

# Preserving and Enhancing the 'Virtual Museum of Minerals & Molecules'

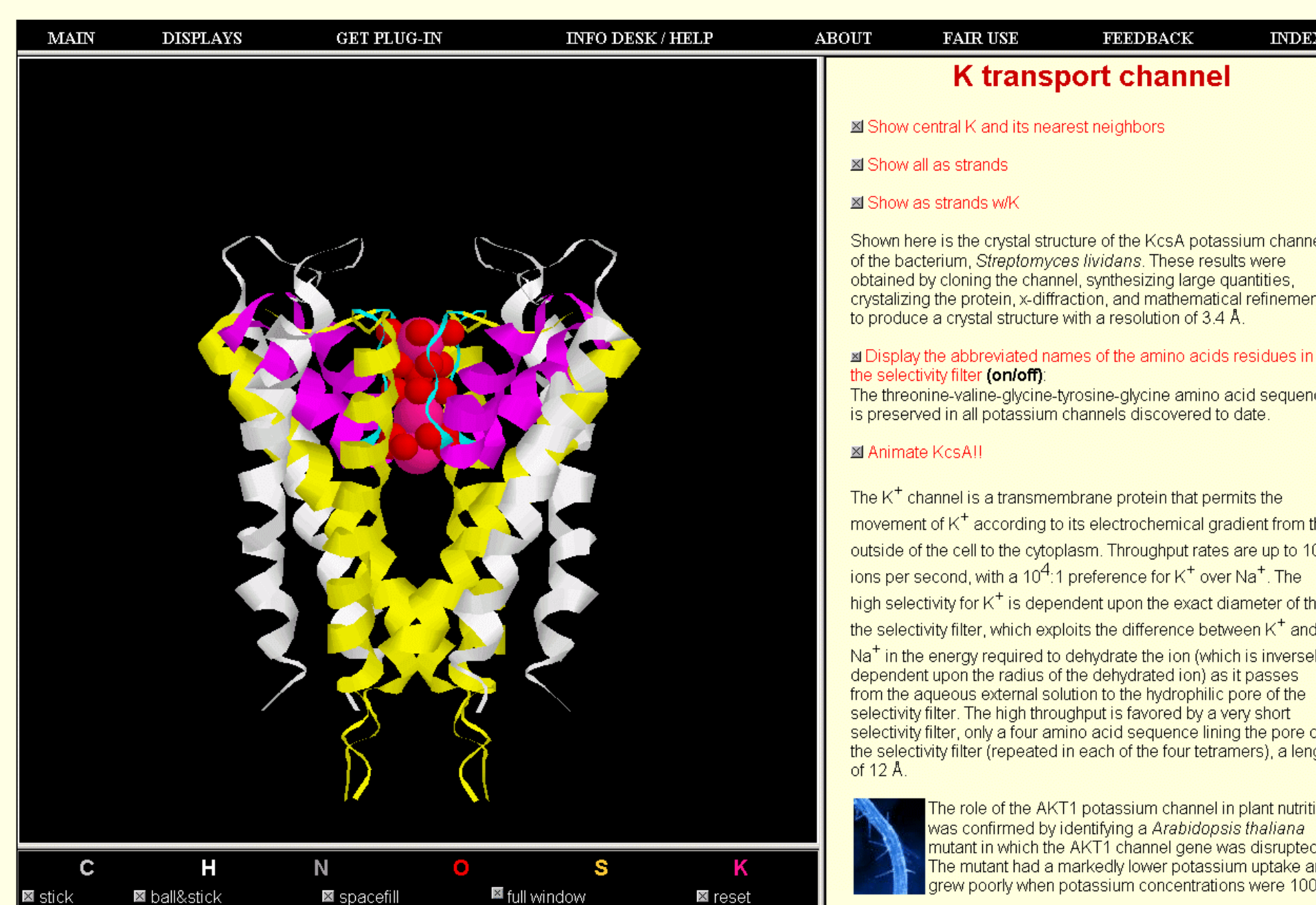
Phillip Barak  
Dept of Soil Science  
Univ of Wisconsin-Madison  
pwbarak@wisc.edu



**Abstract:** Innovative teaching approaches that employ technology-enhanced learning require consideration of replacement cycles to avoid technological obsolescence. The Virtual Museum of Minerals & Molecules, placed on line in 1998 as a web-based interactive display of 3D structure of minerals and molecules of environmental interest, originally operated on all major computer operating systems and browsers of the time, using proprietary browser plugin technology. In the intervening years, platform interoperability has been reduced to a single operating system and single browser, and user resistance to installing plugins has increased. Fortunately, an open source molecular visualization community has arisen and, using Java and javascript, has allowed the VMMM to be completely rewritten and reformulated for the entire breadth of modern operating systems and browsers. After a year of preparation, on a single day, the entire VMMM was transformed from its plugin-based former self to a Jmol-enabled version. Over 35,000 unique visitors are served annually at <http://virtual-museum.soils.wisc.edu>.

## INTRODUCTION:

**The Virtual Museum of Minerals & Molecules (VMMM)** is a web-based educational resource presenting interactive, 3D, research-grade molecular models to help visualize the sub-microscopic intricacies of mineral and organic substances and explore the connections between structure and function.



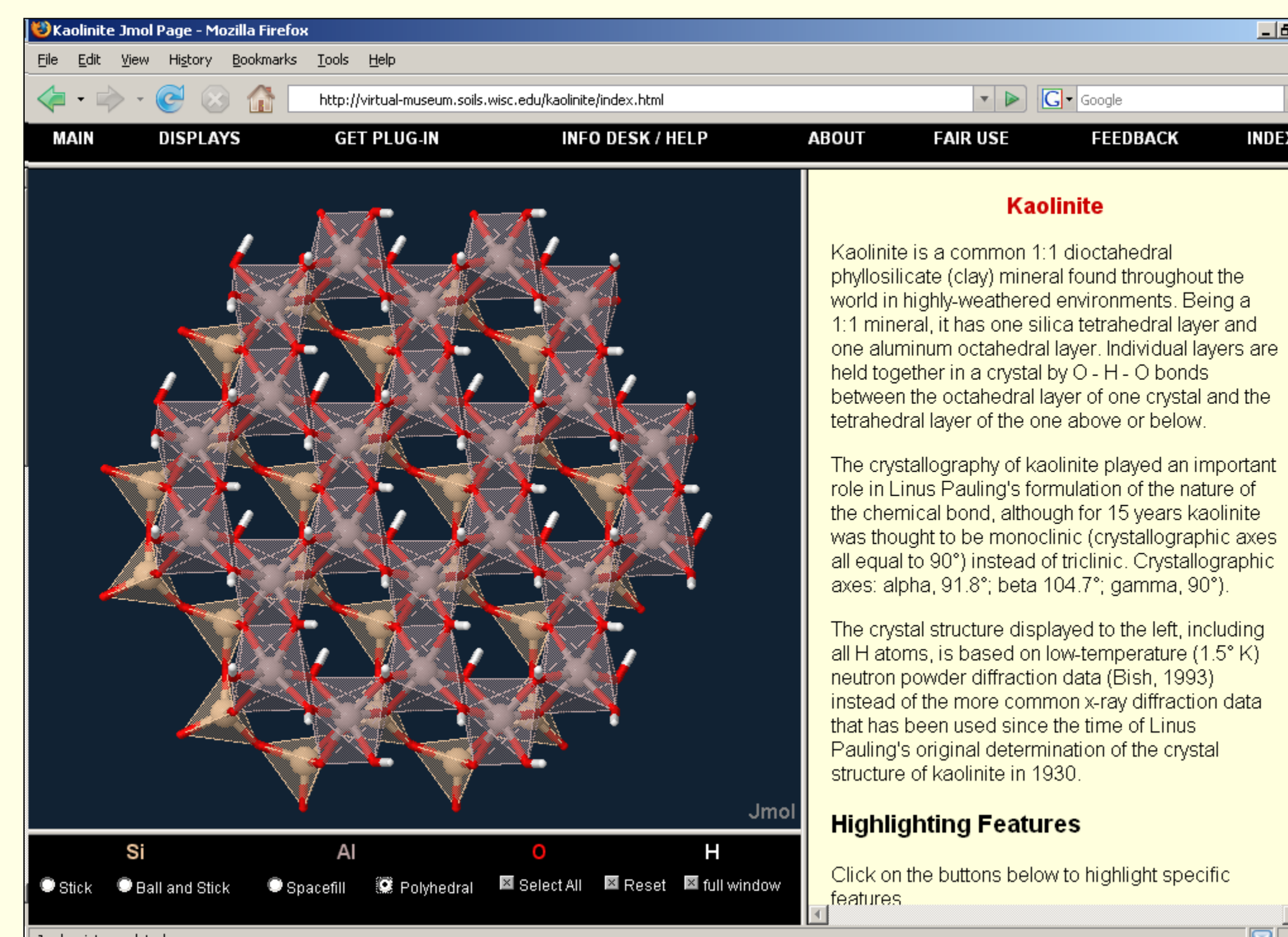
**K transport channel**

Show central K and its nearest neighbors  
Show all as strands  
Show as strands w/ k  
Show here is the crystal structure of the KcsA potassium channel of the bacterium *Streptomyces lividans*. These results were obtained by cloning the channel, synthesizing large quantities, crystallizing the protein, in diffraction, and refinement of electron to produce a crystal structure with a resolution of 3.6 Å.  
Display the abbreviated names of the amino acid residues in the select box (left).  
The threonine-valine-glycine-tyrosine-glycine amino acid sequence is preserved in all potassium channels discovered to date.  
Animals KcsA11  
The K<sup>+</sup> channel is a transmembrane protein that permits the movement of K<sup>+</sup> according to its electrochemical gradient from the outside of the cell to the cytoplasm. Throughput rates are up to 10<sup>7</sup> ions per second, with a 10<sup>3</sup> preference for K<sup>+</sup> over Na<sup>+</sup>. The high selectivity for K<sup>+</sup> is dependent upon the exact diameter of the selectivity filter, which excludes the difference between K<sup>+</sup> and Na<sup>+</sup> in the energy required to dehydrate the ion (which is inversely dependent upon the radius of the dehydrated ion). As a cation from the aqueous external solution to the hydrophilic pore of the selectivity filter, only a four amino acid sequence lining the pore of the selectivity filter (repeated in each of the four tetramers), a length of 12 Å.  
The role of the AKT1 potassium channel in plant nutrition was confirmed by identifying a Arabidopsis thaliana mutant in which the AKT1 channel gene was disrupted. The mutant had a markedly lower potassium uptake and grew poorly when potassium concentrations were 100

The electronic medium of the VMMM allowed quick updates of instructional material. The potassium transport channel (left) was posted three months after print publication. An aquaporin display was put up within a month after publication. (Lead researchers for both papers shared the Nobel Prize in Chemistry a few years later.)

Created in response to an increasingly visual audience attuned to high-quality computer-generated 3D imagery, the VMMM is designed to be not only educational, but also entertaining. Innovations in web-based 3-D visualization are making their way pervasively into the biotechnology and engineering fields – why not use these visualization packages to illustrate the essential building blocks of our living world?

The VMMM went on-line in 1998 with funding from USDA-HEC and used the proprietary Chime plug-in, which had versions for Netscape 4.7 and Internet Explorer v.4 browsers on Windows and Mac operating systems. The VMMM soon received notice and commendations from EduCause, the editors of *Scientific American*, and Sigma Xi (*American Scientist Online*).



**Kaolinite**

Kaolinite is a common 1:1 dioctahedral phyllosilicate (clay) mineral found throughout the world in highly-weathered environments. Being a 1:1 mineral, it has one silica tetrahedral layer and one aluminum octahedral layer. Individual layers are held together in a crystal by O-H...O bonds between the octahedral layer of one crystal and the tetrahedral layer of the one above or below.

The crystallography of kaolinite played an important role in Linus Pauling's formulation of the nature of the chemical bond, although for 15 years kaolinite was thought to be monoclinic (crystallographic axes all equal to 90°) instead of triclinic. Crystallographic axes: alpha, 91.8°, beta 104.7°, gamma, 90°.

The crystal structure displayed to the left, including all H atoms, is based on low-temperature (1.5° K) neutron powder diffraction data (Bish, 1992) instead of the more common x-ray diffraction data that has been used since the time of Linus Pauling's original determination of the crystal structure of kaolinite in 1930.

**Highlighting Features**

Click on the buttons below to highlight specific features.

A valuable feature of the VMMM is the ability to not only highlight individual features of molecules but to alter the molecular view smoothly, for example, from ball&stick to spacefilling or polyhedral presentation (left). The VMMM is particularly valuable to visual and active learners, but does not force a single conceptual model of atomic representation on the viewer.

## OUTCOMES to date include:

- 35,000 unique viewers a year (virtual-museum.soils.wisc.edu), closely following the academic calendar
- 600+ weblinks to the VMMM, mostly from the dot-edu domain
- Inclusion in at least two textbooks
- Source material used for NSF workshops and GeoWall
- Citations in the scientific literature
- Use in over a dozen classrooms worldwide, in front of over 1100 students annually!

## PROBLEM:

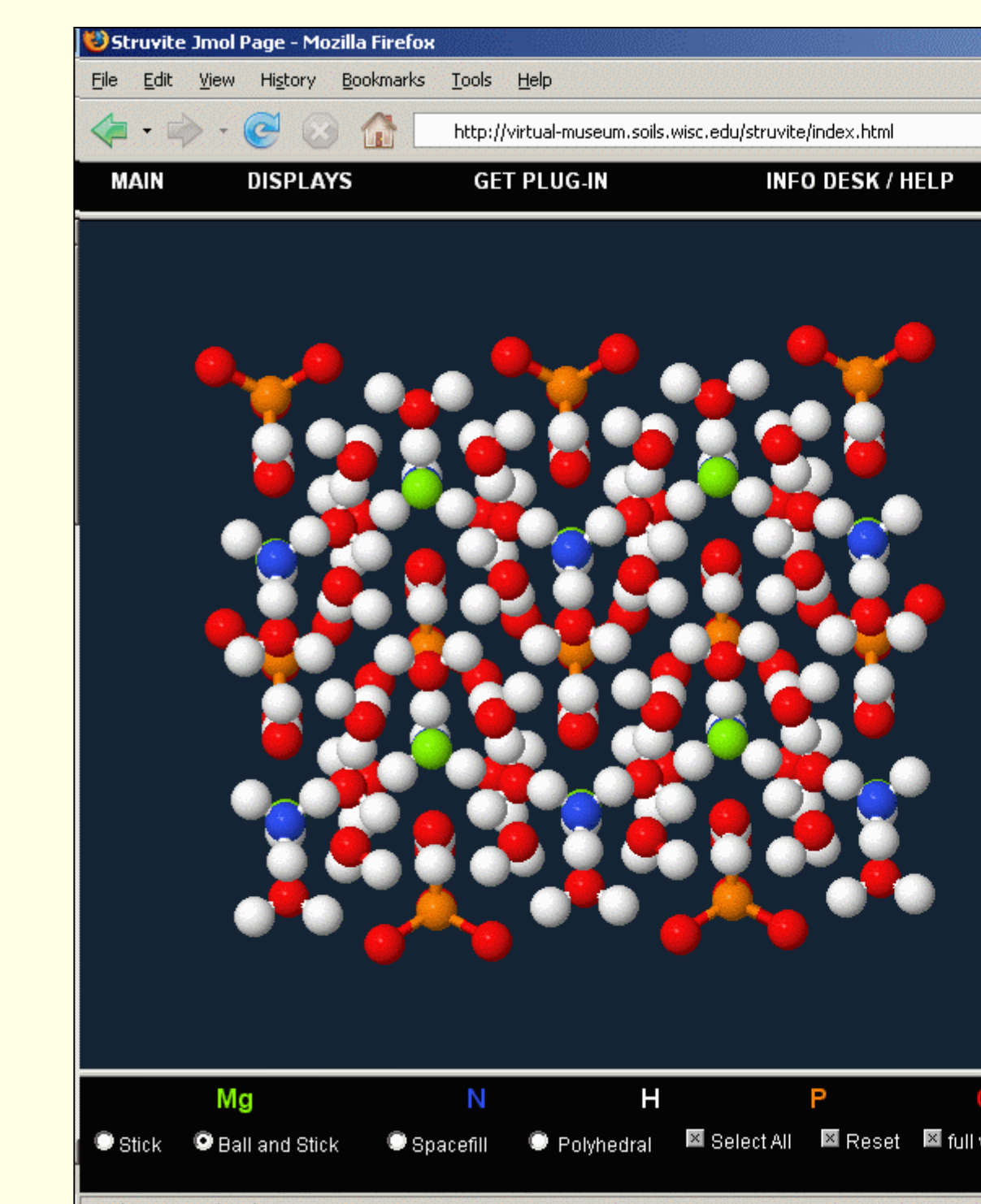
What is the technological lifespan of a successful teaching technology?

The proprietors of the Chime plugin have been sold twice since 1998 and seemed disinterested in the development of a free product. No new features of consequence had been added since 1998. All development had stopped except for IE for Windows, leaving all other browsers and platforms unsupported. Furthermore, users were increasingly resistant to installing unfamiliar plugins.

## SOLUTION:

The development of the open source chemical visualization community linked electronically and working collaboratively produced Jmol, a Java-based molecular visualization applet and application that has a chemical scripting language and JavaScript functionality. The open source nature of the project allowed it to rapidly add functionality from other open source projects, such as crystal symmetry operations and molecular optimization calculations.

The USDA-HEC funded a second project 'To Preserve and Enhance the VMMM' following proof-of-concept conversion of several VMMM displays from Chime to Jmol. The content of the VMMM displays were rewritten into XML (eXtensible Markup Language), an open, tagged format that would facilitate any further conversions and alterations. Using XLST (eXtensible Stylesheet Language Transformations), the XML file for each display can be written into the required files for VMMM usage.



**Struvite**

aka, Guanite; Magnesium ammonium phosphate hexahydrate (MgNH<sub>4</sub>PO<sub>4</sub>·6H<sub>2</sub>O), d<sub>s</sub>=1.71

**Highlighting Features:**

- Show Mg: Each group consists of four H arranged in near perfect tetrahedral geometry around a central N. (Mean O-N-O, 110°, compare with angle subtended by an edge at the center of a tetrahedron, 109.1°, mean N-H, 0.92 Å.) Three of four H atoms in each group are hydrogen bonded to either O of nearby water (2.16 Å) or phosphate (1.87 Å).
- Show PO<sub>4</sub>: Each group consists of four O arranged in near perfect tetrahedral geometry around a central P. (Mean O-P-O, 109.8°, compare with angle subtended by an edge at the center of a tetrahedron, 109.1°, mean P-O, 1.54 Å.)
- Show H<sub>2</sub>O: Each group consists of four O atoms, each from an H<sub>2</sub>O molecule, form an octahedron of (near)tetrahedral (near) tetrahedra and a sphere of

Struvite is likely to play a role in nutrient recovery from wastewater streams, both manure and sewage treatment plants. The mineral structure includes tetrahedral arrangements of phosphate (PO<sub>4</sub>) and ammonium (NH<sub>4</sub><sup>+</sup>) and octahedral arrangement of water around the magnesium ion (Mg·6H<sub>2</sub>O) reflecting the dipole moment of water. Struvite is a biogenic mineral and has also been crystallized on molecular templates.

## What's Next?

We are continuing to work on improving the use of crystallographic symmetry in our mineral displays and adding materials of interest to our wide viewership (--ask about meridianite!) We are also looking at the use of the Nintendo WiiRemote as a controller for pseudo-stereoscopic viewing and would like to help visitors build their own displays on our site by using our XML templates and storing their results on our servers.

## Curators of the Virtual Museum of Minerals & Molecules:

Phillip Barak, Univ of Wisconsin-Madison  
Ed Nater, Univ of Minn-Twin Cities  
Cindy Stiles, USDA-NRCS-SSL

URL: <http://virtual-museum.soils.wisc.edu>