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# Specification of Structural Viewer and Analytical Tool (JECP/SVAT)

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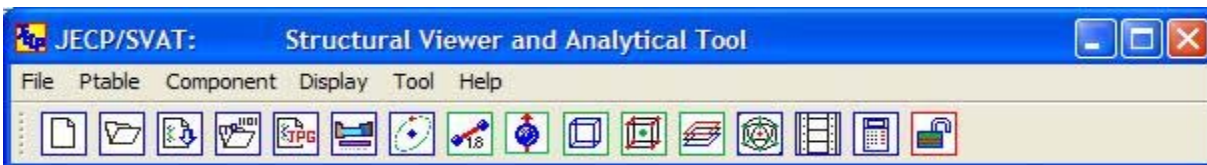
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# Specification of Structural Viewer and Analytical Tool (JECP/SVAT)

by X.Z. Li

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Table of Contents

- [1. Purpose](#)
- [2. Graphic user interface](#)
- [3. Features](#)
- [4. Installation](#)
- [5. Basic operation](#)
- [6. Contact the author](#)
- [7. References](#)

## 1. Purpose

Java Electron Crystallography Package (JECP) is a collection of programs for crystallography and electron diffraction analysis. The package is designed and written by Dr. X.Z. Li. The software can be used as a research tool as well as a teaching aid.

The need of a structural viewer/an analytical tool, using the same input data format as the JECP and proJECT software, becomes obvious with the growth of the JECP and proJECT programs and users.

There exist many programs for structural design and/or display in various levels developed by individual, research group or software company. Some of them are expensive software with multi-purpose and advanced graphics, which maybe not be suitable for beginners. Others are simply programs for building/dislaying crystal structures. The motivation for the development of JECP/SVAT is to provide a structure viewer and also working as a analytical tool.

JECP/SVAT provides mouse/arrow-key driven real-time 3D display of crystal structure in a unit-cell, including the chemical bonds and magnetic moments. The structure can also be displayed in animated modes including rotation or wobble. The structure can be analyzed (i) as a projection in a user selected [uvw] direction or layer by layer, (ii) as a local structure (or polyhedral cluters) by defining a center atom, and a radius of spherical range. Tools for calculate the bond length/angle are included. **One important feature** is that user's work on the structure can be saved to a file, which can be reloaded for a quick display next time or continue on an unfinished work. The display of a structure can be sent directly to printer for printing or saved as JECP and TIFF image files. More details of the features are described below.

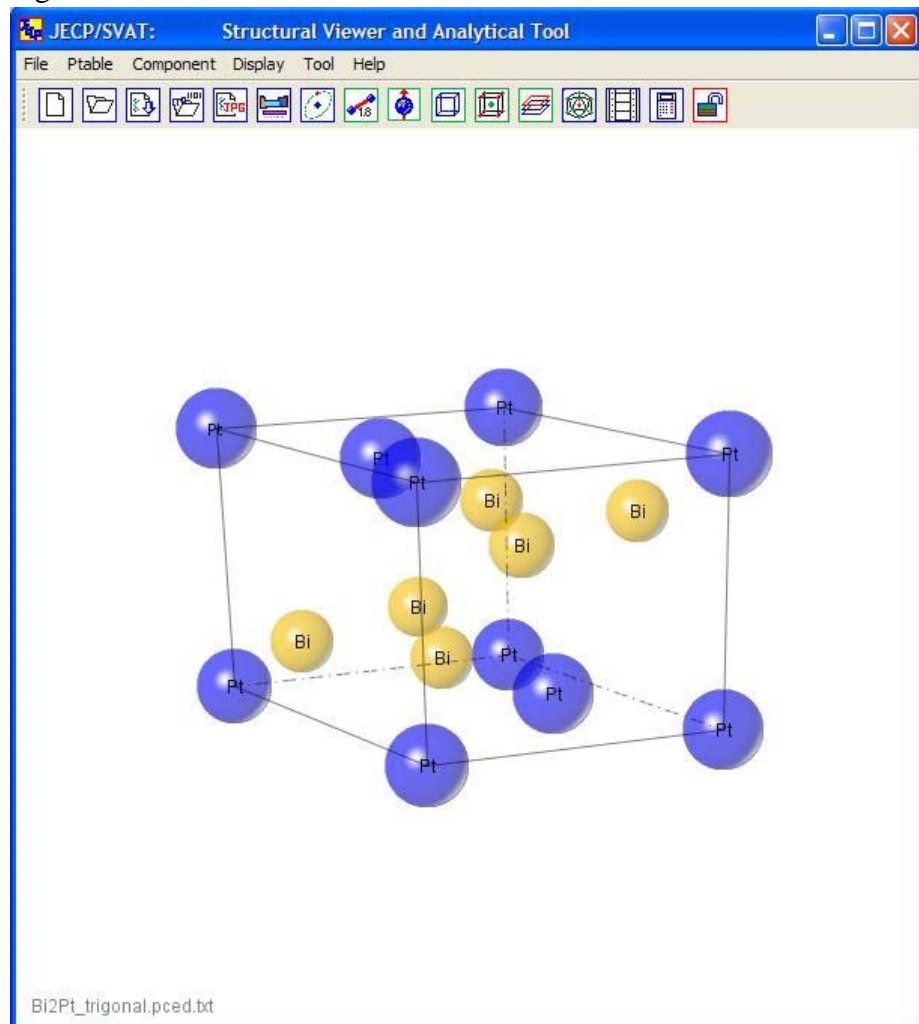
[\[TOC\]](#)

## 2. Graphic user interface

The GUI of JECP/SVAT consists of a drop-down menu, a menu bar, a display panel and several operational panels. The drop-down menu provides all the options and the menu bar provides more frequently used ones. The display panel and control operational panel are always on, while other operational panels can be turned

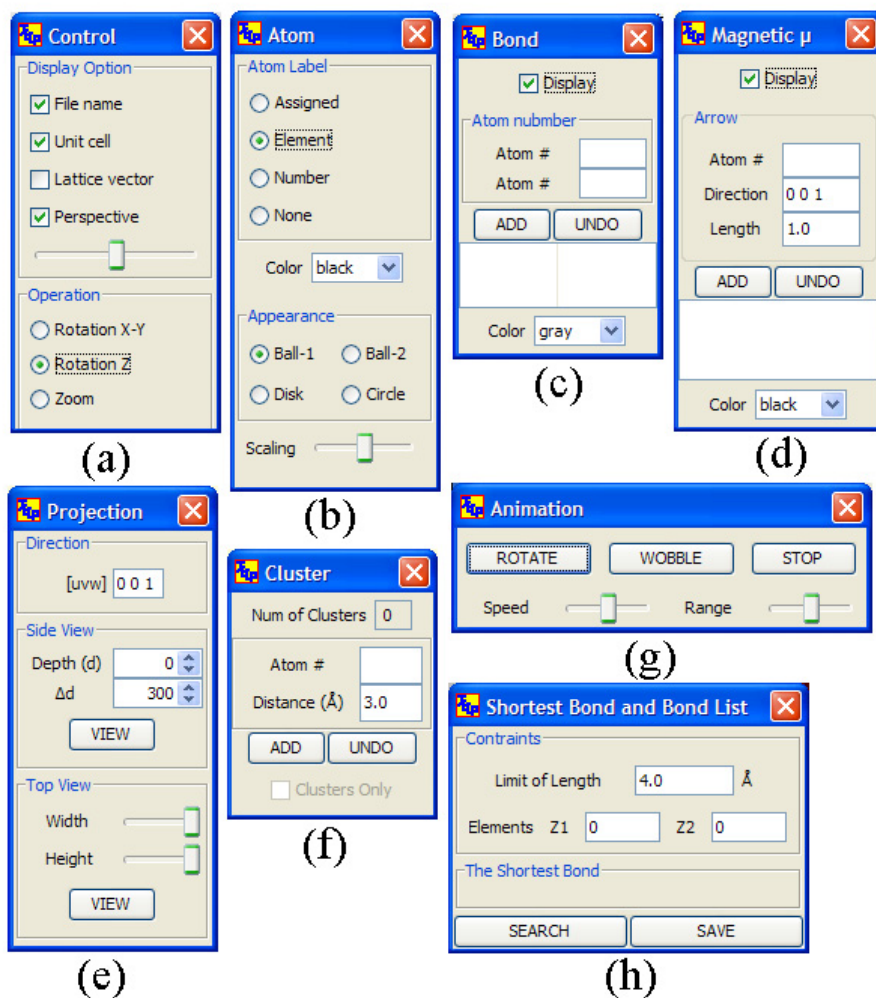
on and off as needed.

Figure 1 shows the GUI of JECP/SVAT with the Bi<sub>2</sub>Pt structure as example.



[\[TOC\]](#)

Figure 2 shows all the operational panels.



[\[TOC\]](#)

### 3. Features

Crystal structure file can be prepared using a built-in template of the input file. All JECP and proJECT software use the same jecp format of input files.

Figure 3. shows (a) the template for creating crystal structure file (the jecp format), (b) the existed crystal structure files in jecp format and other formats (e.g, CIF, JEMS, PowderCell) can be edited and saved in the jecp format.

**JECP Template of Crystal Structure**

Description  
new crystal structure

Bravais Lattice  
Crystal system: Triclinic Lattice type: P

Lattice parameters  
a = [ ] (Å) b = [ ] (Å) c = [ ] (Å) α = [ ] (°) β = [ ] (°) γ = [ ] (°)

Space group  
Number: 1~2 Symbol: c1c1c1

Coordinates of Atoms

atom	elem #	x	y	z	occ.
		0.0	0.0	0.0	1.0

Add Remove Clear View

Number of atom in the list: 0 Global isotropic temperature factor: 0.0

Notes  
References etc.

New Edit Save Close

**File Format**

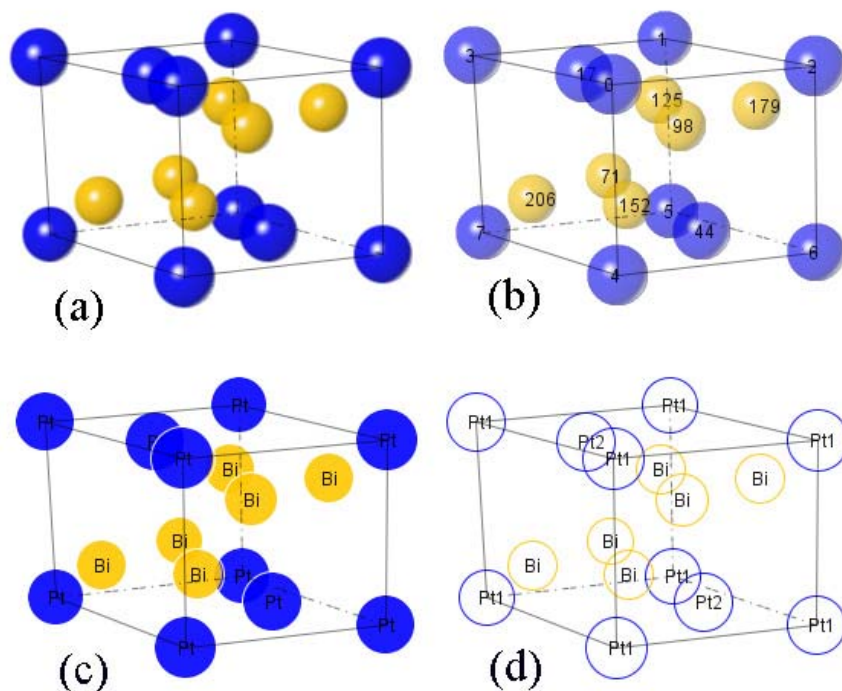
JECP (.jec; .txt)  
 CIF (.cif)  
 jems (.txt)  
 PowderCell (.cel)

NEXT BACK

[\[TOC\]](#)

Crystal structure can be displayed in 3D view with an adjustable perspective constant. Various options for the atomic label and atomic appearance are available. Chemical bonds and magnetic moments can be added on for numeric atomic labels.

Figure 4 shows the structure of Bi<sub>2</sub>Pt with various appearance, atom as (a) solid ball, (b) transparent ball, (c) disk and (d) circle; atomic label as (a) off, (b) numerical, (c) element and (d) atom label.

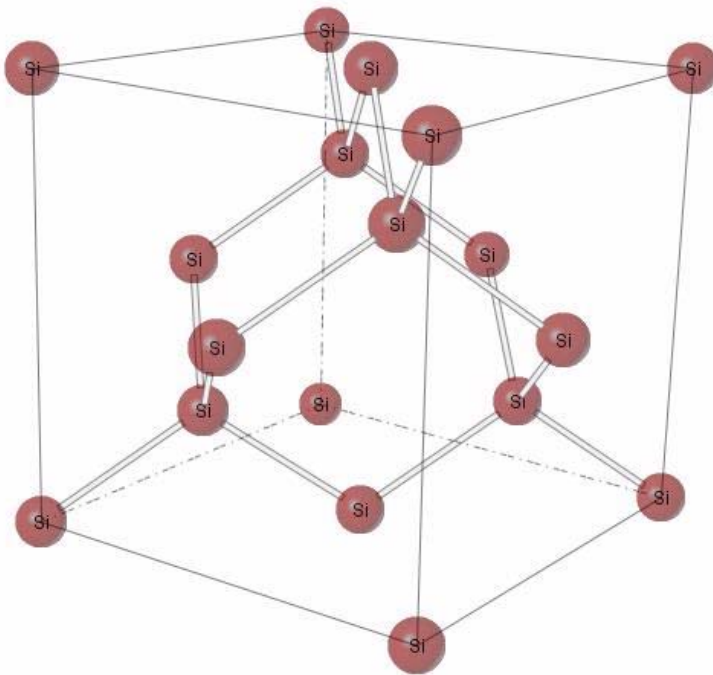


Bi2Pt\_trigonal.pced.txt

[\[TOC\]](#)

For a computer with a relatively slow speed CPU, it is suggested firstly to manipulate the structure using the atomic appearance of disk or circle and then reset the atomic appearance of solid ball.

Figure 5 shows the structure of Si with chemical bonds.

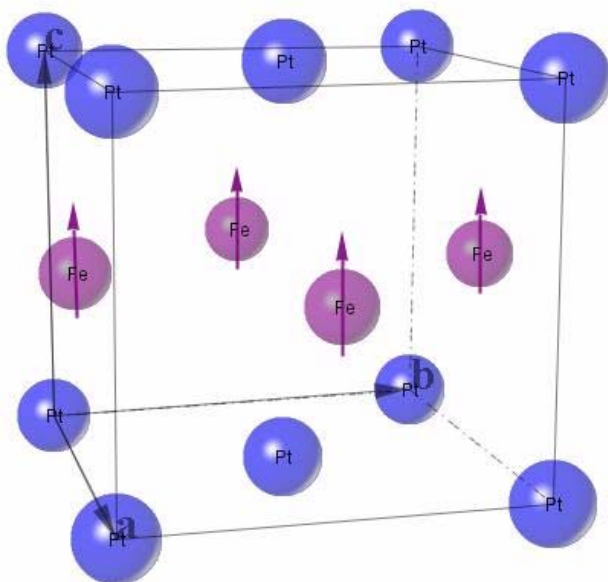


Si.dat.txt

[\[TOC\]](#)

Figure 6. shows the structure of FePt  $L1_0$  phase with magnetic moments on Fe atoms.



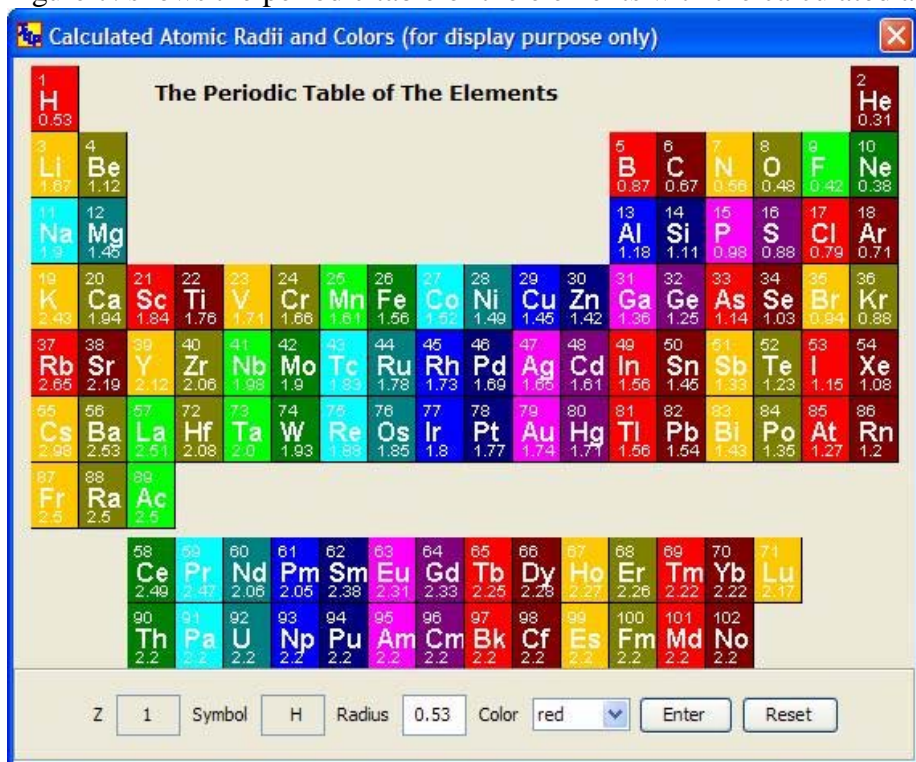


FePt\_L10\_full.enc.dat.txt

[\[TOC\]](#)

The software provides the data sets of calculated and empirical measured atomic radii in the periodic table of the elements. Both atomic radius and atom display color can be customized.

Figure 7. shows the periodic table of the elements with the calculated atomic radii.

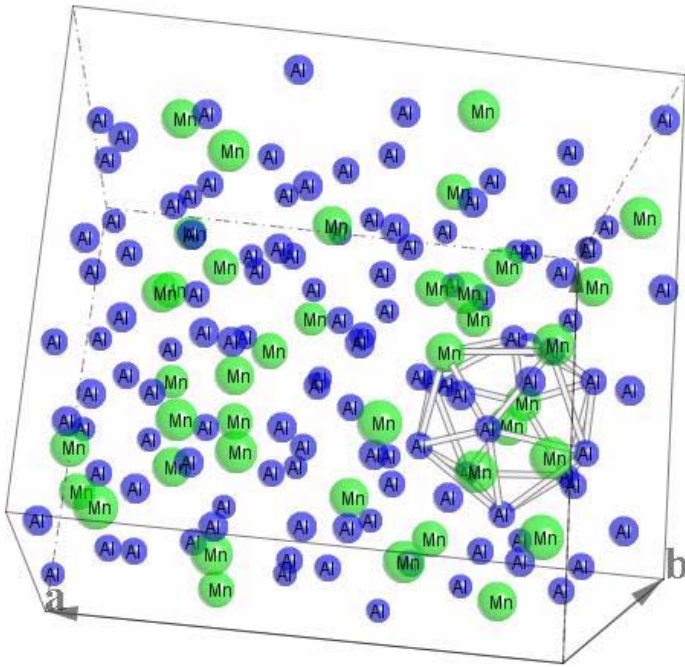




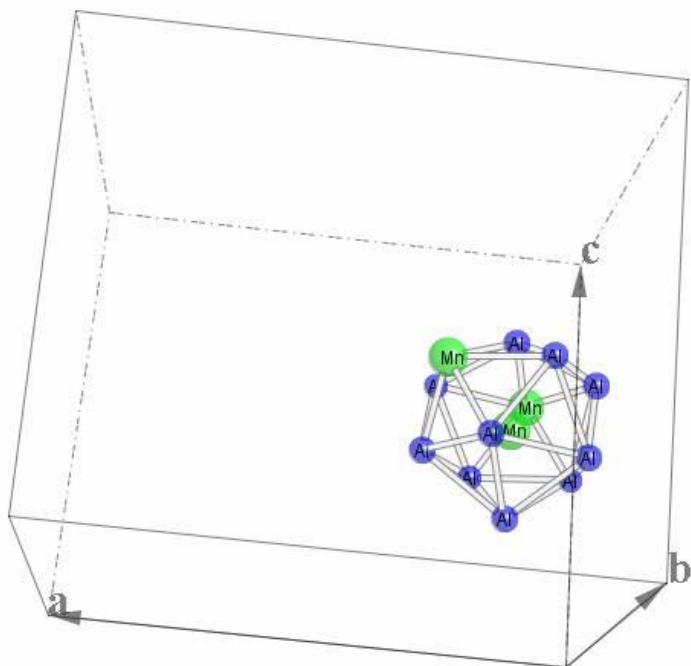
[\[TOC\]](#)

Crystal structures can be displayed with lattice only or 3D structure in the unit-cell. Crystal structures can also be displayed/analyzed using projection/layer and local structure/polyhedral cluster. This is an important way to display/analyze complex structures.

Figure 8. shows the structure of the  $\text{Al}_3\text{Mn}$  phase, a crystalline approximant of the Al-Mn decagonal quasicrystal.



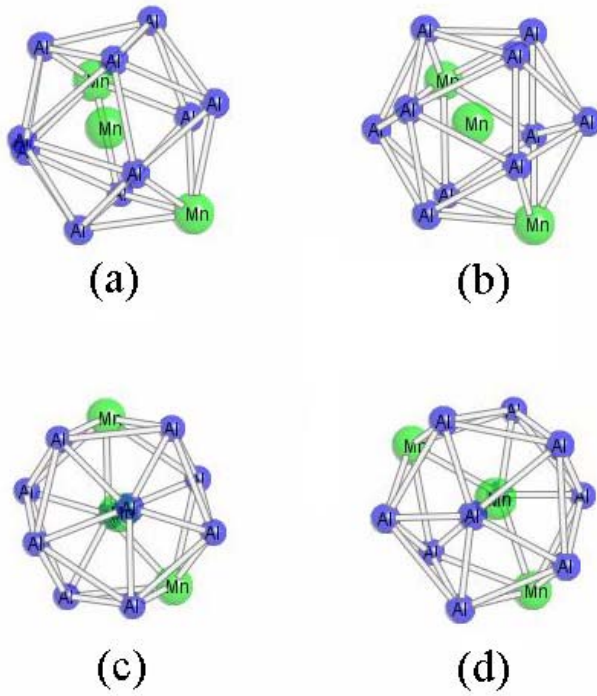
Al3Mn.str.bt



Al3Mn.str.txt

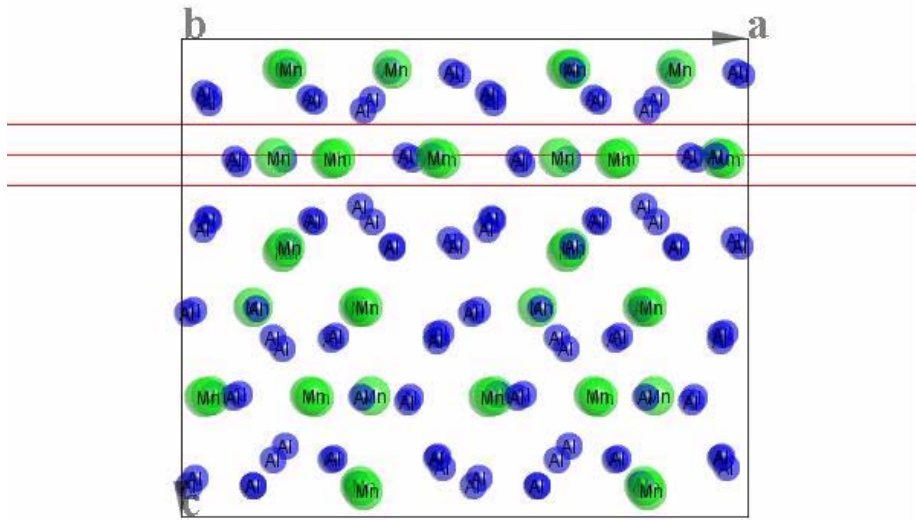
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Figure 9. shows the polyhedral cluster marked in Figure 8 viewed at four different angles.



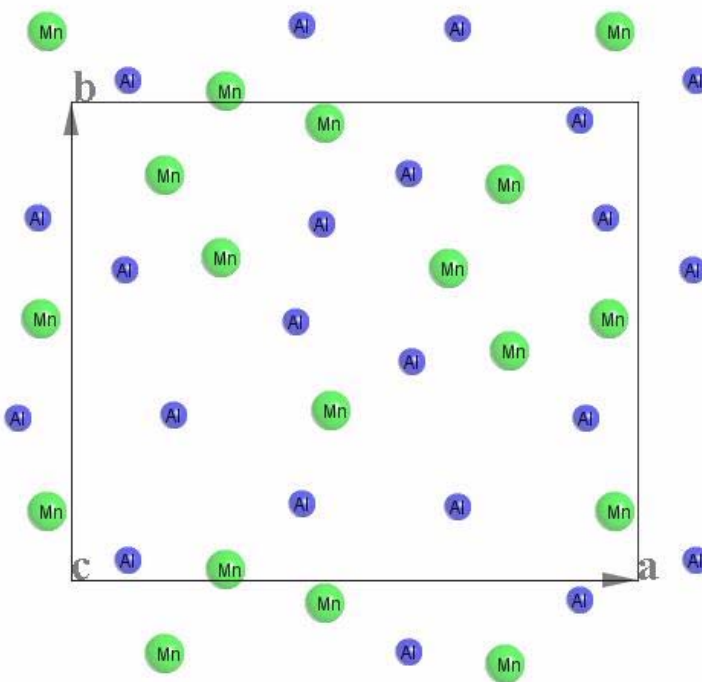
Al3Mn.str.txt

Figure 10. shows a structural projection of the  $\text{Al}_3\text{Mn}$  structure (the lower part) for a specifically selected the layer, as shown in the upper part.



Al3Mn.str.txt

[\[TOC\]](#)



Al3Mn.str.txt

[\[TOC\]](#)

As shown in Figure 2(g), JECP/SVAT can show the structure in animated rotation or wobble. Besides an operational panel in Figure 2(h) is for calculating bond length and bond angle, the other operational dialog is for calculating the shortest bond length and a bond list within a given bond length.

#### 4. Installation

Java virtual machine, i.e., J2RE, must be installed for running JECP/SVAT. The 3D vision is generated using 3D geometical calculation and Java2D functions, so Java3D library is not needed.

The executable bytecodes, together with the data files for testing and this specification file is available in compressed form (jecp\_svat.rar) at <http://www.unl.edu/CMRAcfem/programs.htm>.

Uncompress jecp\_svat.rar in a user defined directory, e.g. c:\jecp\_svat\ and execute jecp\_svat.jar (double click in window or type 'java -jar jecp\_svat.jar in command line).

The software works in two levels, basic (trial) level and full level. A license file is required for running in the full level. Without the license file, the software can be run in the basic level. The software is fully operational at basic level, but all functions for save and print are blocked. A coded structure file is required for the software in basic level. **The code is free available for the first-time users and continue available if the users provides a picture of the structure created by JECP/SVAT together with a link to JECP/SVAT site in their webpages.** Both normal and coded structure file can be used in the full mode.

[\[TOC\]](#)

#### 5. Basic operation

i) As mentioned above, new crystal files can be prepared using the editing panel. Crystal structures can be loaded using the menu bar or the drop-down menu.

ii) In addition to the structure file, there is a second type of input file, which contains the information of previous work on a structure. A work file of the same crystal file can be loaded subsequently to display the work done previously or to continue an unfinished work. The work file can be loaded in both modes, but can only saved in the software with a license.

iii) Most operations are self-explanatory but some may need guidance. For example, atom radius and atom displayed color can be edited by users for current work and can also be saved into a work file and reloaded as a customized data set for later works. A user manual for the details for all operation is in preparation now.

[\[TOC\]](#)

#### 6. Contact the author

For the license file and the code of a structure file, please contact the author (xli2@unl.edu). Suggestion and bug reports are welcome.

[\[TOC\]](#)

#### 7. References

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[\[TOC\]](#)