic model kit and construct various types of molecules of organic nature that use only covalent bonds.

In the past students have used the ball-and-stick and Styrofoam models to represent their individual bond types, the molecule or compound formed, and the resultant possible crystalline patterns. From these models the students would attempt to grow expanded crystalline structures. Since it is impossible to do this in this fashion, the students always failed and this added to their frustration with chemistry.

Eventually they were required to cut one of these Styrofoam crystals and attempt to put it in a unit cell to determine the actual chemical formula of the compound or molecule being studied. This was never a very realistic project and the students seldom accomplished this activity.

COMPUTERIZED STRUCTURES

The actual implementation of the system described above is a tedious series of boring lectures. These are followed by a few nondescriptive activities that may or may not show the desired effect. The effect of the too few actual experiments that produce good results are clouded by the bad ones. The average student fails to grasp the concept, the purpose of the activity or the experimental results of the good lab experiment. The evolution of this into the AutoCAD Program is to guide the instructor into a visualization of the topic and develop a way for the average student to develop an understanding of a complex topic. The outcome should produce the model that freely shows the atoms, their bonds, the crystalline structures they form, and the unit cell embedded in them. Even the average student will be able to explore the ramifications of the program and recognize the chemical principle being expressed in it. The actual AutoCAD Program Release 12 is available for a few dollars and easily installed in any personal computer with 25 MB of storage. The program is accessible enough to allow the average student to begin drawing set models of three-dimensional structures as soon as they turn it on. This program can create an immediate bridge between the drafting, technical arts, and design drafting course work taught at any high school. The ability to combine such different disciplines will attract additional students and instructors to assist in the design of these programs. The ability to create a three-dimensional graphic that rotates about the three principle axis of rotation, while displaying angles of different proportions, is excellent. The student is able to create the several different atomic models of the crystalline pattern within the first hour of instruction. The ability to change these models is the main reason this program is so useful to both students and teachers.

The ability to color, delineate size and shape, and bond atoms makes this program a natural choice for chemists. The ability to change the model in the computer in real time teaches the concepts of bonding and structure while reinforcing and modeling the outcomings at the same time. This ability to define the different structures and new subparts allows us to naturally pick this program to model the unit cell and the way that the atomic parts are arranged in the cell. The subset can be isolated without interference from the rest of the model or delineated in the structure drawn. The crystals formed in this program can then be used to show the growth rate and direction of crystalline structure through the array command. The applications of the program are only limited by the imagination of the user.

This program will only enhance the students' ability to use the knowledge and expertise of their instructor as never before. They will be able to finally draw and see the structures that were only suggested previously.

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Lab 16 Shapes of Covalent Molecules and Polarity: This lab reviews the way hybridized orbitals bond together to form Molecules. It shows the student how to predict molecular polarity .

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Will help to explain the development of the periodic chart and its trends.

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Lab 19 Molecular Shapes and Structures are explored through model sets and the Lewis Dot Theory.
Lab 20 Properties of Some Representative Elements are explored and reinforced through the study of the periodic chart
Lab 21 Classes of Chemical Reactions will be determined by the type of bond formation exhibited by the atoms involved. These will be reduced to the specific type of reaction pattern they conform to in nature.

Super Models from Ryler Enterprises. Ryler Enterprises, Inc. P.O. Box 881 West Chester, OH. 45071-0881
They sell different types of stick and ball model sets from Buckyball to general coordination chemistry.

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Develops the effect of the transfer of the electron from one substance to another as an electric change that occurs because of the reaction and the side affect possible with different vessels that are used to contain the reaction

Wilbraham, Anthony C., Dennis D. Staley, C.J. Simpson and Michael S. Matta. *Chemistry: Laboratory Manual*. New York: Addison-Wesley, 1987.
Page 50, Lab 6: Allows the student to use inductive reasoning to explain the internal structure of atoms and bonds they form.
Page 147, Lab 24: Demonstrates and allows the students to develop the atomic theory used to explain the periodicity used on the periodic chart today.
Page 153, Lab 25: Explains the geometry of crystal structures using Styrofoam balls.
Page 157, Lab 26: Develops the structure ideas of bonding using stick and ball models.
The last three labs are exceptional for use with concrete or visually impaired learners, who need positive and immediate reinforce of their learning.

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Page 287, Chapters 7-9: This is a college-level discussion of the way atoms bond, the types of bonds formed and the reason they bond that way only. This is a serious discussion for abstract learners only.
Page 941, Chapter 20: This is the most intense discussion of coordination chemistry I have read in years. It highlights the who, what, when, where and how of bonding in a coordination compound.

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These are inexpensive sets of the various stick and ball models described and used in the labs presented in the paper.
Acids and Bases Model Set (#G15158) $22.55 - shows student how
to construct models that illustrate the molecular basis of acids and bases.
Atom Building Game (#G1913081) $139.95 - helps student understand the atom and different chemical properties.
Atomic Mobiles (#G11155) $34.95 - materials to construct models of the first 36 elements as mobiles.
Atomic Modelic Kit (#G21855) $95.20 - represents concept of space-filling electron clouds.

Atomic Models Set (#G19146) $118.95 - shows students the interrelationship of protons, electrons, and neutrons.
Basic Magnetic Atomic Model Set (#G1900575) $71.40 - students can build various molecules with magnetic spheres.
Basic Structures Model Kit (#G15934) $63.45 - provides materials for the construction of molecular and crystal structures.
General Chemistry Model Kit (#G15937) $61.25 - an intodutory model making kit.
Inorganic and Organic Chemistry Kit (#G15935) $60.95 - advanced molecular kit for organic and inorganic molecules.
Orbital Set (#G16408) $207.50 - provides materials for the study of orbital configurations.