Instructions

George C. Lisensky

to accompany the

Polyhedral Model Kit

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Contents

Getting Started

This kit will allow you to build models of a great many crystal structures. By examining the models you can learn where atoms are located and how to visualize three-dimensional crystal lattices. The model kit makes complex structures easy to build and see.

☛ To get started, open the box and examine the parts, identified and shown on page 4, Model Kit Parts. Assemble the units as shown on page 5, Assembling the Units. Read and master the introductory materials on pages 7-9, "Why Polyhedra?" and "What You Need to Know." Then you are ready to build some representative structures such as NaCl (page 10), ZnS (page 12) and $Al_2(OH)_6$ (page 14).

For instructions on building additional models see

http://mrsec.wisc.edu/Edetc/pmk

Preface

The breathtaking speed with which science and engineering are advancing reflects our increasing sophistication in understanding how the structures of solids influence their physical and chemical properties. These structures have taken on enhanced significance with the many recent exciting advances in materials and nanoscale science and engineering. From an educational perspective, the three-dimensional extended structures that are characteristic of many of these solids are particularly challenging to visualize.

This Polyhedral Model Kit was developed to complement the ICE Solid-State Model Kit, which, since 1994, has allowed teachers and students to investigate the three-dimensional structures of solids that comprise the world around us. Using spheres, rods, and templates, the ICE Solid-State Model Kit permits construction of solids whose atomic arrangements are guided by sphere packing. Many of these same solids can be represented in a powerful, alternative way by linked polyhedra. This new kit also allows one to build less symmetric structures not possible using sphere packing. The ability to shift between these different viewing perspectives is an important pedagogical objective, as it can produce new insights into structure-property relationships. The Polyhedral Model Kit provides the means to investigate these important spatial relationships.

There are many opportunities for integrating the Polyhedral Model Kit into the curriculum. It can be used to build many structures that would commonly be discussed in science and engineering courses such as chemistry, chemical engineering, geology, environmental science, materials science, soil science, and physics.

This kit owes its conception and original implementation to the eminent solid-state chemist, A. F. Wells. Nearly fifty years ago, Wells convincingly demonstrated the power of polyhedral models to create simple and complex structures. The authors are grateful to Drs. M. Stanley Whittingham of Binghamton University and Terrell A. Vanderah of the National Institute of Standards and Technology for bringing the kit to their attention and to Dr. Wells' family for permission to re-release the kit. Advances in polymer science and computer-aided design and manufacturing have resulted in this enhanced version of the kit.

The Polyhedral Model Kit serves as part of the educational infrastructure for an effort, supported by the National Science Foundation and the Camille and Henry Dreyfus Foundation, to integrate materials and nanoscale science and engineering into the curriculum. The guidance and advice of Retlaw Industries has been invaluable in manufacturing this educational product. Ryan Nygard designed the cover art for the kit.

While many individuals contributed to the realization of this Kit, including Phillip Barak, Mithra Beikmohamadi, Cindy Carter, Olivia Castellini, Tony Cina, Keenan Dungey, Andrew Greenberg, Janice Hall, Robert Lichter, Ken Lux, John Moore, Don Neu, Jim Rougvie, Matt Vander Zanden, Jen Walz, and Greta Zenner, it is our pleasure to acknowledge especially the many teachers and students around the country who auditioned the Kit and whose comments have greatly enhanced its effectiveness.

We hope that you enjoy and learn from the Kit, and we welcome your comments and suggestions.

Wendy C. Crone
Arthur B. Ellis
George C. Lisensky

About the Kit

Safety

Please exercise normal care in handling the plastic pieces and connectors; while they are sturdy, they can be broken. The kit should be kept away from small children, who might accidentally ingest the small parts.

Protecting Your Kit

Use and store the kit in a dry environment: water could damage the cardboard box; organic solvents can attack the plastic parts. Keep the plastic pieces away from excessive heat which could damage the parts or soften the connectors.

Allowed Uses

Since some users may wish to incorporate the directions for building a model into their own written materials for students, permission is hereby granted for such use, provided that it is for local, non-commercial distribution. Anyone considering for-profit reproduction of any of these images or of the model-building directions must obtain written permission from the Institute for Chemical Education.

Checking the Model

This booklet contains computer-generated illustrations of some of the structures. Since these images are static, they do not serve as a substitute for the models; to see all features of a structure, the model must be built. The companion web site to this model kit shows interactive views of the models and can be used both for building structures and checking their accuracy.

http://mrsec.wisc.edu/Edetc/pmk/

Living Product

We encourage the development of new structures. If you devise new structures, let us know (lisensky@beloit.edu), and we will try to include the structures in the on-line manual.

Funding

We are grateful for funds from the National Science Foundation through Materials Research Science and Engineering Center (MRSEC) on Nanostructured Interfaces (DMR-9632527, DMR-0079983 and DMR-0520527) and The Camille and Henry Dreyfus Foundation.

Inspiration

This model kit was inspired by a kit originally prepared in the 1960s by A. F. Wells, the author of *Structural Inorganic Chemistry,* Oxford University Press.

Field Trials

The model kit has been used in field trials by the following individuals and their chemistry and geology classes: Mike Condren (Christian Brothers University), Keenan Dungey (U. of Illinois-Springfield), Bill Durham (University of Arkansas), Maggie Geselbracht (Reed College), George Lisensky (Beloit College), Karen Nordell (Lawrence University), James Rougvie (Beloit College), Mark Van Baalen (Harvard University), Eric Voss (Southern Illinois University-Edwardsville). We thank these individuals and their students for helpful contributions.

Model Kit Parts

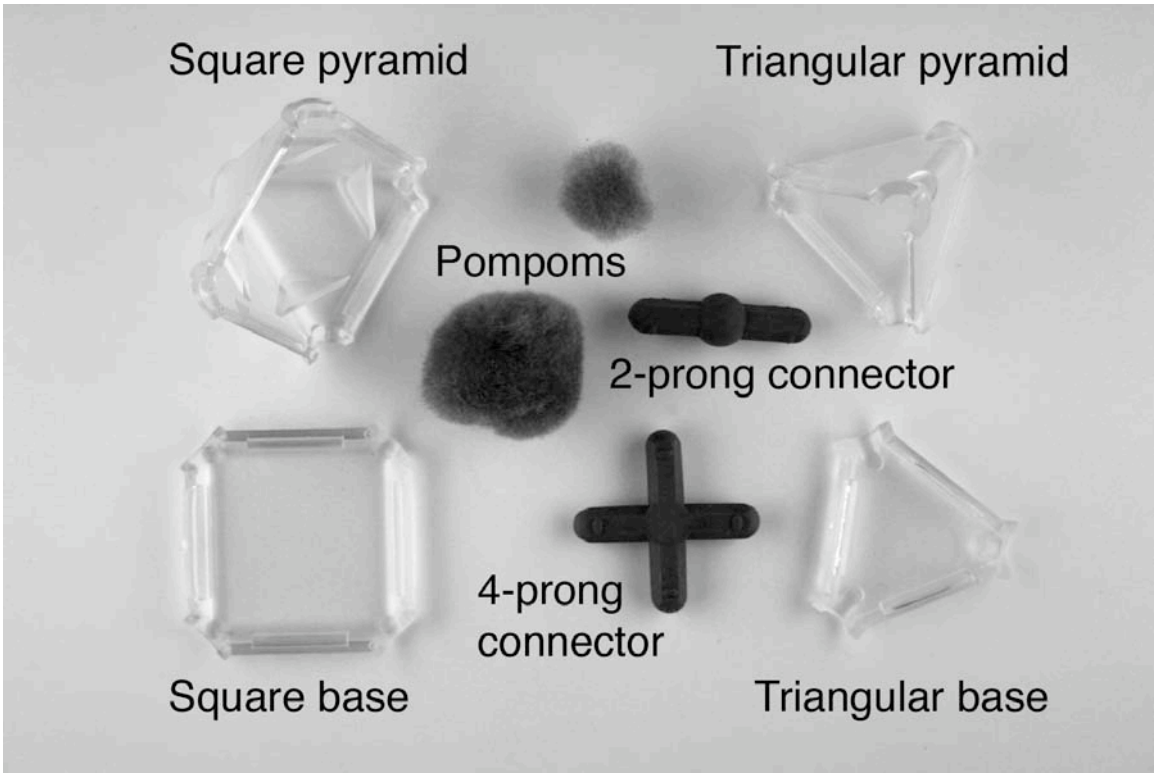


Figure 1. Unassembled Units

Triangular pyramid (tetrahedron top)	60	Blue pompoms (1/2")	100
Triangular base (tetrahedron bottom)	60	Assorted pompoms (1/2")	100
Square pyramid (octahedron half)	180	Yellow pompoms (1")	100
Square base (square half)	60	Assorted pompoms (1")	100
2-prong connector	230		
4-prong connector	230		

These pieces permit assembly of 60 tetrahedral units, 78 octahedral units, 24 square pyramidal units, and 18 square planar units. Two or three kits are adequate for 20 students working in small teams, especially if larger structures are built by teams working together.

The blue pompom is normally used as the center atom for the tetrahedral units. The yellow pompom is normally used as the center atom for the octahedral units. Additional assorted colors are provided to represent more than one kind of atom (see Table 1 on page 17.)

See the directions on the next page to assemble the pieces into structural units that can be used for model building. A movie showing the units being prepared is at

http://mrsec.wisc.edu/Edetc/pmk/preparation.html

Assembling the Units

Assembling tetrahedral units.
Put a 1/2" blue pompom (or other color if desired) in a triangular pyramid. Snap a triangular base onto the triangular pyramid to form tetrahedral pieces. Note the alignment pins on the parts. It is generally easier to align one edge and then use that edge as a hinge to fold the parts together. Substantial pressure must be applied to snap the pieces together.

Assembling octahedral units.
Put a 1" yellow pompom (or other color if desired) in a square pyramid. Snap two square pyramids together to form octahedral pieces. Note the alignment pins on the parts. It is generally easier to align one edge and then use that edge as a hinge to fold the parts together. *Be sure to reserve 24 square pyramids for assembling square pyramidal units.*

Assembling square pyramidal units.
Put a 1" pompom in a square pyramid. Snap the square base onto the square pyramid to form square pyramidal pieces. Note the alignment pins on the parts. It is generally easier to align one edge and then use that edge as a hinge to fold the parts together.

Assembling square planar units.
Put a 1/2" pompom in a square base. Snap a square base onto the square base to form square planar pieces. Note the alignment pins on the parts. It is generally easier to align one edge and then use that edge as a hinge to fold the parts together.

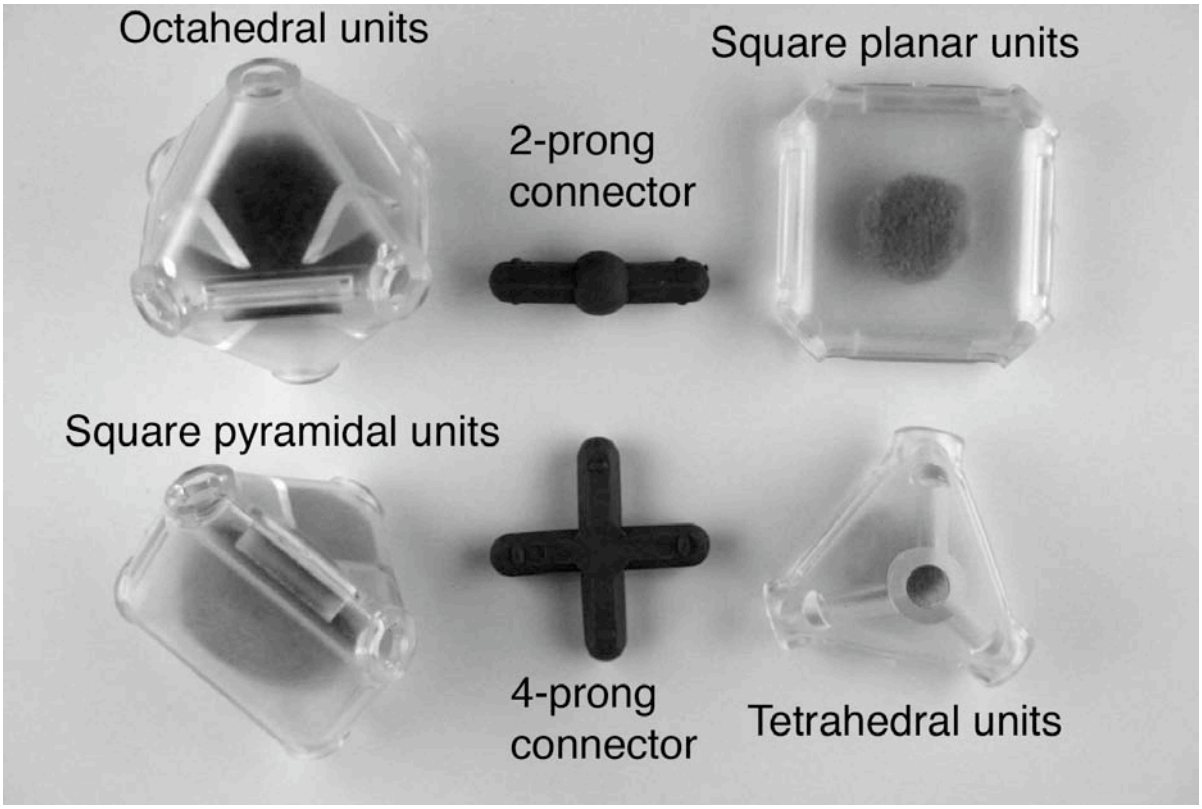


Figure 2. Assembled units

Choosing connectors

Which connector to use is not a critical issue and the choice is not specified in the directions. In general the 2-prong connector works well with the tetrahedra and the 4-prong connector works well with the octahedra. In some structures six vertices meet and a 6-prong connector would be ideal. In this case you will need to use the 4-prong connector and leave some vertices adjacent but unconnected. Again the choice of which vertices to connect is not critical but can be guided by the need to hold layers together.

To disassemble a unit

While not a routine step, disassembly can be done a few times without damage to the pieces. Insert a pointed cylinder such as a pencil or pen into the opening next to a joint (not the apex of the square or triangular pyramid piece) and pry off the base. Reassemble as before, perhaps with a different color pompom inside.

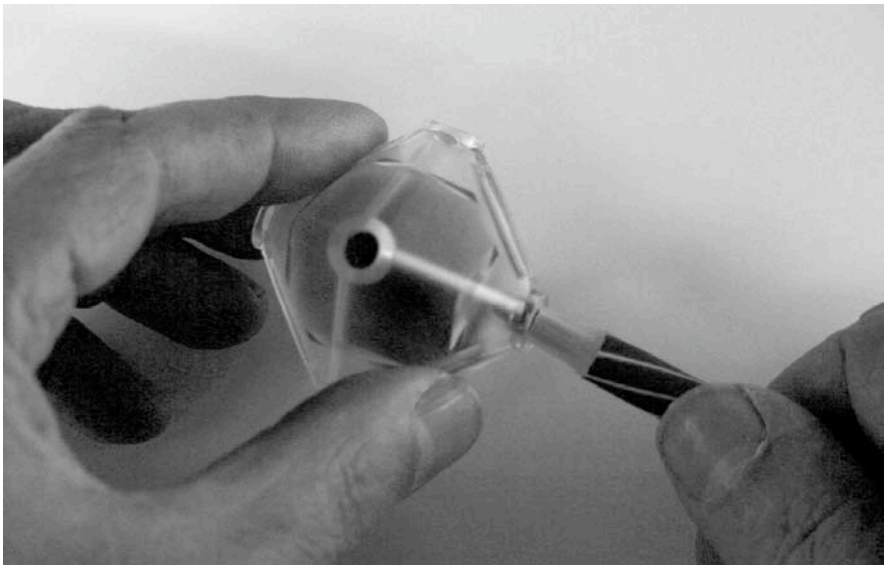


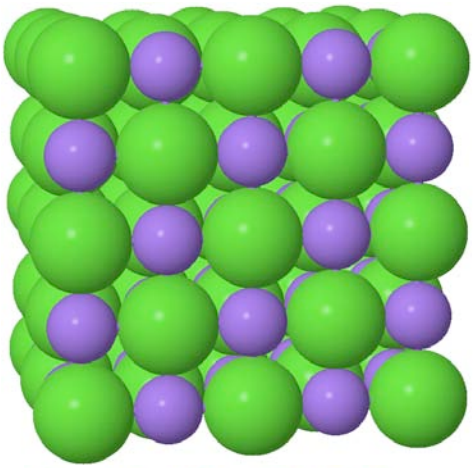
Figure 3. Unit disassembly.

Introduction: Why Polyhedra?

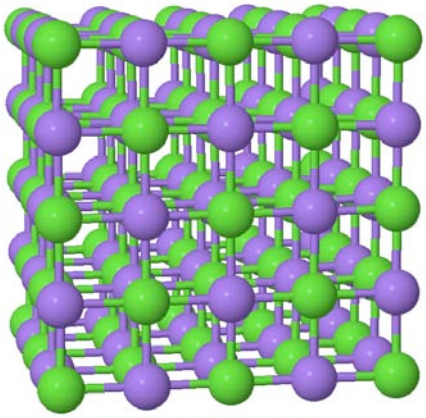
Most simple inorganic compounds consist of atoms that alternate indefinitely rather than existing as discrete molecules in the solid state. The formula of a molecule gives the actual number of atoms in the molecule. How do we give the number of atoms in a solid? In such cases the empirical formula is used as the chemical formula.

An example is NaCl which does not consist of just one sodium ion and just one chloride ion. Rather, in NaCl each sodium ion is surrounded by an octahedron of chloride ions and each chloride ion is surrounded by an octahedron of sodium ions in an extended structure. There are multiple ways to represent the structure of such a solid.

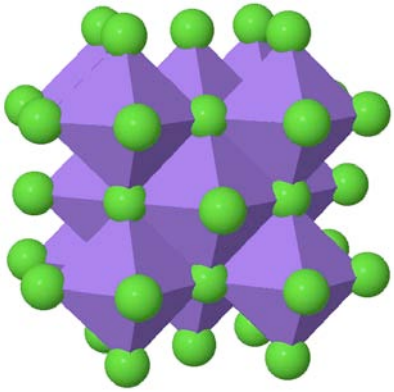
The space-filling model is best for showing relative atom sizes and how the atoms fill space.



The ball-and-stick model is best at showing distances and angles. The sticks do not represent localized electron bonds in this ionic solid.



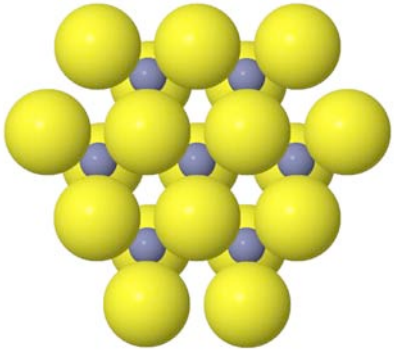
The polyhedral model, where a cation surrounded by its anions is represented by a single polyhedron, is useful for visualizing how structural components fit together. Only atoms belonging to complete polyhedra are shown.



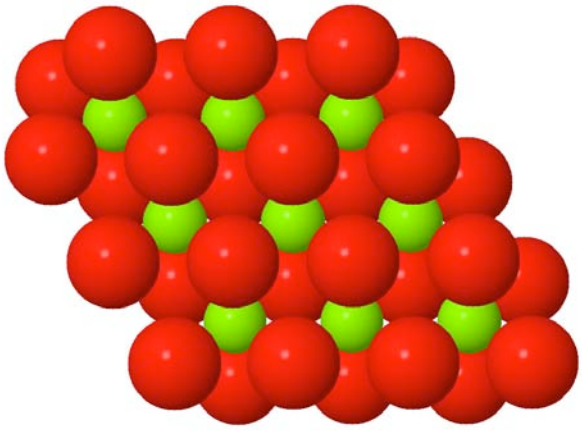
All of the figures on this page show the same structure at the same scale. Which is easier to describe?

What You Need to Know

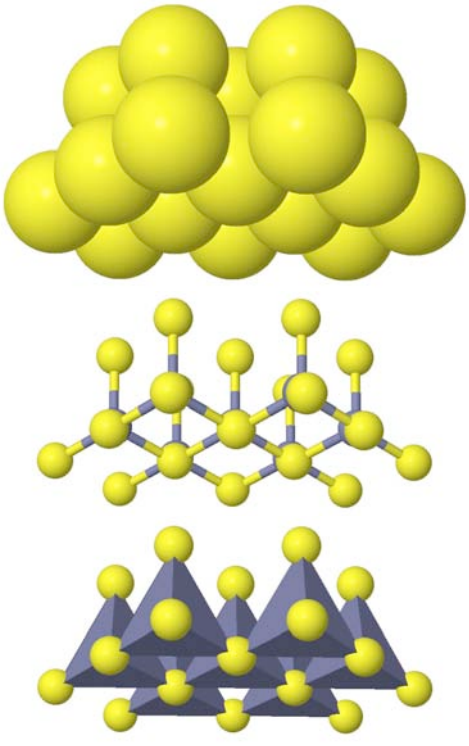
Anions are generally larger than cations. Many solids can be viewed as a close-packed array of anions with the spaces between the anions occupied by cations. Those spaces have tetrahedral and octahedral geometries – the same geometries as the structural units in this model kit.



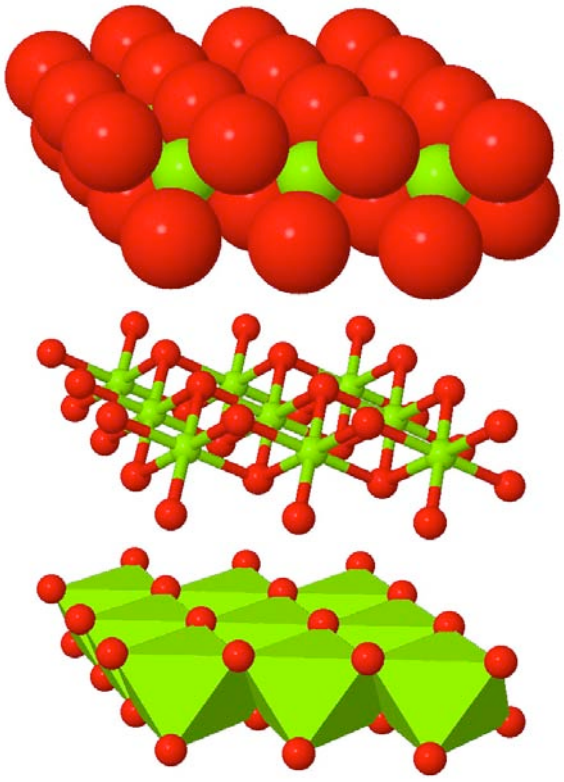
Tetrahedral spaces between two anion layers in the zinc blende, ZnS, structure.



Octahedral spaces between two anion layers in the brucite, $Mg_3(OH)_6$, structure.



Side view of two anion layers in the zinc blende, ZnS, structure. Which representation best helps you to visualize the structure?



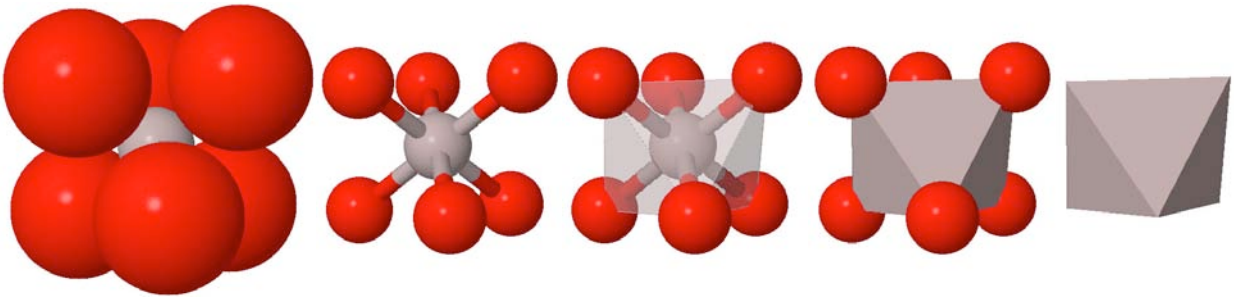
Side view of two anion layers in the brucite, $Mg_3(OH)_6$, structure. Which representation best helps you to visualize the structure?

Since in some respects all of these representations are valid, the important question is not really which representation is correct. What is important is what you can learn from each and that using multiple representations will enhance your visualization and understanding of the structure.

Models are designed to represent some features of the world. Models that show arrangements of atoms have their limitations, since atoms are not spheres and bonds are not sticks. Polyhedral models are designed to show how atoms arranged in structural units such as tetrahedra and octahedra fit together. *Because they consist of structural units instead of individual atoms, polyhedral models can be assembled quickly. By focusing on units larger than atoms, patterns in complex structures can be more easily discerned.*

Since models are simplifications they also introduce errors. This is not a problem if you remember that models are just models and you realize the following.

1. In most cases the cations in this model kit are located at the center of the polyhedron and the anions are located at the corners of the polyhedron. The edges of the polyhedra do not represent bonds but do serve to define the polyhedral shape. Because the connectors that hold adjacent polyhedra together are at the corners, they can be thought of as representing atoms or ions.



Which of these best represents an octahedral arrangement of atoms? For what purpose? Close packed arrays of oxide ions are the basis of many mineral structures and are important for understanding geochemistry. Geochemists routinely use the representation at the far right.

2. Anions are generally larger than cations. (See the discussion at the beginning of this section.) This means that the atom represented by the colored pompom at the center of the polyhedron is actually *smaller* than the atoms represented by the corners of the polyhedron. The space-filling view (above left) more correctly indicates relative ion sizes.

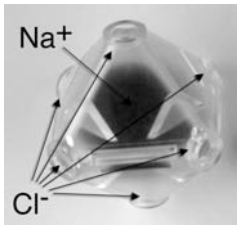
3. The tetrahedra and octahedra in this model kit are highly symmetric. In real crystals all six anions surrounding a cation may not be at the same distance and not all the bond angles may be the 90° expected for an octahedron. Four anions surrounding a cation may not be a perfect tetrahedron or even square planar. The models you build will however be close enough to help you visualize the atomic relationships that are more accurately shown in the illustrations. The computer-generated illustrations in this manual and in its online companion are based on actual atomic positions determined by x-ray crystallography.

4. The tetrahedra and octahedra in this model kit come in only one size. Real crystals can be constructed from many different elements with different degrees of ionic and covalent bonding, resulting in variations in atomic size. The computer-generated illustrations in this manual and in its online companion are based on average ionic radii for the observed coordination number and oxidation state as assigned by Shannon and Prewitt based on x-ray crystallographic data (*Acta Cryst.*, **A32**, 751 (1976) and *J. Amer. Chem. Soc.*, **111**, 5707 (1989)). In our illustrations we have, however, used an ionic radius for H^+ of 0.5 Å (0.05 nm or 50 pm). This too-large value was chosen so that hydrogen could still be observed in the space-filling view. Again the models you build are to help you visualize the atomic relationships that are more accurately shown in the illustrations.

NaCl Example

Names: Sodium chloride, Halite or Rock Salt.

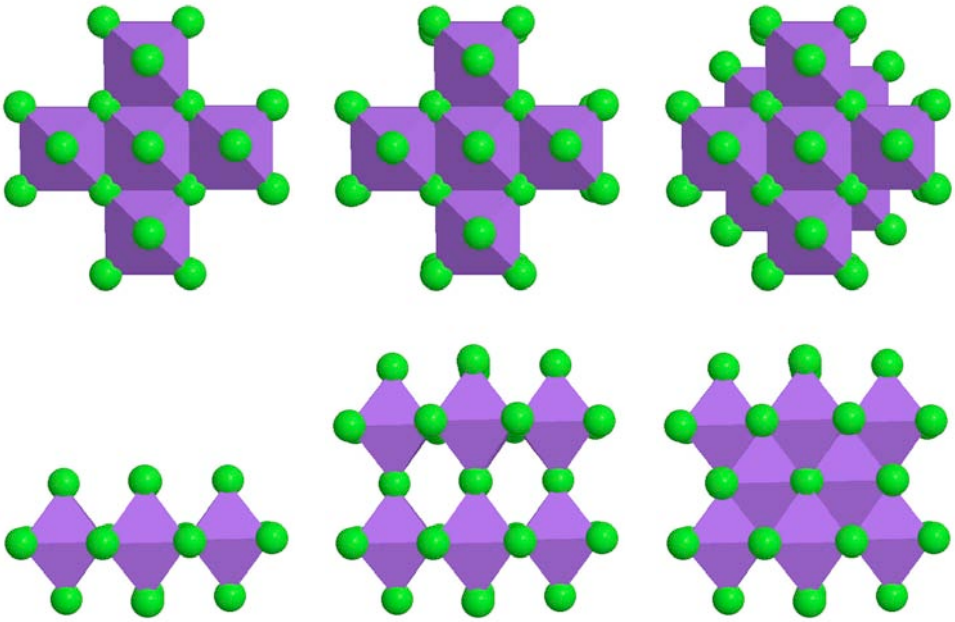
This structure is built from octahedral units. The pompom inside represents a sodium ion and the clear octahedron represents six chloride ions in an octahedral arrangement around the sodium.



Construction

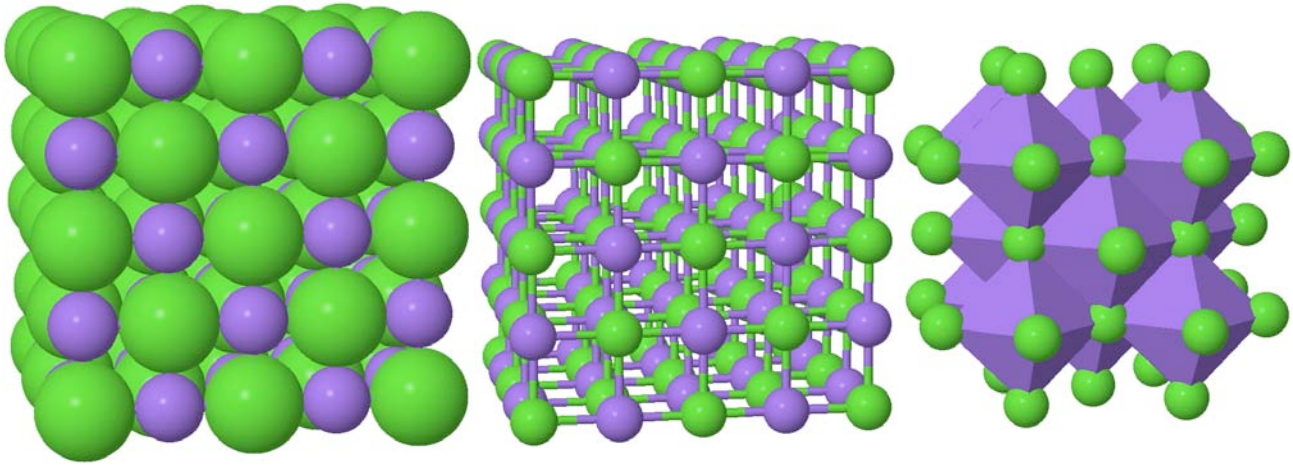
Top view

Side view



1. Build an edge-shared octahedral layer.
2. Build another octahedral layer directly on top of the first layer.
3. Fill in all the space between octahedral layers to form a middle octahedral layer.

Alternate representations for this structure (all views show identical structures):



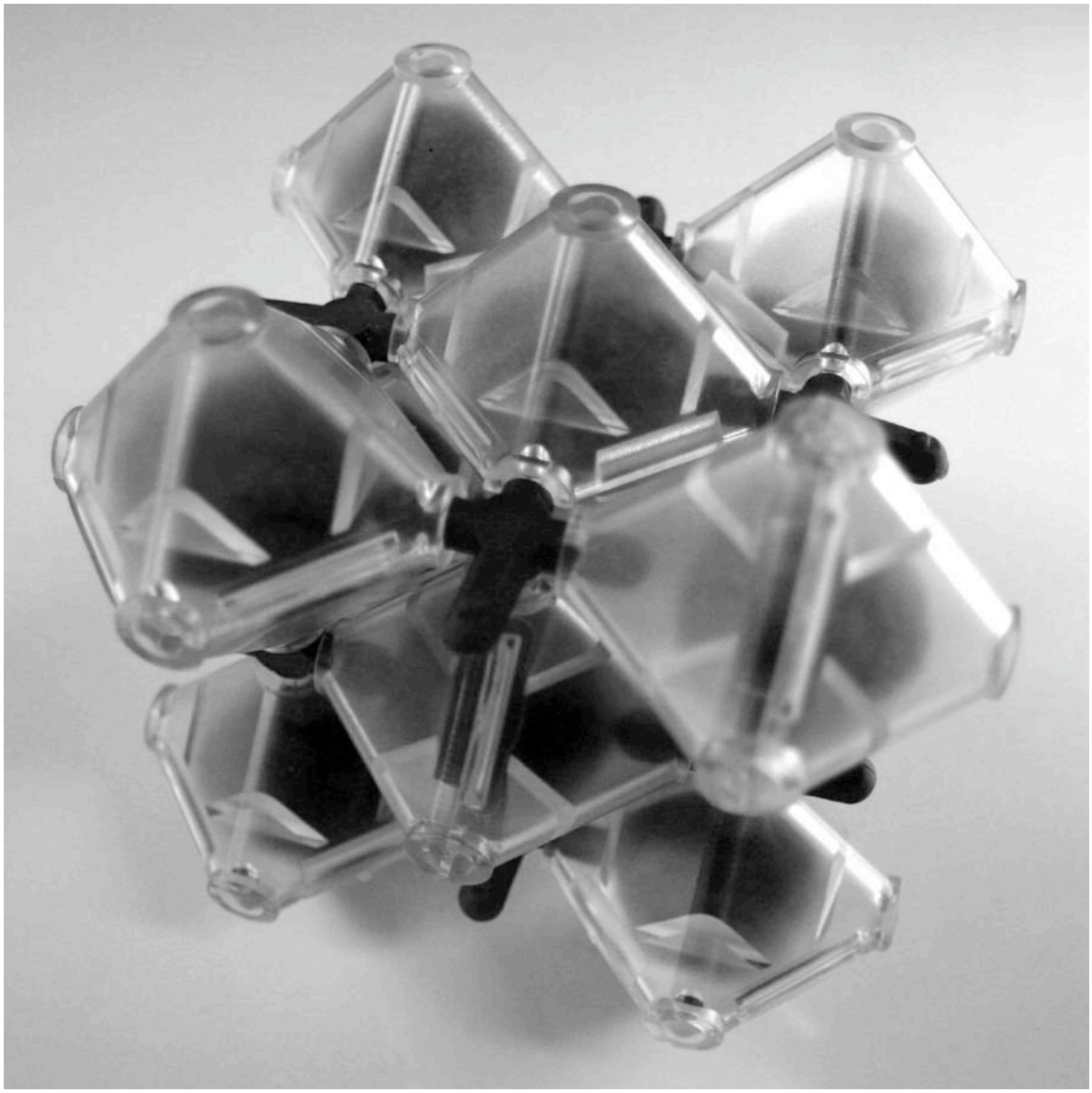
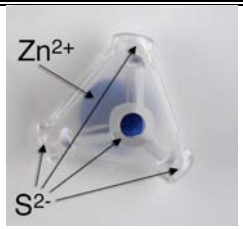


Figure 4. Polyhedral NaCl model assembled using the kit.

ZnS Example

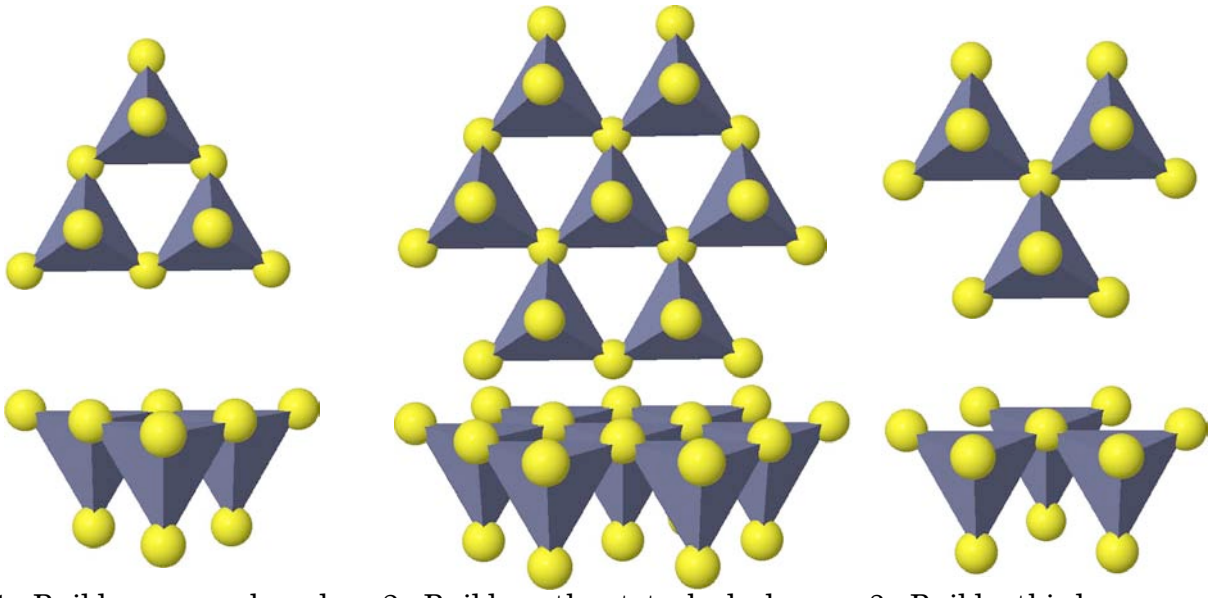
Names: Zinc Sulfide or Zinc Blende.

This structure is built from tetrahedral units. The pompom inside represents a zinc ion and the clear tetrahedron represents four sulfide ions in a tetrahedral arrangement around the zinc.



Top view

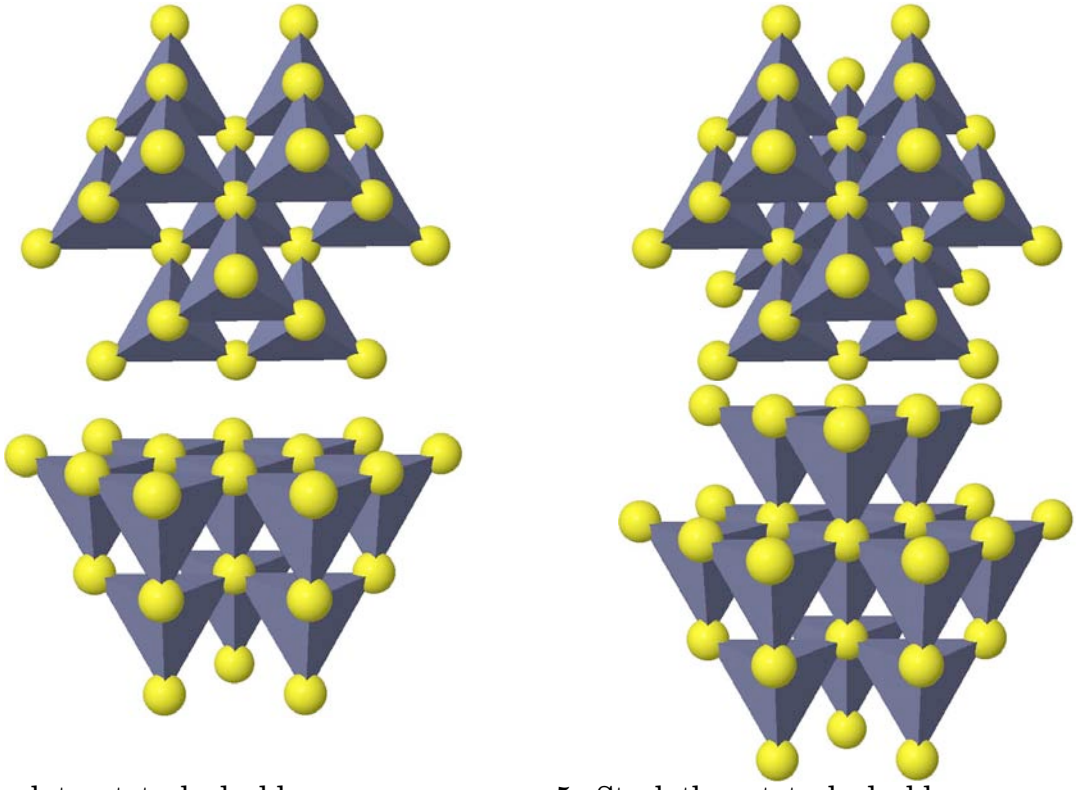
Side view



1. Build a corner-shared tetrahedral layer.
2. Build another tetrahedral layer.
3. Build a third tetrahedral layer.

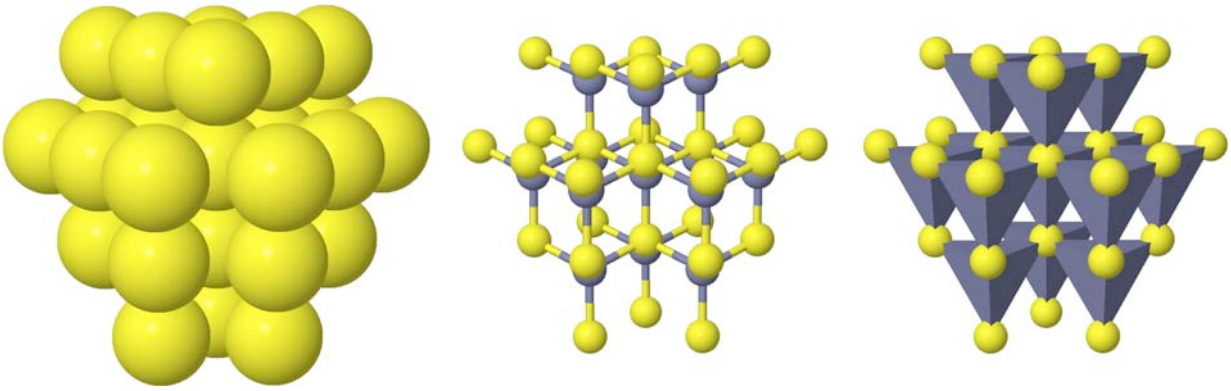
Top view

Side view



4. Stack two tetrahedral layers
5. Stack three tetrahedral layers

Alternate representations for this structure (all views show identical structures at the same scale):



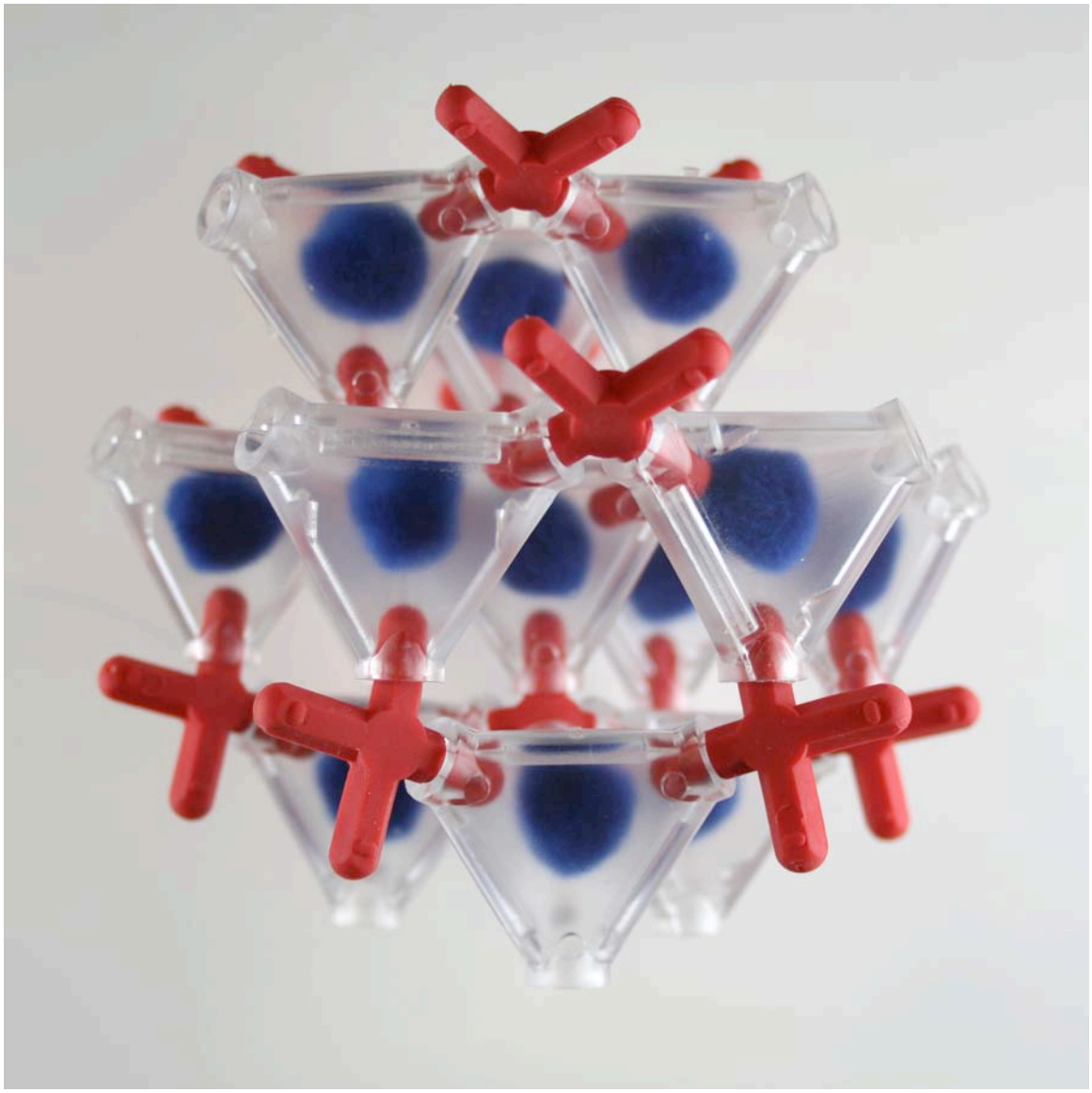
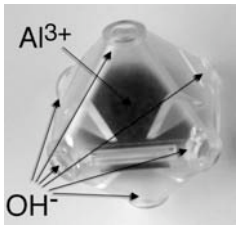


Figure 5. Polyhedral ZnS model assembled using the kit.

$Al_2(OH)_6$ Example

Names: Aluminum hydroxide or Gibbsite.

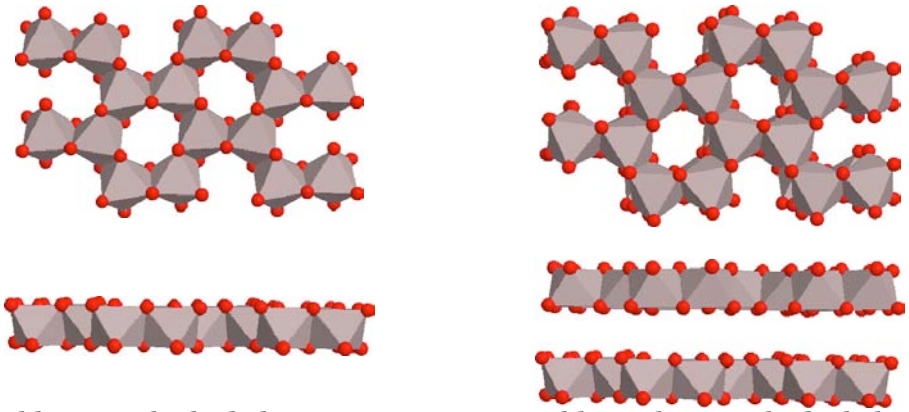


This structure is built from octahedral units. The pompom inside represents an aluminum ion and the clear octahedron represents six hydroxide ions in an octahedral arrangement around the aluminum. The motif of an octahedral sheet is found in many soil minerals.

Construction

Top view

Side view



1. Build an octahedral sheet.
2. Build another octahedral sheet.

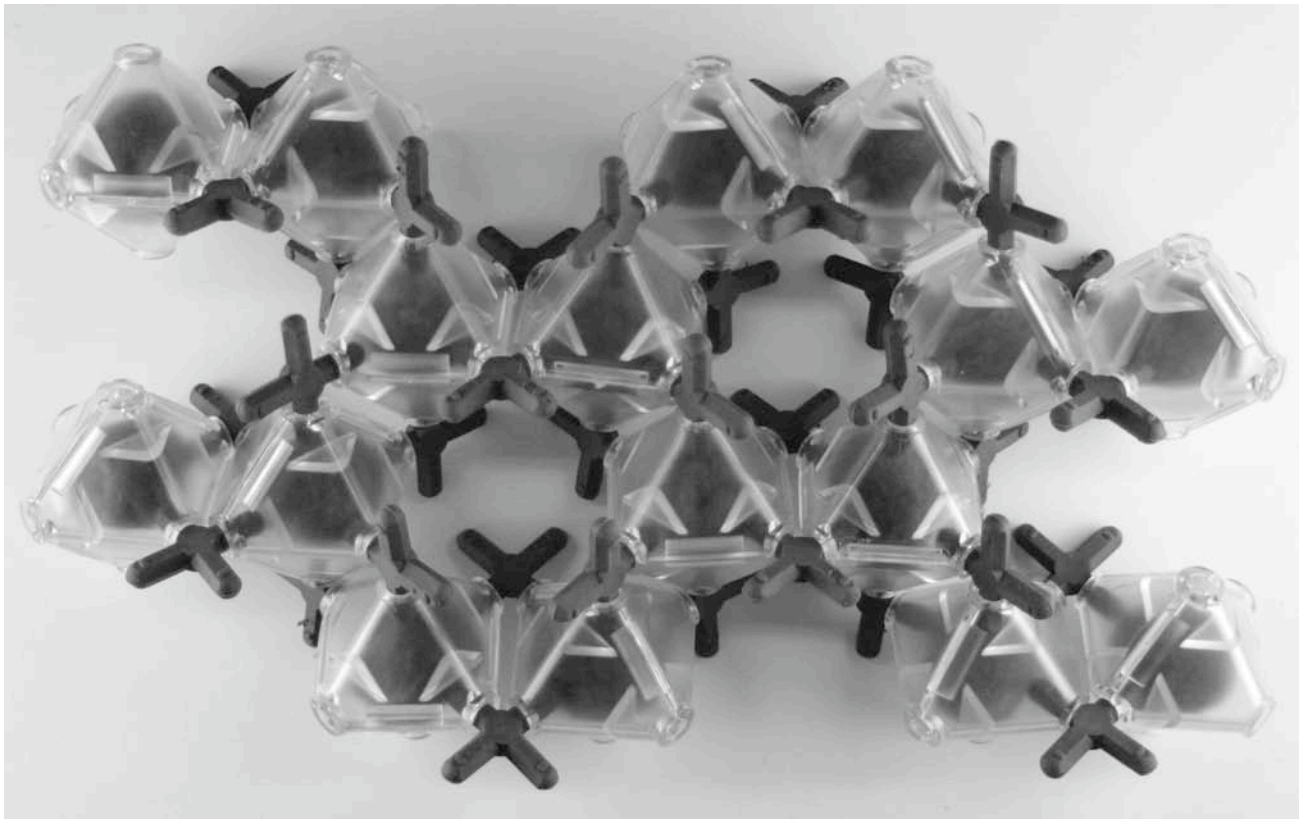
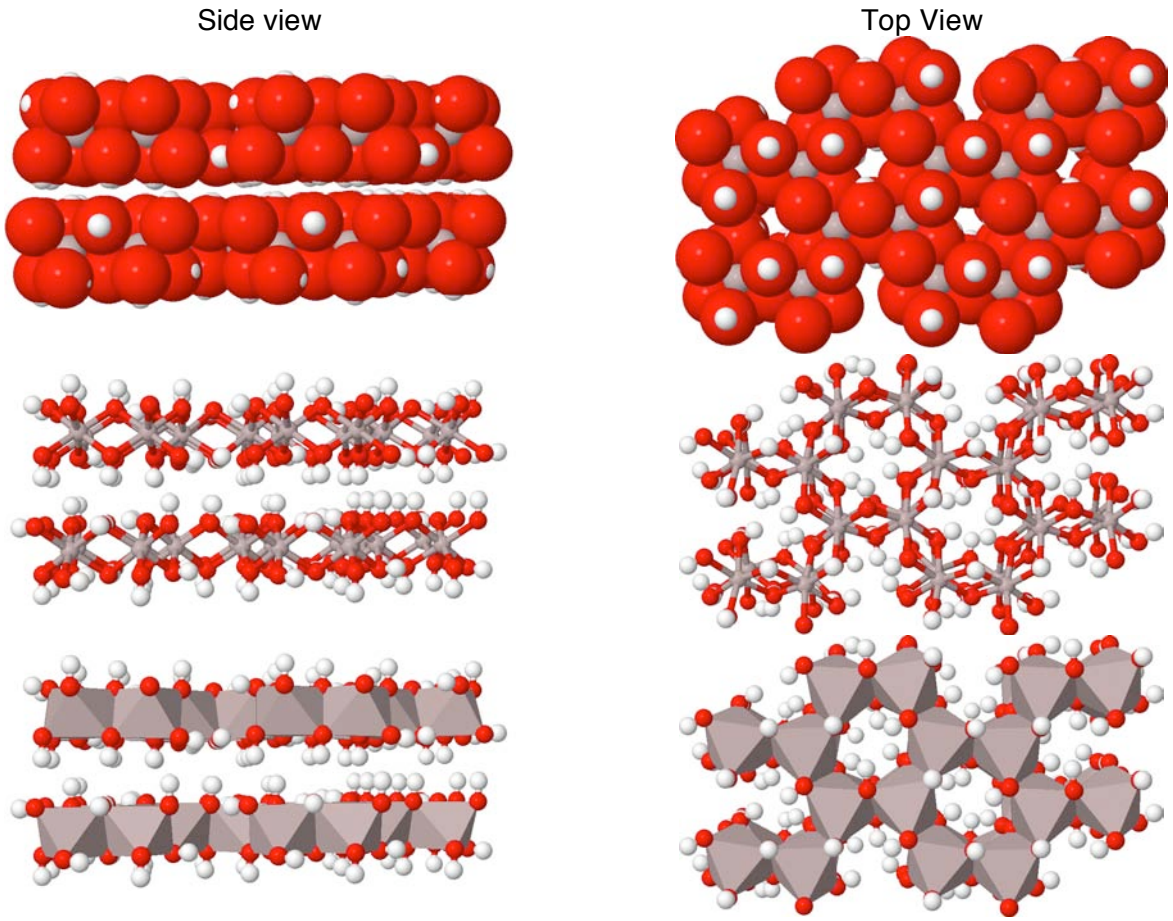


Figure 6. Polyhedral $Al_2(OH)_6$ layer assembled using the kit.

Alternate representations for this structure (all views show identical structures):



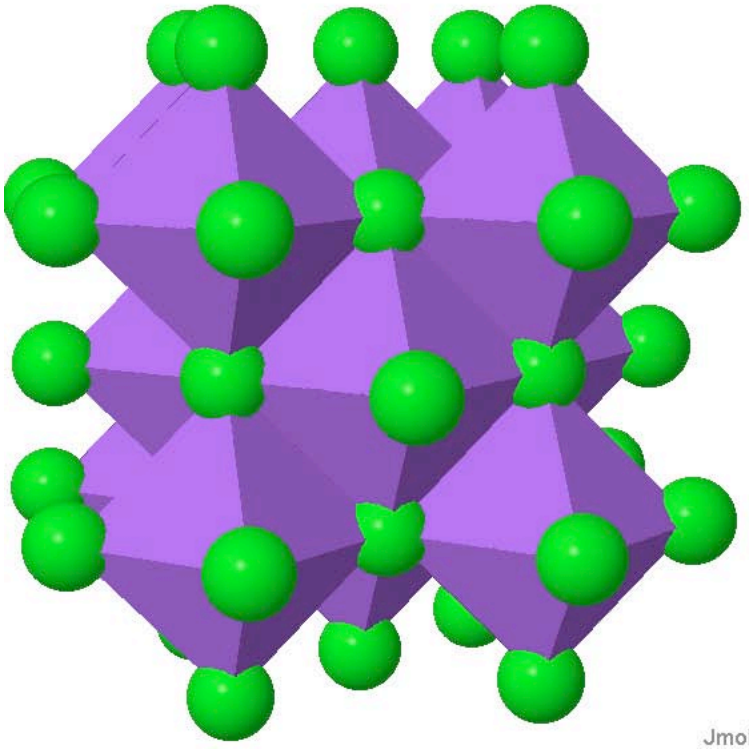
These views also show the hydrogen atoms that are part of $Al_2(OH)_6$. In the space-filling representations too large a value has been used for the H^+ ionic radius so that hydrogen can be observed.

Key to the Online Directions

This model kit has a companion web site at

http://mrsec.wisc.edu/Edetc/pmk/

The screen capture below shows the online controls for the internet companion representation of the NaCl structure. The numbered section on the right is a set of controls that are specific to each particular structure. Step 0 for each structure indicates the polyhedral units involved in that structure. The numbered steps indicate the order for assembling layers. Click the button to change the view to that step. Use the mouse to drag and rotate the molecule; shift-drag to zoom. Usually several layers are built and then assembled.



The controls at the top and bottom are common to all of the structures. The **Reset** and **Center** buttons at the top allow the default settings to be restored if zooming or rotating has gotten you confused.

The bottom set of controls allows the viewer to toggle between transparent-polyhedral, solid-polyhedral, ball-and-stick or space-filling representations, and various sizes of atom labels. Stereo draws two images, either (1) separate images meant to be viewed separately by each eye ("wall view"), (2) overlaid views which require red and blue glasses ("red and blue"), or (3) separate images showing the front and side views at the same time ("90º"). At any time the representation can be made to spin. This rotation will continue until toggled off.

Some of the functions of the bottom controls may be altered by the numbered set of controls. To reselect an option, click the button again.

Use the Large Screen link to increase the figure size on large format monitors.

Table 1. Number of pieces required to match the directions at http://mrsec.wisc.edu/Edetc/pmk

Structure	**Octahedral units**	**Tetrahedral units**	**Square pyramidal units**	**Square planar units**
Kit contents	78	60	24	18
Halite, NaCl	14			
Halite alternate	22			
Cadmium Iodide, CdI_2	4*			
Sphalerite, ZnS		13		
Sphalerite alternate		10		
Chalcopyrite, $CuFeS_2$		27 (two types)		
Platinum Sulfide, PtS				14*
Nickel Arsenide, NiAs	12			
Tellurobismuthite, Bi_2Te_3	36			
Ice, $H_2O(s)$		36		
Antifluorite, Li_2O		8		
Rutile, TiO_2	14			
Corundum, Al_2O_3	24			
Vanadium Pentoxide, V_2O_5			24	
Rhenium Trioxide, ReO_3	8			
Perovskite, $BaTiO_3$	8			
Superconductor, $YBa_2Cu_3O_7$			12*	6*
Spinel, $MgAl_2O_4$	7	8		
Magnetite, Fe_3O_4	16	17		
Brucite, $Mg_3(OH)_6$	9*			
Lizardite, $Mg_3(OH)_4[Si_2O_5]$	16*	12*		
Talc, $Mg_3(OH)_2[Si_2O_5]_2$	13*	26*		
Biotite, $K(Mg,Fe)_3(OH)_2[Si_3AlO_{10}]$	16* (two types)	29*		
Gibbsite, $Al_2(OH)_6$	16*			
Kaolinite, $Al_2(OH)_4[Si_2O_5]$	14*	15*		
Pyrophyllite, $Al_2(OH)_2[Si_2O_5]_2$	18*	43*		
Muscovite, $KAl_2(OH)_2[Si_3AlO_{10}]$	10*	28*		
Montmorillonite, $(Na,Ca)_x(Al,Mg)_2(OH)_2[Si_2O_5]_2$	12*	24*		
Albite, $NaAlSi_3O_8$		32 (two types)		
Olivine, $Mg_xFe_{1-x}[SiO_4]$	21	8		
Diopside, $CaMg[Si_2O_6]$	12	36		
Tremolite, $Ca_2Mg_5[Si_4O_{11}]_2(OH)_2$	36	80		
Sodalite, $Na_4Al_3Si_3O_{12}Cl$		24 (two types)		
Beryl, $Be_3Al_2[Si_6O_{18}]$	20	58 (two types)		
Topaz, $AlF(OH)SiO_4$	30	10		
Quartz, SiO_2		49		

*This is a layered structure. The web site shows two layers which would require twice as many pieces.