VENUS System for Three-Dimensional Visualization of Crystal Structures and Electron/Nuclear Densities

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Preface

Despite the availability of many good structure-drawing programs, cross-platform free software that is directly based on OpenGL technology (http://www.opengl.org/) is few. We have been distributing our own premier system VENUS: **V**isualization of **E**lectron/ **NU**clear densities and **S**tructures.

VENUS bears the bell in three-dimensional (3D) visualization, rendering, and manipulation of crystal structures and electron/nuclear densities determined not only by X-ray/neutron diffraction but by electronic-structure calculations.

VENUS fully utilizes the OpenGL Application Programming Interface (API). Video cards equipped with GPUs supporting hardware acceleration for the OpenGL are desired to rotate, expand, and translate objects fast in three dimensions.

The VENUS system comprises three independent programs:

VICS: **VI**sualization of **C**rystal **S**tructures
VEND: **V**isualization of **E**lectron/**N**uclear **D**ensities
PRIMA: **P**ractice of **I**terative **M**EM **A**nalyses

That is, VEND and VICS deal with electron/nuclear densities and crystal structures, respectively. VEND also supports the 3D visualization of electrostatic potentials and wave functions that have both positive and negative values, which allows us to obtain additional information about electronic states. The present document does not deals with MEM analysis program, PRIMA, that yields 3D electron and nuclear densities from X-ray and neutron diffraction data, respectively.

We are convinced that heavy users of RIETAN are very pleased that VENUS can input and output user-input files, ∗.ins, of RIETAN. After releasing VENUS, such a 3D visualization package will be regarded as an indispensable tool for those who utilize a Rietveld-analysis program like RIETAN-2000 and a MEM analysis program like PRIMA. We must understand crystal structures, electron/nuclear-density distribution, and electronic states not two-dimensionally but three-dimensionally!

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About This Manual

This manual consists of two parts: (1) VICS: Visualization of Crystal Structures and (2) VEND: Visualization of Electron/Nuclear Densities. We repeated part of descriptions twice, considering that the two programs are mostly used independently. Nevertheless, some descriptions are placed below because they are general notabilia common to these two.

License Agreement

I have benefited from a number of free software packages. I am, hence, willing to deliver VENUS as free software licensed under the GNU General Public License. That is, VENUS is 'copylefted' with its source code freely available to everyone in the world. The source code included in the distribution file is indispensable for debugging the program, learning techniques of crystallographic computing, and implementing new features in VENUS.

Anyone is free to copy, modify, redistribute, and sell it under the terms of the GPL plus the following additional condition.

Drawings produced by VICS and/or VEND may be used in any publications provided that proper acknowledgement is given; for example,

> Figure 1 was drawn with VENUS developed by Dilanian and Izumi.

Operating Systems

At present, VENUS can be run only on Windows and UNIX/Linux. Its source programs will serve to learn techniques to develop crystallographic programs for 3D visualization and add new features. VENUS for Windows were compiled and linked with Microsoft Visual C++ in Microsoft Visual Studio 6.0 (Service Pack 5) on Windows 2000, and VENUS for Linux with GCC 3.1.1 (http://gcc.gnu.org/) and GTK+ 2.0 (http://www.gtk.org/) on Redhat Linux 7.3.

To run VICS and VEND, Windows NT/2000/XP is preferred to Windows 98/Me for decent performance. Windows NT/2000/XP is robust, supporting the Command Prompt that is much inferior to various shells in UNIX but not so bad. On the other hand, Windows 98 and, particularly, Windows Me have some serious problems including the absence of

memory protection, memory leak, and MS-DOS Prompt of less features. Frankly, Windows 98/Me is now obsolete.

Minimum Requirements of Hardware for the Windows Version

CPU: MMX Pentium 233 MHz or faster
RAM: 64 MB or more
Video RAM: 16 MB or more is desirable
Video card: A video card equipped with a GPU supporting hardware acceleration of the OpenGL API is highly desired. Without this hardware component, both 3D graphics and the GUI become slow-moving, and it takes more time to save 3D images in graphic data files. At present, such video cards can be purchased at relatively low price.

Folder and Files Included in the Windows Version

The current version of VENUS can be run on Microsoft Windows 98/Me/NT/ 2000/XP.

Archive fils, VENUS.tbz, Examples.tbz, and PRIMA.tbz, have to be uncompressed with an archiver supporting the tbz (=tar.bz2) format. For information about archivers available on Web sites, refer to http://hompage.mac.com/fujioizumi/rietan/angle_dispersive/angle_dispersive.html#Archive_utilities.

VENUS.tbz, Example.tbz, and PRIMA.tbz are uncompressed to give folders VENUS, Examples, and PRIMA, respectively. Move folders Examples and PRIMA into folder VENUS.

Executable binary files, VICS.exe and VEND.exe, are stored in folder VENUS\Programs with some additional files, and all the source code files and libraries (glut, glui, JPEG, and JasPer) in folder VENUS\Source_code. A variety of input files are placed below VENUS\Examples. Folder VENUS\Documents contains two PDF files including the present document (VENUS.pdf) while folder VENUS\contrd stores folders and files related to a file converter, contrd, for a DV-X□ method program, SCAT. Refer to Readme_contrd.txt in Folder VENUS\contrd to learn how to use contrd. VENUS\PRIMA stores folders and files relevant to a program, PRIMA, for the maximum-entropy method;

nothing is described regarding PRIMA in this document.

Folder VENUS may be located anywhere lest the total length of names for the absolute path and the input/output file exceeds 256.

A dynamic-link library (DLL), glut32.dll (Ver. 3.7.6, released on November 8, 2001), placed in folder VENUS\Programs was downloaded from http://www.xmission.com/~nate/glut.html. This DLL may alternatively be located in C:\Windows\system32 (Windows 98/Me/XP), C:\WINNT\system32 (Windows 2000), or C:\WINNT40\system32 (Windows NT). If another file of glut32.dll is included in one of these folders, please delete it.

You can drag and drop various input files, *e.g.*, ∗.vcs, ∗.cif, ∗.pdb, ∗.den, and ∗.rho, directly onto the icons (or shortcuts) of VICS.exe and VEND.exe. Of course, input files opened with this feature must have default extensions of VICS and VEND (refer to Appendixes A.1).

The above feature can be utilized only when the absolute path of folder VENUS\Programs is given to an environment variable 'VENUS'. In Windows NT/2000/ XP, the environment variable can be defined with a control panel named System (Advanced → Environment Variables in the case of Windows 2000). For example, 'VENUS' is set at C:\Program Files\VENUS\Programs\ when the VENUS folder is stored under folder C:\Program Files\ in the C drive. Never forget to put '\' as the last character. In Windows 98/Me, open AUTOEXEC.BAT at the root of a drive where Windows has been installed with a text editor and add a line for the environment variable, *e.g.*,

```
SET VENUS=C:\Program Files\VENUS\Programs\
```

After rebooting your PC, you can drag & drop input files onto the executable files.

Notes on the Graphical User Interface of VENUS

The Graphical User Interface (GUI) of VENUS has been constructed with GLUT (http://www.opengl.org/developers/documentation/glut.html) and GLUI (http://www.cs.unc.edu/~rademach/). GLUT is the OpenGL Utility Toolkit, a window system independent toolkit for writing OpenGL programs. It implements a simple windowing application programming interface (API) for OpenGL. GLUT makes it considerably easier to learn about and explore OpenGL programming. GLUT provides a portable API so that we can

write a single OpenGL program that works on both Win32 PCs and X11 workstations. GLUI is a GLUT-based C++ user interface library that provides controls such as buttons, checkboxes, radio buttons, and spinners to OpenGL applications. It is a window system relying on GLUT to handle all system-dependent issues, such as window and mouse management.

After launching VICS or VEND, two bars and two windows appear: Menu Bar ("VICS: Menu" or "VEND: Menu"), Dialog Bar, Graphics Window, and Output Window. In the case of the Output Window, the absolute path plus the program name appears as a title. An Info Bar is attached to the bottom of the Graphics Window to give the current size of the Graphics Window.

Sizes of the Graphics and Output Windows can be changed by dragging its edge or corner whereas those of the Menu and Dialog Bars cannot be changed manually. The Graphic Window is displayed in a full size by clicking the minimization–maximization button in its title bar; clicking this button once more reproduces the previous window size. The size and position of the Output Window can be stored by right-clicking its title bar and selecting Properties, where they can be specified (in the cases of Windows NT/2000/XP). The content of the Output Window can be copied to a clipboard and then pasted in a window for a file in a text editor or a word processor in the same manner as with the Command Prompt Window.

The Output Window corresponds to the DOS/Command Prompt Window when running VICS (or VEND) on Microsoft Windows.
If the GPU of your PC does not support the hardware acceleration of OpenGL, a message

```
Video configuration: GDI Generic
```

appears in the Output Window just after launching VICS (or VEND). If you PC includes a video card ELSA GLoria DCC supporting OpenGL acceleration, a message

```
Video configuration: DCC/AGP/SSE2
```

is issued in the Output Window. In the case of a notebook-type PC, Toshiba DynaBook 6/U22PDEW, equipped with GeForce4 460 Go, the following message is output:

```
Video configuration: GeForce4 460 Go/AGP/SSE2
```

Throughout this document, three symbols are used to show kinds of input data:

[ ]: a button (dotted lines appear after clicking it)

" ": a radio button and check box (words following it may be clicked to select it)

{ }: an input item (*e.g.*, a value or a name) including spinners and list boxes; you must sometimes press <Enter> to input a value certainly.

< >: a key in the keyboard

The current positions of all the dialog boxes excluding the Open/Save/Expoprt Dialogs are automatically saved during running VICS or VEND. They can further be saved in the Preferences Dialog Box.

Troubleshooting

A variety of important information including error messages is displayed in the Output Window. Please browse it whenever you encounter some troubles.

VENUS may not function properly with part of video cards; most of such troubles seem to arise from bugs of their drivers. Updating drivers to latest ones may solve the problems. If some failures occur with VENUS, please try to run it on another machine to check whether or not the trouble is caused by a bug in it.

Never click the close button at the upper right corner of the title bar in each window/bar! Clicking it not only closes the window but also terminates VICS/VEND without any warning. At present, we cannot solve this problem arising from a specification of the GLUT API. You should click [OK] or [Close] to close a dialog box, and click [exit] to quit VICS/VEND.

If you touch the keyboard or the mouse during saving a graphic data file, it may partly be damaged. Such a trouble most probably stems from a bug in the driver of your video card. In such cases, please wait until all the data have been saved in the file.

Feedback and Suggestions

The development of VENU has been led by user feedback. Its phenomenal success results from the response from around the country. I assume that things are working fine provided

that no feedback is received. If its users were so selfish as to behave like “black holes,” VENUS would not be improved very much. Please feel free to inform us of any bugs and your thoughts. Sending us files relevant to your troubles could facilitate the debug.

Encouraging responses would present us with driving forces for further development and refinement of VENUS.

Acknowledgments

We wish to thank the Independent JPEG Group (http://www.ijg.org/) and the JasPer Project (http://www.ece.ubc.ca/~mdadams/jasper/) for presenting the source codes of JPEG and JasPer libraries, respectively. Thanks are also due to Paul Bourke of the Swinburne Centre for Astrophysics and Supercomputing for providing us with valuable information about visualization technique and formats of graphic files, and some useful source codes at http://astronomy.swin.edu.au/~pbourke/. Masao Arai and Masataka Mizuno kindly coded file converters, wien2venus.py for WIEN2k and contrd for SCAT, respectively. Takuji Ikeda gave us example files for VEND. The development of VENUS was financially supported by the superconductivity research project of NIMS.

VICS: Visualization of Crystal Structures

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1. Outline of VICS

VICS is a program to visualize and manipulate crystal structures in three dimensions.

Crystal-structure files with a variety of formats can be imported by VICS. All the settings described in “International Tables for Crystallography,” Vol. A [1] are supported, including up to six different settings per space group in monoclinic and orthorhombic systems.

VICS allows you to represent crystal structures with five different models: ball-and-stick, space-filling, coordination polyhedra, wire-frame, and stick models.

Unique and powerful features of searching atoms and bonds beyond a boundary box are supported, making it possible to specify boundaries of drawing crystal structures flexibly and easily.

With VICS, graphic data files with nine image formats can be exported with a user-specified number of pixels.

2. Bars and Windows

2.1 Menu Bar

The Menu Bar includes the following buttons used to input, output, and edit various data:

[New]	Create a new data file
[Open]	Load crystal data from a file
[Save]	Save crystal data and various parameters/settings to a file with a VICS format
[Export]	Export crystal data to a file
[Image]	Export an graphic data to a file
[Edit]	Edit crystal data
[Bonds]	Specify and search bonds
[Preferences]	Show, edit, and save current and default settings
[About]	Short description on VICS
[Exit]	Exit VICS

2.2 Dialog Bar

The Dialog Bar is used to change various settings, manipulate and render objects in the Graphics Window, and calculate geometric data such as interatomic distances, bond angles, and torsion angles.

2.2.1 Properties Rollout

The Properties rollout includes the following buttons (see Section 4):

[General]	Open the General Dialog Box
[Atoms]	Open the Atoms Dialog Box
[Bonds]	Open the Bonds Dialog Box
[Polyhedra]	Open the Polyhedra Dialog Box
[Unit cell]	Open the Unit Cell Dialog Box

2.2.2 Models Panel

In the Models Panel, one of the following structure-drawing models (see Section 3) is selected:

"Ball-and-stick"
"Space-filling"
"Polyhedra"
"Wire-frame"
"Stick"

2.2.3 Plot Range

A boundary box within which objects are drawn is specified in the Plot Range Dialog Box that appears by clicking [Plot range].

2.2.4 Orientation

Clicking [Orientation] opens the Orientation Dialog Box to specify a direction of viewing objects.

2.2.5 Lattice Plane

A lattice plane is specified in the Lattice Plane Dialog Box resulting from clicking [Lattice Plane].

2.2.6 Manipulations Panel

The Manipulations Panel includes

buttons related to moving objects:

[Rotate]

[Magnify]

[Translate]

buttons to calculate

[Distance] (interatomic distances)

[Angle] (bond/torsion angles)

a button to

[Select] atoms, bonds, polyhedra, and a lattice plane

2.2.7 Rotation Modes Panel

Using the Rotation modes panel, you can select a rotation mode

"Drag"

"Push"

"Click"

and a rotation axis:

[Free]	Rotate objects around an arbitrary axis
[X axis]	Rotate objects around the *X* axis (from the left to the right in the Graphics Window)
[Y axis]	Rotate objects around the *Y* axis (upward direction in the Graphics Window)
[Z axis]	Rotate objects around the *Z* axis (perpendicular to in the Graphics Window)

2.3 Graphics Window

The Graphics Window is used to display crystal structures in three dimensions.

2.4 Output Window

The Output Window displays a title and crystal data described in Section 6. It also shows information about selected atoms and coordination polyhedra, *e.g.*, fractional coordinates, symmetry operations, and translation vectors.

3. Model Types

The Models panel in the Dialog Bar lists five models of representing crystal structures.

3.1 Ball-and-Stick Model

In the [Ball-and-stick] model, all the atoms are expressed as solid spheres or thermal ellipsoids (see Subsection 4.2). Default radii of spheres depend on the type of {Radii} in the General Dialog Box (see 4.1.6). They are equal to atomic/ionic radii multiplied by 0.4 for “Atomic” or “Ionic” and van der Waals radii multiplied by 1/4 for “van der Waals”. Bonds are expressed as either cylinders or lines (see Subsection 4.3).

3.2 Space-Filling Model

In the [Space-filling] model, atoms are drawn as solid spheres. Default radii of spheres depend on the type of {Radii} in the General Dialog Box (see 4.1.6). They are equal to atomic/ionic radii multiplied by 1.3 for “Atomic” or “Ionic” and van der Waals radii for “van der Waals”. This model is useful to understand how atoms are packed together in the structure.

3.3 Polyhedral Model

Click [Polyhedra] to show a polyhedral model, which is effective in understanding crystal structures by representing them with coordination polyhedra where central atoms, bonds, and apex atoms may also be included. Bonds between central and apex atoms have to be searched with the Search Bonds Dialog Box to display coordination polyhedra comprising them. Needless to say, the transparency of the coordination polyhedra must be high enough to make it possible to see the central atoms and bonds. One of six different modes for representing polyhedra can be specified in the Polyhedra Dialog Box described in Subsection 4.4.

3.4 Wire-Frame Model

In the [Wire-frame] model, atoms with no bonds are drawn as wire-frame spheres. Default radii of spheres depend on the type of {Radii} in the General Dialog Box (see 4.1.6). They are equal to atomic/ionic radii multiplied by 0.4 for “Atomic” or “Ionic” and van der Waals radii multiplied by 1/4 for “van der Waals”. Atoms bonded to other atoms are never drawn. All the bonds are presented as lines with gradient colors. This model is useful to see and manipulate complex and/or large structures.

3.5 Stick Model

In the [Stick] model, atoms with no bonds are drawn as solid spheres. Default radii of spheres depend on the type of {Radii} in the General Dialog Box (see 4.1.6). They are equal to atomic/ionic radii multiplied by 0.4 for “Atomic” or “Ionic” and van der Waals radii multiplied by 1/4 for “van der Waals”. Atoms bonded to other atoms are never drawn. All the bonds are expressed as cylinders, whose properties can be change in the Bonds Dialog Box. This model serves to see frameworks or molecular geometry.

3.6 Dot surface

In the ball-and-stick, wire-frame, and stick models, dot surface spheres are added with van der Waals radii in the same manner as with the space-filling model if "Show dot surface" is checked. This mode of showing van der Waals dots is designed to accentuate the outer surface. Individual spheres are represented as though they are hollow shells, with a mesh of dots on the surface. The combination of dot surface with the stick model is useful to understand how atoms are combined with each other in the molecule.

You will profit from a technique of altering the appearance of dot surface spheres by changing {Stacks} and {Slices} in the Parameters panel in the Atoms Dialog Box (see Subsection 4.2).

4. Properties of Objects

This section describes how to input/change various properties of objects in the Graphics Window.

Click the [Properties] rollout (with ‘+’) to open a subpanel including five buttons: [General], [Atoms], [Bonds], [Polyhedra], and [Unit cell]. To close the Properties subpanel, click the Properties rollout (with ‘–’) again.

VICS has a very convenient feature to redraw the current crystal structure in real time after changing any settings (preview mode). By default, the preview mode is active. It is, however, pointed out that a large amount of video memory is desirable to enjoy this feature when dealing with a large-scaled structure. This feature will slow down the redrawing of the structure. Unless you want to update objects on the fly, just uncheck "Preview" in Dialog Boxes Atoms (Subsection 4.2), Bonds (Subsection 4.3), and Polyhedra (Subsection 4.4). There is also check box "Preview" in the Lattice Planes Dialog Box (Section 10).

4.1 General Dialog Box

Click [General] to open the General Dialog Box. This dialog box is used to specify the color rendering of light and a background and objects such as atoms, bonds, coordination polyhedra, and unit cell, by changing reflectance properties and the direction of light.

4.1.1 Materials Panel

The Materials panel lets you change various properties of selected Objects, *i.e.*, atoms, bonds, polyhedra, or lattice plane, by changing the following four reflectance coefficients:

{Ambient} is a light that does not come from any particular direction. It has a source, but the rays of light have bounced around the room or scene and become directionless. Objects illuminated by ambient light are evenly lit on all surfaces in all directions.

{Diffuse} is a light that comes from a particular direction but is reflected evenly off a surface. Even though the light is reflected evenly, the object surface is brighter if the light is pointed directly at the surface than if the light grazes the surface from an angle.

{Specular} is a directional light, like diffuse light, but it is reflected sharply and in a particular direction. A highly specular light tends to cause a bright spot on the surface it shines upon, which is called the specular highlight.

{Shininess} is a property, which specify how small and focused the specular highlight. A value of 0 specifies an unfocused specular highlight. If this value is set, you reduce the size and increase the focus of the specular highlight, which causes a shiny spot to appear. The larger the value, the more shiny and pronounced the surface.

4.1.2 Light Panel

The Light panel is used to change light rendering: {Ambient} and {Diffuse} described above. The {Light direction} is changed using an arcball.

4.1.3 Background Panel

The background color is changed in this panel.

4.1.4 Projection Panel

Either of the following two projection modes is specified:

"Perspective projection"

"Parallel projection"

You can also set {Perspective}, which is a measure of the distance between your eyes and objects in the perspective projection mode.

4.1.5 "Show Compass" and "Show Axis Labels"

"Show compass" is used to turn on/off a display of three arrows indicating *a*, *b*, and *c* axes (or *x*, *y*, and *z* axes in the case of Cartesian coordinates).

"Show axis labels" is used to turn on/off a display of ‘a’, ‘b’, and ‘c’ (or ‘x’, ‘y’, and ‘z’ in the case of Cartesian coordinates).

4.1.6 Radii

List box {Radii} is used to select a type of default atomic radii from the following three:

Atomic	Metallic or covalent radii. Most values were taken from Ref. 2.
Ionic	Effective ionic radii compiled by Shannon [3] for representative oxidation states and coordination numbers
van der Waals	van der Waals radii [4]

The atomic, ionic, and van der Waals radii are contained in a text file elements.ini in folder VENUS\programs\ and edited using a text editor.

4.1.7 Depth-Cueing

The degree of depth-cueing (fog) is specified using the {Depth-cueing} spinner. Width depth-cueing, colors of objects can be changed, depending on distances from the eye. VICS supports linear depth-cueing according to equation:

$$\text{fog} = (\text{end} - l) / (\text{end} - \text{start}), \quad (1)$$

where l is the distance from the eye, start is the distance between the eye and the foremost object, and end is determined with the equation

$$\text{end} = l(\text{foremost object}) + f \times [l(\text{rearmost object}) - l(\text{foremost object})] / 2 \quad (2)$$

$$f = 1 + 2 \times (\{\text{depth-cueing}\} - 1) / 99. \quad (3)$$

The color of fog is the same as that of the background color.

4.2 Atoms Dialog Box

Click [Atoms] to open the Atoms Dialog Box.

4.2.1 Symbol and Radius

Select a symbol of an element from list box {Symbol} and specify its {Radius}.

4.2.2 Color Panel

The Colors panel is used to change colors of atoms.

4.2.3 Parameters Panel

{Stacks} and {Slices} are parameters common to all the atoms, allowing you to change the resolution (quality) of atoms displayed in the screen. {Stacks} denotes the numbers of subdivisions along the *Z* axis (similar to lines of latitude). {Slices} denotes the number of subdivisions around the *Z* axis (similar to lines of longitude). {Stacks} and {Slices} should be equal to each other in ball-and-stick and space-filling models where atoms are represented with perfect spheres.

4.2.4 Atom Style Panel

Select either of the following two radio buttons for the mode of displaying atoms on the Graphics Window: (1) "Show as balls" or (2) "Show as thermal ellipsoids".

Below these two, there are check box "Show outlines of ellipsoids" and {Probability}. The {Probability} for atomic nuclei to be included in the ellipsoids is common to all the atoms when drawing thermal ellipsoids.

For convenience, H and D (deuterium) atoms are always drawn as solid spheres even if the mode of displaying atoms is "Show as thermal ellipsoids". In this case, the radius of H or D can be changed according to the way described in 4.2.1

4.2.5 Preview

If "Preview" is checked, atoms in the Graphics Window reflect changes in settings in the Atoms Dialog Box in real time.

4.3 Bonds Dialog Box

Click [Bonds] to open the Bonds Dialog Box.

4.3.1 Bond Style Panel

One of four types of bonds can be selected in this panel:

"Unicolor cylinder"	Each bond is drawn as a cylinder, whose color can be changed in the Color panel.
"Bicolor cylinder"	Each bond is drawn as a cylinder with colors of two atoms connected with each other. This is the default setting when ∗.cc1, ∗.cc2, ∗.mol, ∗.pdb, and ∗.mld …(see Appendix A.1). To change the colors of the bond, those of atoms have to be changed (see Subsection 4.2).
"Color line"	Each bond is drawn as a line, whose color can be changed in the Color panel.
"Gradient line"	Each bond is drawn as a line connecting two atoms with gradient distribution of colors. To change this gradient color distribution, colors to be changed (see Subsection 4.2).

In addition, each H···X bond in the X–H···X hydrogen bond can be plotted with one of the following three line types in the Hydrogen bond style panel:

"Solid line"

"Dotted line"

"Dashed line"

The color of these lines is specified in the Color panel, and their width in {Line width} in the Parameters panel.

4.3.2 Parameters Panel

{Stacks} and {Slices} are the same parameters as described in Subsection 4.2.

The {Radius (B&S, poly)} of each cylindrical bond in the ball-and-stick (B&S) and polyhedra (poly) models may be changed on selection of {1-color cylinder} or {2-color cylinder} in the Bond type panel.

The {Radius (stick)} of each cylindrical bond in the stick model may be changed. This value has to be input independent of {Radius} described above because of a large difference between appropriate radii for the ball-and-stick/polyhedra and stick models.

The {Line width} of each bond represented with a line may be changed when {Color line}

or {Gradient line} is selected in the Bond type panel in the ball-and-stick and polyhedra models or when the wire-frame model is selected.

4.3.3 Color Panel

The Color panel is used to change colors of bonds.

4.3.4 Preview

If "Preview" is checked, bonds in the Graphics Window reflect changes in settings in the Bonds Dialog Box in real time.

4.4 Polyhedra Dialog Box

Click [Polyhedra] to open the Coordination Polyhedra Dialog Box.

4.4.1 Polyhedral Style

Click [Polyhedral style] to open the Polyhedral Styles Dialog Box. Click one of six styles to express coordination polyhedra:

Show atoms and bonds without any coordination polyhedra
Show atoms, bonds, and coordination polyhedra (default)
Show atoms and coordination polyhedra
Show central atoms and coordination polyhedra
Show only coordination polyhedra
Show only bonds represented as lines (for lines, see Subsection 4.3)

4.4.2 Opacity

The {Opacity} of coordination polyhedra is input with the value of 100 % corresponding to opaque planes (the inside of each coordination polyhedron is invisible) and that of 0 % corresponding to fully transparent faces (the coordination polyhedra are invisible).

4.4.3 Outlines

The {Outline width} for coordination polyhedra is input here. There is also a {Show outlines} check box.

4.4.4 Outline Color

The Outline Color panel is used to change colors of outlines for coordination polyhedra.

4.4.5 Preview

If "Preview" is checked, coordination polyhedra in the Graphics Window reflect changes in

settings in the Coordination Polyhedra Dialog Box in real time.

4.5 Unit Cell Dialog Box

Click [Unit cell] to open the Unit Cell Dialog Box, where some settings related to the outlines of the unit cell are changed.

4.5.1 Unit Cell Edges

Check box "Show unit cell edges" enables you to turn on/off displaying outlines of the unit cell in the Graphics Window.

4.5.2 Line Type

Unit cell edges can be plotted with three types of lines: "Solid lines", "Dotted lines", and "Dashed lines".

4.5.3 Width

The {Width} of the unit cell edges can be changed here. When a high-resolution image file is desired, a large width, *e.g.*, 4.0, must be input.

4.5.4 Colors

The Colors panel is used to change the color of outlines for the unit cell.

5. Load a Crystal Structure File

An Open Dialog Box appears by clicking [Open] in the Menu Bar. Select a file format (see Appendix A.1) and a file. Then, click [OK].

6. Create/Edit a Crystal Structure File

A new crystal structure file is created either by inputting all the crystal data in the New Data Dialog Box or by editing existing crystal data in the Edit Data Dialog Box.

Note that Cartesian coordinates have to be input from files with one of the following formats: Chem3D, MDL Molfile, MOLDA, Protein Data Bank, and XMol XYZ. For convenience, the space group in the Edit Data Dialog Box is always set at *P*1 (No. 1), with a result that lattice parameters and fractional coordinates displayed there are not actual

ones but virtual ones converted appropriately from the Cartesian coordinates by VICS. For XMol XYZ, The maximum coordinate, X_{max}, is determined from all the Cartesian coordinates, which are then divided by $1.5X_{max}$ regarded as a lattice parameter of the virtual cubic unit cell. If you want to change atomic coordinates, edit numbers recorded in the original files using a text editor.

To create a new crystal structure file, click [New] in the Menu Bar to open the New Data Dialog Box.

Click [Edit] to change an existing structure. Then, an Edit Data Dialog Box is opened.
The New Data and Edit Data Dialog Boxes have contents similar to each other, comprising several parts described below.

6.1 Title
A {Title} up to 70 characters is input for a structure to be visualized.

6.2 Space-Group Symmetry Panel
This panel contains information about crystal symmetry.

There are two ways of specifying the space group: using spinner {Number} and list box {Std. Symbol}.

List box {Std. symbol} contains all the standard settings of 230 space groups compiled in Ref 1. If a non-standard setting of the selected space group is preferred to the standard setting, your cell choice has to be specified in list box {Setting}.

As described above, structures for which Cartesian coordinates are input are always regarded as belonging to *P*1 (No. 1) having only one equivalent position (*x*, *y*, *z*) for convenience.

The number of available settings is automatically determined for the selected space group with the name and system of the space group for the current setting displayed automatically in two text boxes.

Before changing the setting number of a unit cell, be sure to check "Update parameters with current settings" prior to changing {Setting}, particularly in orthorhombic crystals.

For the monoclinic system, settings of **ab<u>c</u>** (*b*-axis unique) and **ab<u>c</u>** (*c*-axis unique) in cell choices listed in Table 4.3.2.1 in Ref. 1 are available. Information about these settings, *e.g.*, multiplicities, Wyckoff letters, and equivalent positions, is described in Chapter 7 in Ref. 1. When the unique axis for a monoclinic crystal is changed from the *b* axis to the *c* axis and *vice versa*, lattice parameters are automatically changed.

For the orthorhombic system, any of six settings, *i.e.*, **abc**, **ba$\bar{c}$**, **cab**, **$\bar{c}$ba**, **bca**, and **a$\bar{c}$b** listed in Table 4.3.2.1 [1] may be selected with setting numbers of 1, 2, 3, 4, 5, and 6, respectively. It is, however, pointed out that Chapter 7 [1] describes information about only the first standard setting, **abc**. Lattice parameters, *a*, *b*, and *c*, are automatically changed according to the new setting number.

On changes in crystal axes, *e.g.*, rhombohedral or hexagonal axes in a trigonal crystal, lattice parameters are automatically varied.

A crystal system and a space-group symbol are displayed below the setting number. The latter differs from the standard symbol when the setting number is not 1.

Regardless of crystal systems, lattice, fractional coordinates, and anisotropic atomic displacement parameters that have already been input are updated in accordance with the current setting of the space group provided that "Update parameters with current settings" has been checked (default setting). Thus, VICS can be used as a utility program to convert crystal data according to a change in crystal axes. Beware that we must click [Apply] to leave these parameters in memories (not in a file, ∗.vcs) after leaving the New Data or Edit Data Dialog Box.

Only in the case of orthorhombic compounds, lattice parameters are not updated by changing the setting number unless "Update parameters with current settings" has been checked.

6.3 Lattice Parameters Panel

In this panel, lattice parameters are input in Å (*a*, *b*, and *c*) or degrees (α, β, and γ). The number of lattice parameters input by the user depends on the crystal system, ranging from one in the cubic system to six in the triclinic system; the other lattice parameters are automatically set by VICS.

6.4 Settings for Thermal Motion

Check "Use anisotropic atomic displacement parameters" provided that anisotropic atomic displacement parameters are assigned to at least one site. Then, the type of anisotropic atomic displacement parameters must be specified in list box {Type}: 'U' to input U_{ij} (U_{11}, U_{22}, U_{33}, U_{12}, U_{13}, and U_{23}), and 'beta' to input β_{ij} (β_{11}, β_{22}, β_{33}, β_{12}, β_{13}, and β_{23}). Using this list box, we can convert U_{ij} into β_{ij} and *vice versa*.

The anisotropic Debye–Waller factor, $T(\boldsymbol{h})$, for the *hkl* reflection (reflection $\boldsymbol{h}$) is defined as

$$\begin{aligned} T(\boldsymbol{h}) &= \exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + \\ &\quad 2hla^*c^*U_{13} + 2klb^*c^*U_{23})] \\ &= \exp[-(h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + 2hk\beta_{12} + 2hl\beta_{13} + 2kl\beta_{23})], \end{aligned} \tag{4}$$

where a^*, b^*, c^*, α^*, β^*, and γ^* are the reciprocal lattice parameters. The isotropic Debye–Waller factor, $T(\boldsymbol{h})$, is defined as

$$T(\boldsymbol{h}) = \exp\left(-B\frac{\sin^2\theta}{\lambda^2}\right) = \exp\left(-\frac{B}{4d^2}\right) = \exp\left(-\frac{2\pi^2U}{d^2}\right), \tag{5}$$

where B and U are the isotropic atomic displacement parameters ($U = B/8\pi^2$), θ is the Bragg angle, λ is the X-ray or neutron wavelength, and d is the lattice-plane spacing. Isotropic and anisotropic atomic displacement parameters defined in different ways must be converted into U_{ij}, β_{ij}, B, and U defined above.

When isotropic and anisotropic atomic displacement parameters are mixed in crystal data of a compound, the type of isotropic atomic displacemen parameters, *i.e.*, B or U, must be specified, too. For this purpose, checkbox "Use B" is used; values of isotropic atomic displacement parameters are automatically changed in response to your selection. When the [Save] button is clicked to output ∗.vcs, U/Å^2 is automatically converted into B/Å^2 (if "Use B" has been unchecked).

6.5 Structure Parameters Panel

The following structural information is input in the Structure parameters panel for each crystallographic site:

{Label}: Site name (up to six characters)

{Symbol}: Symbol of an element (up to two characters)

{x}, {y}, and {z}: Fractional coordinates, *x*, *y*, and *z*, for which appropriate signifi-cant digits should be given, *e.g.*, 0.333333 for 1/3 and 0.666667 for 2/3.

{esd(x)}, {esd(y)}, and {esd(z)}: Estimated standard deviations, *s*, of the fractional coordinates (default values: zero). Note that the whole real number may be invisible; then you must slide the cursor to see up to its tail.

{g}: Occupancy, *g* (optional, unity for full occupation)

{B} or {U}: Isotropic atomic displacement parameter, *B* or *U* (in Å^2, optional)

{U11}, {U22}, {U33}, {U12}, (U13), and {U23}: Anisotropic atomic displacement parameters, U_{ij} (in Å^2, optional)

{beta11}, {beta22}, {beta33}, {beta12}, {beta13}, and {beta23}: Anisotropic atomic displacement parameters, β_{ij} (dimensionless, optional)

In addition to the above input data, the total number of atoms (sites) and an atom number for each atom (site) are displayed in the Structure parameters panel.

If the occupancy of a site is less than unity, atoms occupying that site are displayed as bicolor balls. If unicolor balls are preferred to bicolor ones, change the occupancy to unity for convenience. On the use of some video cards, dirty dots may appear on spheres for partially occupied sites. In such cases, change their occupancies at unity for convenience.

A site number is automatically assigned to each site in the asymmetric unit. Needless to say, U_{ij} or β_{ij} values described above must be input to represent a structure with thermal ellipsoids.

In sites for which anisotropic atomic displacement parameters, U_{ij} or β_{ij}, have been input, equivalent isotropic atomic displacement parameters, B_{eq} (if "Use B" has been checked) and U_{eq} (if "Use B" has been unchecked), converted from them are respectively displayed as *B* and *U* (nonchangeable).

6.6 Buttons for Manipulating New and Existing Sites

After entering all the data for the current site, click

[Add] to accept them.

[Update] to accept changes for an existing site (saved in the ‘memory’).

[Delete] to delete the site that has already been input.

Use navigation buttons

[>>]	Last site
[>]	Next site
[<]	Previous site
[<<]	First site

or list box {Site No.} to navigate through the sites that have already been entered.

6.7 Draw a Crystal Structure with the Current Structural Information

After entering all the crystal data, a new or modified crystal structure can be displayed by clicking [OK] in the New Data Dialog Box or [Apply] in the Edit Data Dialog Box, respectively. It should be noted that all the crystal data are stored in a scratch file at this moment; you need to save ∗.vcs by clicking [Save] to record them permanently. Atoms, bonds, coordination polyhedra, and so forth are calculated from the current lattice and structure parameters.

7. Interactive Manipulations

7.1 Rotate Objects

Click [Rotate] in the Dialog Window to rotate objects displayed on the Graphics Window. Four different rotation modes are available: [Stepwise], "Drag", "Push", or "Click". When "Drag", "Push", or "Click" is clicked, specify a rotation axis by clicking [Free], [X axis], [Y axis], or [Z axis]. [Free] means that objects can be rotated around arbitrary axes. On selection of the [X axis], [Y axis], or [Z axis], objects are rotated around each screen axis (refer to 2.2.7).

7.1.1 Stepwise Rotation

Click [Stepwise] to open the Stepwise Rotation Dialog Box. There are two modes for stepwise rotation: "Single step" and "Continuous". Objects are rotated only once by a step specified in {Step (deg)} in the "Single step" mode while they are rotated continuously with the step in the "Continuous" mode until the Stepwise Rotation Dialog Box is closed by Clicking [OK].

Input {Step (deg)} with which objects are rotated around each axis.

There are three buttons for the rotation axis: [X axis], [Y axis], and [Z axis]. Objects in the Graphics Window are rotated around the clicked axis.

7.1.2 Drag Mode

In the "Drag" mode, move the mouse while pressing the left mouse button to rotate objects in the Graphics Window. The objects are rotated, keeping with the mouse. They are never rotated after the mouse button has been released. In the [Free] rotation mode, the rotation axis becomes normal to the direction along which the mouse is moved.

7.1.3 Push Mode

In the "Push" mode, press the left mouse button at point 1 and move the mouse to point 2. In the [Free] rotation mode, objects are rotated around an axis perpendicular to a line connecting points 1 and 2, continuing to rotate even after the mouse button has been released. The rotation speed is proportional to the speed of moving the mouse.

The objects stop to rotate immediately by clicking the left mouse button at any point in the Graphics Window. On the use of a slow computer, it may be necessary to keep the mouse button pressed for a short time.

7.1.4 Click Mode

In the "Click" mode, click the left mouse button to rotate the objects. In the "Click" plus [Free] rotation modes, the rotation axis is perpendicular to a line connecting the click position and the central point. Note that selection of [Z axis] in the click mode practically results in that of [Free].

In this mode, the rotation speed depends on the rotation step, which can be changed in either the Stepwise Rotation Dialog Box or the Preferences Dialog Box.

To stop the rotation of the objects, (1) select either the "Drag" (recommended) or "Push" mode and (2) click the left mouse button at any point in the Graphics Window. Operation (1) is required because only clicking the left mouse button in the Graphics Window leads to a change in the rotation axis in this mode.

7.2 Magnify Objects

Click [Magnify]. Press the left mouse button and move the mouse. Objects are magnified in proportion to the distance of moving the mouse upward. On the other hand, objects are shrunk in inverse proportion to the distance of moving the mouse downward.

7.3 Translate Objects

Click [Translate]. Press the left mouse button and move the mouse. The objects will be

moved with the mouse along the same direction.

7.4 Select Objects

Click [Select] in the Dialog Bar and click an object such as an atom, a bond, or a coordination polyhedron to highlight it. Information about the selected object, *i.e.*, site name, fractional coordinates, symmetry operations, translation vector, interatomic distances (bond and coordination polyhedron), and so forth are output in the Output Window. When the atom is selected, its label, symbol, and fractional coordinates (x, y, z) are displayed on the Info Bar. When the bond is selected, its length is displayed with its estimated standard deviation, if any, on the Info Bar. Press <Shift> to select multiple objects; in this case, only information about the first object is displayed in the Output Window.

When a coordination polyhedron with a coordination number of n is selected, the following geometric information is displayed in the Output Window:

The volume of the coordination polyhedron.

The quadratic elongation, $\langle \lambda \rangle$ [6] (only for tetrahedra, octahedra, cubes, dodecahedra, and icosahedra)

$$\langle \lambda \rangle = \sum_{i=1}^{n} \frac{l_i / l_0}{n} \tag{6}$$

where n is the coordination number of the central atom, l_i is the distance from the central atom to the ith coordinating atom, and l_0 is the center-to-vertex distance of a regular polyhedron of the same volume.

The bond angle variance, σ^2 [6] (only for tetrahedra, octahedra, cubes, dodecahedra, and icosahedra),

$$\sigma^2 = \sum_{i=1}^{m} \frac{(\theta_i - \theta_0)^2}{m - 1} \tag{7}$$

where m is (number of faces in the polyhedron)×3/2 (*i.e.*, number of bond angles), θ_i is the ith bond angle, and θ_0 is the ideal bond angle for a regular polyhedron (for example, 90° for an octahedron or 109°28′ for a tetrahedron).

The volume of the coordination polyhedron, $\langle \lambda \rangle$, and σ^2 are useful when investigating structural changes under high/low temperature and high pressure.

A bond valence sum, *V*, is also obtainable in the [Select] mode. If a coordination polyhedron is clicked while pressing <Ctrl>, you are asked to input a bond valence parameter, l_0, [7] for its central metal. A CIF file storing bond valence parameters is available for download at http://www.ccp14.ac.uk/ccp/web_mirrors/i_d_brown/. A bond valence sum [7] for the central atom is calculated and displayed in the Output Window from all the bond lengths, l_i, for the current polyhedron and the bond valence parameter:

$$V = \sum_{i=1}^{n} \exp\left(\frac{l_0 / \text{Å} - l_i / \text{Å}}{0.37}\right) \tag{8}$$

Then, VICS prompts you for an oxidation number corresponding to *V* in Eq. (8); pressing the <return> key skips the subsequent calculation. After entering its value, an bond length expected with Eq. (8) is calculated and given in the Output Window.

To hide (not delete) the selected object(s), press <Delete>. To undo this operation, simply press <Esc>. If coordination polyhedra with central atoms and bonds for a specific chemical species are hidden manually, you can mix balls and sticks for those central atoms with coordination polyhedra of other chemical species.

7.5 Calculate Interatomic Distances

Click [Select]] in the Dialog Bar if another mode, *i.e.*, [Rotate], [Magnify], or [Translate], is effective. Click [Distance] in the Dialog Bar, and select two atoms A and B to highlight them. The interatomic distance (Å) between A and B is displayed on the Info Bar, and a line connecting atoms A and B is plotted on the screen. The estimated standard deviation of the interatomic distance [5] is output in a pair of parentheses if those of lattice and structure parameters have been input. The Output Window gives more detailed information about the interatomic distance. When more accurate estimated standard deviations of interatomic distances are desired, increase effective digits of lattice parameters and fractional coordinates in the Edit Data Dialog box (the same as with bond and torsion angles). To obtain a bond length in a ball-and-stick model, selecting the relevant bond (see 7.7) is faster than clicking two atoms.

7.6 Calculate Bond Angles

Click [Select]] in the Dialog Bar if another mode, *i.e.*, [Rotate], [Magnify], or [Translate], is effective. Click [Angle] in the Dialog Bar, and select three atoms A, B, and C to highlight them. The bond angle (degree) with atom B at the apex is displayed on the Info Bar with its estimated standard deviation, if any, and two lines connecting the three atoms are plotted on the screen. The estimated standard deviation of the bond angle [5] is output

in a pair of parentheses if those of lattice and structure parameters have been input. More detailed information about the bond angle is displayed in the Output Window.

7.7 Calculate Torsion Angles

For a sequence of four atoms A, B, C, and D, the torsion angle is defined as the angle between the normals to the planes to the planes ABC and BCD. By convention, the torsion angle is positive if the sense of rotation from BA to CD, viewed down BC, is clockwise; otherwise, it is negative.

Click [Select]] in the Dialog Bar if another mode, *i.e.*, [Rotate], [Magnify], or [Translate], is effective. Click [Angle] in the Dialog Bar and select four atoms, A, B, C, and D to highlight them while pressing <Shift>. The torsion angle (degree) for atom D and a plane on which atoms A, B, and C lie is displayed on the Info Bar with its estimated standard deviation, if any, and three lines connecting the four atoms are plotted on the screen. The estimated standard deviation of the torsion angle [5] is output in a pair of parentheses if those of lattice and structure parameters have been input. More detailed information about the torsion angle appears in the Output Window.

7.8 Move a Lattice Plane

Click [Select] in the Dialog Bar and press the left mouse button on a lattice plane to drag it. This operation is possible only when the Boundaries mode (Section 11) is active.

7.9 Display Atom Vectors

Click [Select] in the Dialog Bar. Press <Ctrl> and click an atom to open the Define Vector Dialog Box. In this dialog box, an arrow (vector) attached to each ball is specified. Such arrows serve to show magnetic moments or directions of static displacements. After attaching arrows to balls, click [Save] in the Menu Bar to save information about the vectors in a VICS text file.

7.9.1 Direction

Input u, v, and w in a lattice vector, $u\boldsymbol{a} + v\boldsymbol{b} + w\boldsymbol{c}$, to specify the direction of the vector.

7.9.2 Length

The {Length} (in Å) of the vector is input here.

7.9.3 Color

A color panel is used to change the color of the vector.

7.9.4 "Show vector"
"Show vector" is used to turn on/off displaying the vector.

Click [Apply] to make new settings (direction, length, and color) active.

8. Plot Range

Click [Plot Range] in the Dialog Bar to open the Plot Range Dialog Box. Input minimum and maximum fractional coordinates, *x*, *y*, and *z*.

9. Orientation

Click [Orientation] in the Dialog Bar to open the Orientation Dialog Box. This dialog box lets you specify a direction of viewing objects.

9.1 Manner of Specifying Directions
This direction may be entered in two different ways:

"Lattice vector"	Input *u*, *v*, and *w* in a lattice vector, $u\boldsymbol{a} + v\boldsymbol{b} + w\boldsymbol{c}$
"Plane normal"	Input indices, *h*, *k*, and *l*, in a reciprocal-lattice vector, $h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*$, perpendicular to the (*hkl*) plane

9.2 Upward Direction Panel
The upward direction on the screen is automatically selected by VICS when "Automatic selection" is checked whereas it is input by the user when "Manual selection" is checked.

9.3 Two Directions
Two directions, *i.e.*, the direction of projection (direction from the viewpoint to the projection plane) and the upward direction on the screen have to be specified:

For "Lattice vector"

Direction of projection	[u1], [v1], and [w1]
Upward direction on the screen	[u2], [v2], and [w2]. Input only when "Manual selection" is checked.

For "Plane normal"

Direction of projection	[h1], [k1], and [l1]
Upward direction on the screen	[h2], [k2], and [l2]. Input only when "Manual selection" is checked.

The current orientation is displayed in real time as a 3×3 matrix at the left-hand side of the Crystal Orientation Dialog Box.

9.4 Apply Button

The current orientation settings are reflected in the Graphics Window by clicking [Apply].

10. Lattice Plane

Click [Lattice plane] in the Dialog Bar to open the Lattice Plane Dialog Box. Click "Show lattice plane" to see a lattice plane specified by you in the Graphics Window.

10.1 Miller Indices

Input Miller indices *h*, *k*, and *l* for the lattice plane. Click [Apply] so that the (*hkl*) plane appears in the Graphics Window; the lattice-plane spacing, *d*, for the (*hkl*) plane changes simultaneously.

10.2 Location Panel

Either of the following two kinds of lattice planes is selected:

"Fixed"	The lattice plane that is the nearest from the origin is drawn within the unit cell.
"Movable"	The lattice plane can be moved within the boundary box by dragging it with a mouse. At first, VICS places the lattice plane with the central point of the boundary box laid on the plane. The direction of moving the plane is parallel to its normal.

10.3 Color Panel

The color of the lattice plane is changed here.

10.4 Opacity and Outline Width

The {Opacity} and {Outline width} of the lattice plane can be changed here.

10.5 Display Options

Check "Show (–h –k –l) plane" to display the $(\bar{h}\bar{k}\bar{l})$ plane instead of the (hkl) plane on the selection of the "Fixed" radio button in Subsection 10.2.

Outlines of the lattice plane will be plotted by checking "Show outlines".

10.6 Preview

If "Preview" is checked, the lattice plane in the Graphics Window reflects changes in settings in the Lattice Plane Dialog Box in real time.

11. Search Bonds

Click [Bonds] in the Menu Bar to open the Search Bonds Dialog Box.

11.1 Add New Bonds Panel

One of the following three search modes is selected in the Search mode subpanel:

"Search A2 bonded to A1"

A2 atoms bonded to A1 atoms inside the boundary box are searched on the basis of the user-specified maximum interatomic distance, {Max. distance}. If "Search beyond the boundary" is checked, A2 atoms outside the boundary box are searched in addition to those within the box. If "Search beyond the boundary" is not checked, A2 atoms only inside the boundary box are searched.

"Search atoms bonded to A1"

All the atoms bonded to A1 atoms lying within the boundary box are searched on the basis of the user-specified {Max. distance} regardless of the box. That is, A2 atoms outside the box are searched in addition to those inside the box. No A2 atom is specified in this case.

"Search molecules"

All the atoms in molecules that contain atoms within the boundary box are searched reiteratively on the basis of the user-specified {Max. distance}. Neither A1 nor A2 is specified in this case.

Atoms {A1} and {A2} are specified in the "Search A2 bonded to A1" mode, only atom {A1} is specified in the "Search atoms bonded to A1" mode, and neither {A1} nor {A2} is specified in the "Search molecules" mode. {Max. distance} has to be input in the unit of Å in all the modes.

For typical interatomic distances in metals and alloys, inorganic, organic, and organometallic compounds, and complexes, refer to Ref. 8.

The "Search atoms bonded to A1" should be used when drawing coordination polyhedra where each A1 atom is coordinated to two or more ligands. For example, Ca in fluorapatite $Ca_5F(PO_4)_3$, is coordinated to six O atoms in phosphate ions and one F atom. A {Max. distance} of 2.7 Å is appropriate in this case.

In the case of "Search molecules", a maximum distance of 1.6 Å is appropriate in typical organic compounds containing H, C, N, and O atoms; Inputting a larger value might lead to generation of unreal bonds. If larger atoms such as P, S, and Cl are involved, it is necessary to add A1–A2 bonds by selecting "Search A2 bonded to A1".

The "Search molecules" mode should never be applied to inorganic compounds or metals because the infinite number of atoms is searched, which will stop VICS.

Click [Add] to add the data in the current Add New Bonds panel to a search list. Beware that [Add] may be clicked only once on selection of "Search molecules".

11.2 Search List

After editing two or more sets of bonds in the Search list panel, click

[Update] to update a set of bonds

[Delete] to delete a set of bonds

Use navigation buttons, [>] (next set) and [<] (previous set), to navigate through the sets that have already been entered.

No coordination polyhedra containing A1–A2 bonds are displayed on the selection of ‘No’ for "Show polyhedra". No A2 atoms are searched beyond the boundary box when selecting ‘No’ for "Beyond the boundary".

After entering all the data related to bonds, we can display a modified crystal structure by clicking [OK].

The Search Bonds Dialog Box cannot be used to edit or input data related to searching bonds when files with Chem3D, MDL Molfile, MOLDA, and PDB formats are input by VICS. These data may be changed after files with VICS format, ∗.vcs, have been saved and input again by VICS.

11.3 Display Hydrogen Bonds

To display X−H···Y hydrogen bonds, select the "Search A2 bonded to A1" mode in the Search mode subpanel, set A1 at H and A2 at Y, input the maximum H···Y distance in {Max. distance}, click [Add], check "Show hydrogen bonds", and click [OK]. Then, X−H bonds are plotted as cylinders or lines in response to the selected bond style (see subsection 4.3.1), and H···Y bonds as solid, dotted, or dashed lines according to the selected hydrogen bond style (see subsection 4.3.1). Unless "Show hydrogen bonds" is checked, the H···Y bonds are drawn in the same way as with the X−H bonds.

12. Save Crystal Data and Various Settings

To save a VICS text file, *.vcs, storing crystal data and various settings, click [Save] in the Menu Bar.

13. Export Crystal Data

VICS allows you to export crystal data with four formats:

Chem3D
CIF
User input file, ∗.ins, for RIETAN-2000/2001T
XMol

To export the structural data, click [Export] in the Menu Bar.

The feature of outputting ∗.ins enables us to read in crystal data files of various formats with VICS, simulate powder diffraction patterns, and carry out subsequent Rietveld refinements with RIETAN-2000. It should be pointed out that fractional coordinates in part of crystal data recorded in databases have too small significant digits, *e.g.*, 0.3333 instead of 0.333333. In such a case, please increase the significant digit to 6 or 7 before outputting ∗.ins.

Outputting files with the XMol format serves for converting fractional coordinates into Cartesian coordnates.

14. Export Structural Images

Structural images drawn in the Graphics Window can be saved in files with a variety of graphics formats.

Click [Image] in the Menu Bar, select an image format from a list, input/specify a file name, and click [OK]. Then, the Export Graphics Dialog Box is opened. Here, {Smoothing} and {Scale} are input. The number of pixels displayed at the Info Bar is multiplied by the scale factor. Click [Save] finally.

The typical value of {Smoothing} is 1–3 in the presence of unit-cell edges, which become more vague with increasing {Smoothing}. For colored edges, {Smoothing} may be somewhat increased. The maximum value of {Scale} is 10, which yields huge images comprising a number of pixels.

A new Export Graphics Dialog Box is opened after saving the structural images. Click [OK] to continue.

15. Preferences

Default settings can be changed in the Preferences Dialog Box.

Click [Preferences] in the Menu Bar. Select "Show default settings" and "Show current settings" radio buttons to see default and current settings, respectively. Default settings can be restored by clicking [Restore default settings]. Current settings can be saved as defaults by clicking [Save as defaults].

Items from "Show compass" to {Default ext.} are common to the default and current settings. VICS has to be restarted to make all the default settings effective.
A template file for ∗.ins (user input file of RIETAN) output by VICS is specified as the first item. Parts of a space group, and lattice and structure parameters are updated on the basis of current crystal data.
Note that resolutions of objects (atoms and cylinders) for graphics files are input only in this dialog box: Atom stacks/slices and Bond stacks/slices.

Select "Background" (default), "Unit cell", "Polyhedra", "Lattice plane", or "Bonds" in the

Settings Panel. Items irrelevant to the current selection are made ineffective.

All the bonds for atoms whose Cartesian coordinates have been input from .cc1/.cc2, ∗.mol, ∗.pdb, and ∗.xyz (refer to Appendix A) are automatically searched on the basis of {Max. distance} just below the check box provided that "Startup search for bonds" is checked and that these files include information on bond. As described in Section 11, a {Max. distance} value of 1.6 Å will be suitable for typical organic compounds comprising H, C, N, and O atoms.

The current positions of the Menu and Dialog Bars, and Graphic Window can be saved by checking "Save bars/window positions" and then clicking [Save] or [Save as defaults]. In the case of the Graphic Window, its dimension is also saved.

The current positions of all the dialog boxes can be saved in the preference file by checking "Save dialog bar positions" followed by clicking [Save] or [Save as defaults].

16. Running VICS Using a Command

VICS is launched not only by double clicking its icon but entering a command containing one or two arguments in the DOS/Command Prompt Window:

```
VICS file_name
VICS file_name file_format_ID
```

The first form may be used provided that the extension of the file name is the same as that listed in Appendix A.1 for each format. For example, VICS can be run by entering the following command:

```
VICS YBa2Cu4O8.cif
```

The second format, where <file_format_ID> is an identification number for a file format (Appendix A.1), is alternatively used for any file name whose extension is arbitrary.

Appendix A. File Formats

A.1 Import-File Formats

file_format_ID	Extension	Format
0	vcs	VICS text file
1	amc	American Mineralogist Crystal Structure Database (AMCSD) [9]
2	cc1/cc2†	CambridgeSoft Chem3D [10]
3	cif	Crystallographic Information File (CIF) [11]
4	cmt	CrystalMaker [12] text file
5	cry	Inorganic Crystal Structure Database ICSD-CRYSTIN [13]
6	cssr	Crystal Structure Search and Retrieval (CSSR) [14]
7	csd/fdt	Cambridge Structural Database [15] CSD/FDAT
8	cube/cub	Gaussian 98 Cube file [16]
9	ics	Inorganic Crystal Structure Database (ICSD) [17]
10	mol†	MDL Information Systems [18] Molfile
11	min	Crystallographic Database for Minerals (MINCRYST) [19]
12	mld†	MOLDA [20]
13	pdb†	Protein Data Bank (PDB) [21]
14	ins	User input file, ∗.ins, of RIETAN-2000/2001T
15	struct	WIEN2k [22] struct file
16	xyz*	XMol XYZ [23]
17	asse	asse [24]
18	n/a	Files named ‘f01’ (input file for MAKEF05) used in SCAT [25,26] for the DV-X□ method. Boundaries and the position of the origin are input from an input file, ‘c04d’, for contrd if any.
19	n/a	File named ‘FILE07.dat’ output by a molecular dynamics program MXDORTO [27,28]

The extensions may also be described in capital letters, but mixing lowercase and capital letters is inhibited. In files with extensions attached with '∗', molecules are automatically searched using the default value of the maximum distance provided that "Startup search for bonds" are checked in the Preferences Dialog Box (time-consuming in large molecules. Refer to Section 11). Information about bonds in files with the formats marked with † is always utilized, if any.

Beware that the default extension appearing in the Open Dialog Box can be specified in the Preferences Dialog Box: {Default ext.}.

Checking space group names is particularly important when importing crystal data. For example, in ∗.cmt, '–' (given instead of 'bar') is never included in space group names, *e.g.*, 'F m 3 m', which should be changed into 'F m –3 m' ($Fm\bar{3}m$) by yourself using a text editor. The lack in '–' in space group names is also the case on the use of the data base file, spgri, where information about 230 space groups were taken from Ref. 29 when specifying space groups in ∗.ins.

Two retrieval programs, RETRIEVE for MS-DOS and FindIt for Windows, of ICSD output text files with quite different formats. VICS is capable of reading in both types of the crystal data files. In these files, ∗.ics, AMCSD text files, ∗.amc, extra characters are sometimes attached to space group names, *e.g.*, 'P 42/n m c S', which should be 'P 42/n m c' ($P4_2/nmc$). In addition, full Hermann-Mauguin space-group symbols are sometimes given in ICSD text files. In such a case, an error message appears either in the Output Window (RETRIEVE format) or in a message box (FindIt format). Read it carefully to proceed to a next operation.

In part of AMCSD and MINCRYST text files, extra characters are attached to space group names, and non-standard space-group symbols are used. In such a case, an error message appears in the Output Window. It is recommended that such space group names are changed appropriately. Then, change the setting number in the Edit dialog box if necessary. Sometimes, you have to convert fractional coordinates by yourself if a non-standard setting that is not described in the International Tables, Vol. A is adopted.

In a file with the CSSR format, a setting numbers may be given after 'OPT ='. Unfortunately, we have no information about setting numbers in this format. Then, please change it in the [Edit] dialog box if necessary.

CIF and PDB have a variety of formats for crystal data. You can get detailed information about CIF and PDB from http://www.iucr.org/iucr-top/cif/ and http://pdb.protein.osaka-u.ac.jp/pdb/info.html#File_Formats_and_Standards, respectively. For example, CIF files may contain Cartesian coordinates, but VICS cannot input them. Note that VICS does not support all the formats allowed in these two formats. For example, Cartesian coordinates included in CIFs cannot be input with VICS; only fractional coordinates should be given in CIFs. For readable formats, refer to ∗.cif in VENUS\examples\VICS\CIF and ∗.pdb in VENUS\examples\VICS\PDB.

In the case of ∗.cif and ∗.ins containing multiphase data, only the crystal data of the first phase are input.

CIFs created by SHELX-97 [30] have to be modifed. First, 'line_chemical_name_common' should be not '?' but a compound name; For example,

```
_chemical_name_common 'Nd2CuO4'
```

Second, a CIF should contain line with the space group number or space group name defined formally; for example,

```
_symmetry_space_group_number 12
_symmetry_space_group_name_H-M 'P 21/n'
```

In ∗.ins, the volume name of International Tables should be not 'I' but 'A'. For example, 'A-230-2' is input for the second setting of space group $Fd\bar{3}m$. The input of 'I-230-2' causes an error. Lattice parameters must be given within one line in the following way:

```
CELLQ  9.36884  9.36884  6.88371  90.0  90.0  120.0  0.0  1010000
```

After Rietveld analysis, lattice and structure parameters in ∗.vcs are automatically updated provided that ∗.vcs and ∗.ins share the same folder.

The main purpose of reading in ∗.cube and f01 is to obtain ∗.vcs which is, in turn, input by VEND to overlap isosurfaces with a ball-and-stick or stick model.

VICS need to read in c04d, which is an input file of contrd, in addition to f01 if a structural model recorded in ∗.vcs is later input by VEND to overlap two different kinds of images (for details in contrd, refer to VENUS\contrd\Readme_contrd.txt). The dimensions of a boundary box (an area where 3D data are output to text files) in c04d are required to make images created with VICS consistent with those displayed with VEND. Of course, c04d and f01 should be placed in the same folder. If c04d has not been input by VICS, the

following error message appears in VEND: “Dimensions of cuboids in ∗.vcs and ∗.scat files do not agree with each other.”

All the atoms recorded in f01 must be included within the above boundary box. Otherwise, the following error message is output: “Part of atoms outside the boundary box specified in c04d.”

Neither space group numbers nor space group names are included in files with the following formats: Chem3D, Gaussian 98 Cube file, MDL Molfile, MOLDA, WIEN2k struct file, XMol XYZ, asse, SCAT f01 file, and MXDORTO FILE07.dat. For convenience, VICS regards the space group as P1 (Triclinic) for these file formats.

A.2 Export-File Formats

cif
ins
pdb
xyz

A.3 Image-File Formats

BMP
EPS
JPEG
JPEG 2000 [31]
PPM
RAW
RGB (SGI)
TGA
TIFF

Sizes and resolutions of images saved in the above formats can be altered with graphic programs and utilities such as Adobe Illustrator (Adobe Systems Incorporated), Paint Shop Pro (Jasc Software, Inc.), GraphicConverter (http://www.lemkesoft.com/), and IrfanView (http://www.irfanview. com/).

Appendix B. Program Specifications

Maximum number of atoms	9 000
Maximum number of atoms in the asymmetric unit	1 200
Maximum number of chemical species	99
Maximum number of bonds	12 000
Maximum number of bonds of each atom	25
Maximum number of bond specifications	21
Maximum number of polyhedra	2 500
Maximum number of polyhedral faces per polyhedron	50
Maximum number of vertices per polyhedral face	100
Maximum number of selected objects	100
Maximum number of deleted objects	500

Appendix C. Files in the Programs Folder

VICS.exe	Executable binary file of VICS
elements.ini	Default values of atomic radii [2–4] and colors
preferences_VICS.ini	Default settings in VICS
spgra.dat	File storing information about 230 space groups [1]
spgro.dat	File storing non-standard settings of the orthorhombic system

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VEND: Visualization of Electron/Nuclear Densities

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Appendix A. File Formats

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References

1. Outline of VEND

VEND is a program to visualize densities of electrons and atomic nuclei in three dimensions.

The electron density (strictly speaking, the number density of electrons) is the number of electrons per unit volume with a unit of $Å^{-3}$ or $(a.u.)^{-3}$, where 1 a.u. = a_0 = 5.2917721□10^{-11} m = 0.52917721 Å (a_0: Bohr radius). For convenience, the value of bound coherent scattering lengths, b_c, per unit volume with a unit of fm $Å^{-3}$ is referred to as the nuclear density here.

With VEND, three-dimensional (3D) distribution of electron/nuclear densities is represented by drawing isosurfaces with a user-selected equi-density level. Two-dimensional (2D) electron/nuclear distribution on boundary sections at unit cell edges is additionally displayed.

One of great advantages of VEND over other visualization tools is a feature to overlap isosurfaces with ball-and-stick and stick models drawn with VICS.

Furthermore, two-dimensional maps and bird's-eye views for densities summed up in a user-specified range along a direction can alternatively be displayed in separate windows.

VEND is capable of reading in data files listed in Appendix A: ∗.den output by MEED [1], MEEDCAB and MEND [2], ENIGMA [3], and our own program PRIMA [4,5] for the maximum-entropy method (MEM), ∗.cube created with Gaussian 98 [6] for *ab initio* molecular orbital methods, 3D data files, ∗.scat, storing results acquired with DVSCAT [7,8] plus contrd [9] for the discrete variational X□ (DV-X□) method plus contrd, and ∗.rho obtained using a full-potential linearized augmented plane wave package, WIEN2k [10]. We are willing to make it possible to read in files with other formats; any suggestions as to new file formats are welcome.

VEND allows us to visualize not only electron/nuclear densities but also electrostatic potentials and wave functions (molecular orbital) calculated with Gaussian 98 and DVSCAT plus contrd. It also enables us to display any other 3D physical quantities such as Patterson functions. Therefore, the word "density" in this manual may mostly be replaced with another physical quantity from now on.

With VEND, graphic data files with nine image formats can be exported with a user-specified number of pixels.

2. Bars and Windows

2.1 Menu Bar

The Menu Bar includes the following buttons used to input, output, and edit various data:

[Open]	Load electron/nuclear densities from a file
[Save]	Save data to a file with the VEND format
[Image]	Export an electron/nuclear-density image (a graphic data) file
[VICS]	Import a ball-and-stick model from a file of the VICS format
[2D]	Open the 2D Projection Dialog Box
[Info]	Show main information
[Preferences]	Show, edit, and save current and default settings for VEND
[About]	Short description on VEND
[Exit]	Exit VEND

2.2 Dialog Bar

The Dialog Bar is used to change various settings, and manipulate and render objects in the Graphics Window.

2.2.1 Properties Rollout

The Properties rollout includes the following buttons (see Section 4):

[General]	Open the General Dialog Box
[Isosurfaces]	Open the Isosurfaces Dialog Box
[Slices]	Open the Slices Dialog Box
[Unit cell]	Open the Unit Cell Dialog Box

2.2.2 Models Panel

In the Models Panel, one of the following radio buttons for drawing models is selected:

"Surface"
"Frame"
"Mesh"

Uncheck "Show Isosurfaces" not to show isosurfaces in the Graphics Window.

Uncheck "Show sections" not to show sections (boundaries) in the Graphics Window. This option is convenient when a structural model and isosurfaces overlap each other because sections of isosurfaces become transparent.

Check "Show model" to overlap ball-and-stick models with isosurfaces (see Section 6).

2.2.3 Orientation

Clicking [Orientation] opens the Orientation Dialog Box to specify a direction of viewing objects.

2.2.4 Manipulations Panel

The Manipulations panel includes the following buttons related to moving objects:

[Rotate]
[Magnify]
[Translate]

2.2.5 Rotation Modes Panel

Using the Rotation modes panel, you can select a rotation mode

"Drag"
"Push"
"Click"

and a rotation axis:

[Free]	Rotate objects around an arbitrary axis
[X axis]	Rotate objects around the *X* axis (from the left to the right in the Graphics Window)
[Y axis]	Rotate objects around the *Y* axis (upward direction in the Graphics Window)
[Z axis]	Rotate objects around the *Z* axis (perpendicular to in the Graphics Window)

2.3 Graphics Window

The Graphics Window displays isosurfaces with or without (1) planes (slices) and/or (2) atoms and bonds. In (1), two-dimensional distribution of densities on the user-specified planes is drawn by changing colors gradually with increasing density. A ball-and-stick model drawn with VICS may be imported in (2).

2.4 Output Window

The Output Window displays a title, numbers of pixels along *a*, *b*, and *c* axes, lattice parameters, numbers of triangles for isosurfaces, and numbers of polygons for slices and so forth.

3. Definitions

This section describes various settings for visualization of electron/nuclear densities.

3.1 Isosurface Level, *d*(iso)

Electron/nuclear densities on isosurfaces are equal to the isosurface level, *d*(iso). All the points with densities larger than *d*(iso) lie inside the isosurfaces whereas those with densities smaller than *d*(iso) are situated outside the isosurfaces.

3.2 Scale Factor, *f*(section), for *d*(iso)

This factor is used to modify the correspondence between densities on boundary sections of isosurfaces and colors in a palette. Its default value is unity. The color index, *I*(color), for a data point with a density of *d* is calculated from the minimum density, d_1 (default value: isosurface level), and the maximum density, d_2:

$$I(\text{color}) = \min\{1, (d - d_1)/[f(\text{section})\times(d_2 - d_1)]\}, \quad (1)$$

where function min{*A*, *B*} is equal to *A* if $A < B$ and to *B* if $A > B$. In the present case, $A = 1$. The color of each point is determined from its color index, *e.g.*, blue for 0, green for 0.5, and red for 1 in the case of the Rainbow Palette (see 3.3.1).

The full-scale density decreases with a decrease in *f*(section). Data points with densities greater than this full scale become red (see 3.3.1 Rainbow Palette), blue (see 3.3.2 Inverse Rainbow Palette), or black (see 3.3.3 Gray Palette).

Color distribution on two-dimensional planes (slices) including boundary ones can be changed by setting *f*(section) at an appropriate value.

3.3 Palettes

Palettes are used to represent two-dimensional density distribution by use of colors. Three different palettes are available: Rainbow, Inverse Rainbow, and Gray.

3.3.1 Rainbow Palette

This is often referred to as “hot-to-cold” palette. In this palette, points with the highest *I*(color) of unity are red, those with the intermediate *I*(color) of 0.5 are green, and those with the lowest *I*(color) of 0 are blue. This method of expressing two-dimensional distribution of physical quantities is very intuitive.

3.3.2 Inverse Rainbow Palette

As the name of this palette shows, colors are assigned reversely in comparison with the Rainbow palette. That is, points with the lowest *I*(color) of unity are red, those with the intermediate *I*(color) of 0.5 are green, and those with the highest *I*(color) of 0 are blue.

3.3.3 Gray Palette

This palette is used to represent density distribution with only black, gray, and white colors. Points with the highest *I*(color) are black while those with the lowest *I*(color) are white.

3.4 Scale Factors for the Isosurface Level and *f*(section)

To browse two-dimensional distribution of electron/nuclear densities, open the Cross Section Window, where two kinds of scale factors are input:

Scale factor for isosurface level
Scale factor for *f*(section)

VEND enables you to see distribution of densities smaller than *d*(iso) on a two-dimensional plane. For this purpose, d_1 must be changed. As described above, the default value of d_1 is the isosurface level, *d*(iso) (see Subsection 3.2). In VEND, d_1 is multiplied by the scale factor, *s*(iso), for the isosurface level

$$d_1 = s(\text{iso}) \times d(\text{iso}). \qquad (2)$$

The default value of *s*(iso) is zero, which means that all the density data are displayed. It should be pointed out that this scaling is not associated with the correspondence between densities and colors described below.

The value of *f*(section) described in Subsection 3.2 is specified such that relatively large densities on sections (unit-cell edges) inside isosurfaces are appropriately visualized. Usually, *f*(section) is too large to visualize distribution of electron/nuclear densities on planes (slices) specified by the user; a decrease in the full-scale density is indispensable to visualization of low-level densities, *e.g.*, those of bonding and delocalized electrons.

Color distribution on two-dimensional plane can be changed by setting a scale factor, *s*(section), for *f*(section). The default value of *s*(section) is unity. The color index, *I*(color), for a data point with a density of *d* is evaluated as

$$I(\text{color}) = \min\{1, (d - d_1) / [s(\text{section}) \cdot f(\text{section}) \cdot (d_2 - d_1)]\}. \quad (3)$$

4. Properties of Objects

This section describes how to change various properties of objects displayed in the Graphics Window by setting various flags and parameters. Click the Properties rollout (with '+') to open a subpanel including a set of buttons. To close the Properties subpanel, click the Properties rollout (with '–') again.

VEND has a convenient feature to redraw objects in real time just after changing any settings (preview mode). By default, the preview mode is active. It is, however, pointed out that a large amount of video memory is desirable to enjoy this feature when dealing with a large-scaled figure. This feature will slow down the redrawing of density distribution. Unless you want to update objects on the fly, just uncheck "Preview" in Dialog Boxes Isosurfaces (Subsection 4.2) and Slices (Subsection 4.3).

4.1 General Dialog Box

With the General Dialog Box, color rendering of light can be adjusted by changing reflectance properties:

4.1.1 Light Panel

{Ambient} is a light that does not come from any particular direction. It has a source, but the rays of light have bounced around the room or scene and become directionless. Objects illuminated by ambient light are evenly lit on all surfaces in all directions.

{Diffuse} is a light that comes from a particular direction but is reflected evenly off a surface. Even though the light is reflected evenly, the object surface is brighter if the light is pointed directly at the surface than if the light grazes the surface from an angle.

The direction of light in this dialog box can also be changed with an arcball.

4.1.2 Background Panel

Background colors for the "Graphics window", "2D map window", and "Bird's-eye view

window" are also changed here.

4.1.3 Projection Panel

Either of the following two projection models is specified:

"Perspective projection"

"Parallel projection"

You can also change {Perspective}, which is a measure of the distance between your eyes and objects.

4.1.4 "Show Compass" and "Show Axis Labels"

"Show compass" is used to turn on/off a display of three arrows indicating *a*, *b*, and *c* axes (or *x*, *y*, and *z* axes in the case of Cartesian coordinates).

"Show axis labels" is used to turn on/off a display of ‘a’, ‘b’, and ‘c’ (or ‘x’, ‘y’, and ‘z’ in the case of Cartesian coordinates).

4.2 Isosurfaces Dialog Box

4.2.1 Number of Cells Panel

Input the numbers of cells along the {a axis}, {b axis}, and {c axis}

4.2.2 Boundaries

Either of two boundary options is selected:

"Shift the origin": The origin is shifted by fractional coordinates, {x}, {y}, and {z}, in the Origin panel

"Change boundaries": Boundaries for displaying densities are input in the Inside boundaries panel

Origin panel: Shift the origin along the *a*, *b*, and *c* axes by {x}, {y}, and {z} (in fractional coordinates)

Inside boundaries panel: Input drawing boundaries as fractional coordinates, {x(min)}, {x(max)}, {y(min)}, {y(max)}, {z(min)}, and {z(max)}, between 0 and 1 after selecting "Change boundaries". These boundaries are set inside the unit cell(s) specified in 4.2.1. To accept the changes, click the [Apply] button.

4.2.3 {Isosurface level} and {*f*(section)}

They have been explained in detail in Subsections 3.1 and 3.2. If the input file contains both positive and negative data, the absolute value of the isosurface level is input. If only positive and only negative data and included in the file, {Isosurface level} should be positive and negative, respectively. To make the changes effective, click the [Apply] button.

4.2.4 Kinds of isosurface level

One of three kinds of isosurface level is selected:

"Positive & negative data": show isosurfaces for both positive and negative data (default)

"Positive data": show only isosurfaces for positive data

"Negative data": show only isosurfaces for negative data

These radio buttons are made active only when the input file contains both positive and negative data.

4.2.5 Rendering of Isosurfaces

The Color panel is used to change the representation of isosurfaces: "Ambient", "Diffuse", "Specular", or "Emission"; we can specify a color to each of these four.

{Opacity}, and {Shininess} are specified below the Color panel.

In the cases of data having both positive and negative values (*e.g.*, electrostatic potentials and wave functions), the color specified in the Color panel is that applied to positive isosurfaces. Red, green, and blue components of the color for negative isosurfaces are automatically determined in the following ways:

Red(–) = 100 % – Red(+)
Green(–) = Green(+)
Blue(–) = 100 % – Blue(+)

For example, if
Red(+) = 100 %, Green(+) = 0 %, and Blue(+) = 0 %: red isosurfaces
then
Red(–) = 0 %, Green(–) = 0 %, and Blue(–) = 100 %: blue isosurfaces

4.2.6 Preview

If "Preview" is checked, isosurfaces in the Graphics Window reflect changes described in

4.2.4 (in the case of Gaussian 98 cube files, click the [Apply] button).

4.3 Slices Dialog Box

The Slices Dialog Box is used to specify two-dimensional sections added to isosurfaces.

4.3.1 Planes Panel

To specify sections, we input their Miller indices, {h}, {k}, and {l}, in the Planes panel or simply select from [(100)], [(010)], and [(001)] planes. The Miller plane can be shifted along a direction perpendicular to it by setting a value in {Shift}.

Click [Show planes] to see the planes specified in this way. If you have selected a (100), (010), or (001) plane, it is automatically shown, extending beyond one unit cell when two or more unit cells are displayed. On the other hand, an (*hkl*) plane is drawn within only one unit cell.

Because atomic nuclei are generally concentrated within small volumes, hardly any atomic nuclei are visible between two crystallographic sites. Nuclear densities spread over large volumes in highly disordered compounds showing static and dynamic disorder, *e.g.*, superionic conductors.

Click [Add to list] to put the specified planes into the planes list. The number in parentheses following [Add to list] is the current number of planes. VEND lets you input up to three different planes. Use check boxes in the Show planes panel to select a plane (or planes) to be displayed.
Click [Clear] to remove the plane(s) from the Graphics Window.

Check box "Select planes" lets you specify visible planes.

4.3.2 Settings Panel

The {Scale factor for isosurface level}, *s*(iso), is also input here. If *s*(iso) is 0 (minimum value, default), the densities on the planes are calculated from all the density data. If *s*(iso) is 1 (maximum value), the densities larger than the isosurface level are drawn. Of course, other values may also be selected.

The *f*(section) factor described above is further multiplied by {Scale factor for *f*(section)}, *s*(section).

In list box "Palette", one of the following three palettes is specified:

Rainbow
Inverse Rainbow
Gray

4.3.3 Opacity

The {Opacity} of the plane can be changed here.

4.3.4 Preview

If "Preview" is checked, slices in the Graphics Window reflect changes described in 4.3.3.

4.4 Unit Cell Dialog Box

Click [Unit cell] to open the Unit Cell Dialog Box, where some settings related to the outlines of the unit cell are changed.

4.4.1 Unit Cell Edges

Check box "Show unit cell edges" enables you to turn on/off displaying outlines of the unit cell in the Graphics Window.

4.4.2 Line Type

Unit cell edges can be plotted with three types of lines: "Solid lines", "Dotted lines", and "Dashed lines".

4.4.3 Width

The {Width} of the unit cell edges can be changed here. When a high-resolution image file is desired, a large width, *e.g.*, 4.0, must be input.

4.4.4 Colors

The Colors panel is used to change the color of outlines for the unit cell.

4.5 Model Dialog Box

Click [Model] to open the Model Dialog Box where properties of atoms and bonds properties, and structural and bonding types are set.

4.5.1 Atoms Panel

The Atoms panel is used to change some settings related to atoms. Select the symbol of an element from list box {Symbol} and specify its {Radius}, {Stacks}, and {Slices}. {Stacks} and {Slices} are parameters common to all the atoms, allowing you to change the

resolution (quality) of atoms displayed in the screen. {Stacks} denotes the numbers of subdivisions along the *Z* axis (similar to lines of latitude). {Slices} denotes the number of subdivisions around the *Z* axis (similar to lines of longitude). {Stacks} and {Slices} are the same parameters as described in Subsection 4.2 (VICS). Next, change the color of the element in the Color subpanel if necessary.

4.5.2 Bonds Panel

The Bonds panel is used to change some settings related to bonds: {Radius (B&S)} of each cylindrical bond in the ball-and-stick (B&S) model, {Radius (stick)} of each cylindrical bond in the stick model, {Stacks}, and {Slices}. Next, change the color of bonds in the Color subpanel if necessary.

4.5.3 Model Panel

In he Model panel, select the "Ball-and-stick" or "Stick" model (see Section 3, VICS).

4.5.4 Bond Style Panel

One of two types of bonds can be selected in the Bond style panel:

"Unicolor cylinder"	Each bond is drawn as a cylinder, whose color can be changed in the Color panel.
"Bicolor cylinder"	Each bond is drawn as a cylinder with colors of two atoms connected with each other. To change the colors of the bond, those of atoms have to be changed.

5. Open a Three-Dimensional Density File

The Open Dialog Box results from clicking [Open] in the Menu Bar. Select a file format (MEM [1–5], Gaussian 98 [6], SCAT [7], WIEN2k [8], VEND script file, or VEND 3D) and a file. Refer to Appendix A.1 for formats MEM and VEND 3D; see Section 10 for VEND script file. Specify the initial isosurface level, which is required because isosurfaces are always displayed in the Graphics Window after reading in the density file. Click [OK] to input the density file and quit from the Open Dialog Box.

6. Import a VICS File

A ball-and-stick or stick model can be imported from a file with the VICS format to overlap it with isosurfaces and/or slices.

A dialog box named Import a VICS File appears by clicking [Atom] in the Menu Bar. Select a file and click [OK]. Then, the Output Window displays

Title
Space group
Lattice parameters
Structure parameters

Turn on "Show model" to see a structure model in the Graphics Window. Turn off "Show model" to erase a structural model in the Graphics Window.

7. Interactive Manipulations

7.1 Rotate Objects

Click [Rotate] in the Dialog Window to rotate objects displayed on the Graphics Window. Four different rotation modes are available: [Stepwise], "Drag", "Push", or "Click". When "Drag", "Push", or "Click" is clicked, specify a rotation axis by clicking [Free], [X axis], [Y axis], or [Z axis]. [Free] means that objects can be rotated around arbitrary axes. On selection of the [X axis], [Y axis], or [Z axis], objects are rotated around each screen axis (refer to 2.2.6).

7.1.1 Stepwise Rotation

Click [Stepwise] to open the Stepwise Rotation Dialog Box. There are two modes for stepwise rotation: "Single step" and "Continuous". Objects are rotated only once by a step specified in {Step (deg)} in the "Single step" mode while they are rotated continuously with the step until the Stepwise Rotation Dialog Box is closed by clicking [OK].

Input {Step (deg)} with which objects are rotated around each axis.

There are three buttons for the rotation axis: [X axis], [Y axis], and [Z axis]. Objects in the Graphics Window are rotated around the clicked axis.

7.1.2 Drag Mode

In the "Drag" mode, move the mouse while pressing the left mouse button to rotate objects in the Graphics Window. The objects are rotated, keeping with the mouse. They are never rotated after the mouse button has been released. In the [Free] rotation mode, the rotation axis becomes normal to the direction along which the mouse is moved.

7.1.3 Push Mode

In the "Push" mode, press the left mouse button at point 1 and move the mouse to point 2. In the [Free] rotation mode, objects are rotated around an axis perpendicular to a line connecting points 1 and 2, continuing to rotate even after the left mouse button has been released. The rotation speed is proportional to the speed of moving the mouse.

The objects stop to rotate immediately by clicking the left mouse button at any point in the Graphics Window. On the use of a slow computer, it may be necessary to keep the left mouse button pressed for a short time.

7.1.4 Click Mode

In the "Click" mode, click the left mouse button to rotate the objects. In the "Click" plus [Free] rotation modes, the rotation axis is perpendicular to a line connecting the click position and the central point. Note that selection of [Z axis] in the click mode practically results in that of [Free].

In this mode, the rotation speed depends on the rotation step, which can be changed in either the Stepwise Rotation Dialog Box or the Preferences Dialog Box.

To stop the rotation of the objects, (1) select either the "Drag" (recommended) or "Push" mode and (2) click the left mouse button at any point in the Graphics Window. Operation (1) is required because only clicking the left mouse button in the Graphics Window leads to a change in the rotation axis in this mode.

7.2 Magnify Objects

Click [Magnify]. Press the left mouse button and move the mouse. Objects are magnified in proportion to the distance of moving the mouse upward. On the other hand, objects are shrunk in inverse proportion to the distance of moving the mouse downward.

7.3 Translate Objects

Click [Translate]. Press the left mouse button and move the mouse. The objects will be

moved with the mouse along the same direction.

8. Orientation

Click [Orientation] in the Dialog Bar to open the Orientation Dialog Box. This dialog box lets you specify a direction of viewing objects.

8.1 Manner of Specifying Directions

This direction may be entered in two different ways:

"Lattice vector"	Input u, v, and w in a lattice vector, $u\boldsymbol{a} + v\boldsymbol{b} + w\boldsymbol{c}$
"Plane normal"	Input indices, h, k, and l, in a reciprocal-lattice vector, $h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*$, perpendicular to the ($hkl$) plane

8.2 Upward Direction Panel

The upward direction on the screen is automatically selected by VICS when "Automatic selection" is checked whereas it is input by the user when "Manual selection" is checked.

8.3 Two Directions

Two directions, *i.e.*, the direction of projection (direction from the viewpoint to the projection plane) and the upward direction on the screen have to be specified:

For "Lattice vector"

Direction of projection	[u1], [v1], and [w1]
Upward direction on the screen	[u2], [v2], and [w2]. Input only when "Manual selection" is checked.

For "Plane normal"

Direction of projection	[h1], [k1], and [l1]
Upward direction on the screen	[h2], [k2], and [l2]. Input only when "Manual selection" is checked.

The current orientation is displayed in real time as a 3×3 matrix at the left-hand side of the Crystal Orientation Dialog Box.

8.4 Apply Button

The current orientation settings are reflected in the Graphics Window by clicking [Apply].

9. Two-Dimensional Map and Bird's-Eye View

9.1 How to Display Objects in Two Dimensions

Two different methods of representing electron/nuclear densities (or any other physical quantities) projected onto a plane are supported in VEND: 2D Map and Bird's Eye View. In both representations, densities in a user-specified range are summed up along a direction projected onto a plane

The 2D Map Window displays two-dimensional distribution of densities on a plane onto which densities in a user-specified range are projected with different colors corresponding to densities in the same way as described in Section 3. If the starting and ending densities are equal to each other, densities on the plane are simply shown without any projection. The maximum density, Z(max), over the user-specified range is displayed at the upper left corner of the 2D Map Window.

Because nuclear densities in compounds containing elements with negative coherent-scattering lengths, electrostatic potentials, and wave functions have positive and negative values, colors corresponding to their absolute values are displayed in 2D maps. In this case the absolute value of Z(max), |Z(max)|, is displayed at the upper left corner of the 2D Map Window.
On the other hand, the Bird's-Eye View Window expresses the same densities in a three-dimensional manner.

In both types of representing densities projected onto planes, all the data are used to show electron/nuclear densities with the full-scale density changed with *f*(section) (see Subsection 3.2) and *s*(section) (Subsection 3.4).

Click [2D] in the Menu Bar to open the 2D Projection Dialog Box.

In the Plane panel, select a type for a Miller plane from "(100)", "(010)", and "(001)", and "(hkl)" planes.

On the selection of "(100)", "(010)", or "(001)", either of two drawing ranges is specified in the Dimension panel: "1□1" and "2□2" (multiplicity of the unit cell).

On the selection of "(100)", "(010)", or "(001)", input a range for summation of densities along the projection direction in the Projection panel: {From} and {To}.

The *f*(section) factor may be further multiplied by *s*(section) in the same manner as described in Subsections 4.2 and 4.3.

The color and width of outlines can be altered in the Outlines color panel and {Outlines width}, respectively.

Turn on checkbox "Show contour lines" to display contour lines in the 2D Map Window. Contour lines are represented in solid lines for positive values and in broken lines for negative ones.

"Scale factor for 2D map" and "Scale factor for bird's-eye view" denote *s*(sections) described in Subsection 3.4.

Turn on "2D Map" and click [Apply] to create a 2D Map Window. Turn on "Bird's-eye view" to create a Bird's-Eye View Window.

Turn on checkbox "Grid" to add grid lines to the 2D Map Window. Grid lines are plotted with steps of (axis length)/10.

For zooming in the 2D Map Window, press the left button of the mouse and drag it.

For zooming in the Bird's-Eye View Window, press the right button of the mouse and drag it. For rotation in the Bird's-Eye View Window, press the left button of the mouse and drag it.

Finally, click the [Apply] button to make all the settings effective and to create the 2D Map Window or the Bird's-Eye View Window.

If "(hkl)" is selected in the Plane panel, additional information will be displayed in the Output Window:

1. Section parameters: lengths (Å) of X- and Y-axes lengths and an angle, phi, formed by the X- and Y-axes.
2. Axis directions
3. Origin.

9.2 Settings to Plot Contour Lines

Click [Settings] in the 2D Projection Dialog Box to open the Contour Lines Dialog Box.

In the Mode panel, select the mode of determining contour levels, "Normal" or "Exponent".

If "Normal" is selected, contour lines are plotted in a region from {MIN} to {MAX}. By default, {MIN} is the minimum value of the data, D_{min}, and {MAX} is minimum value of the data, D_{max}. The number of contour lines, N, is calculated from the {Step} of contour lines:

$$N = (MAX - MIN) / Step. \quad (4)$$

The contour level, Z, for *j*th step is computed by

$$Z = MIN + (j - 1) \times Step. \quad (5)$$

On selection of "Exponent", {N} contour lines are plotted with the contour line level, Z, for *j*th step calculated with

$$Z = C \times X^{j-1}. \quad (6)$$

By default, C is D_{min}, X is 3, and N is evaluated as

$$N = 1 + [\log D_{max} - \log D_{min}] / \log 3. \quad (7)$$

The Colors panel is used to change the color of contour lines, and the {Width} of the contour lines can also be changed here.

Turn on checkbox "Show only contour lines" to display only a contour map in the 2D Map Window.

10. VEND Script File

The following information is stored in a VEND script file, ∗.vnd:

Drive + absolute path + file name for ∗.den
Isosurface level and *f*(section)
Number of cells along *a*, *b*, and *c* directions
Origin and Inside boundaries
Palette (rainbow, inverse rainbow, or gray)
Colors (rendering of isosurfaces)
Background color
Orientation

Be careful lest the drive + absolute path in the second line of ∗.vnd remains unchanged when copying a pair of ∗.vnd and ∗.den to another folder or another PC.

11. Export Electron/Nuclear-Density Images

Electron/nuclear-density images displayed in the Graphics, 2D map, and Bird's-Eye View Windows can be saved in files with a variety of graphics formats.

At first, click on the Graphics, 2D Map, or Bird's-Eye View Window whose graphic data are output in a file, which is necessary to indicate which graphic data are to be saved.

Click [Image] in the Menu Bar, select an image format from a list, input/specify a file name, and click [OK]. Then, the Export Graphics Dialog Box is opened. Here, {Smoothing} and {Scale} are input. The number of pixels displayed at the Info Bar is multiplied by the scale factor. Select a window whose graphic data will be saved in the Export from panel. Click [Save] finally.

The typical value of {Smoothing} is 1–3 in the presence of unit-cell edges, which become more vague with increasing {Smoothing}. For colored edges, {Smoothing} may be somewhat increased. The maximum value of {Scale} is 10, which yields huge images comprising a number of pixels.
The following settings are preferred for 2D maps including contour lines:

Outlines width (see Subsection 9.2)	3–4
{Smoothing}	1
{Scale}	3–4

A new Export Graphics Dialog Box is opened after saving the electron/nuclear-density images. Click [OK] to continue.

12. Preferences

Default settings can be changed in the Preferences Dialog Box.

Click [Preferences] in the Menu Bar. Select Show default settings and Show current settings radio buttons to see default and current settings, respectively. You can change all

the settings to defaults by clicking [Restore default settings]. Current settings can be saved as defaults by clicking [Save as defaults].

Items in the Settings Panel are common to the default and current settings. VEND has to be restarted to make all the default settings effective.

The current positions of the Menu and Dialog Bars, and Graphic Window can be saved by checking "Save bars/window positions" and then clicking [Save] or [Save as defaults]. In the case of the Graphic Window, its dimension is also saved.

The current positions of all the dialog boxes can be saved in the preference file by checking "Save dialog bar positions" followed by clicking [Save] or [Save as defaults].

13. Running VEND Using a Command

VEND is launched not only by double clicking its icon entering a command containing one or two arguments in the DOS/Command Prompt Window:

VEND file_name
VEND file_name file_format_ID

The first form may be used provided that the extension of the file name is the same as that listed in Appendix A.1 for each format. For example, VEND can be run by entering the following command:

VEND YBa2Cu3O7.den

The second format, where <file_format_ID> is an identification number for a file format (Appendix A.1), is alternatively used for any file name whose extension is arbitrary.

Appendix A. File Formats

A.1 Input-File Formats

file_format_ID	Extension	Format
0	den	Density file formats of MEM-analysis programs MEED [1], MEEDCAB and MEND [2], ENIGMA [3], and PRIMA [4,5] which are given a general name of "MEM" in the Open Dialog Box and automatically distinguished by VEND.
1	cube/cub	Gaussian 98 Cube format [6]
2	scat	Format of files created by contrd [9] that converts files F09 and F39 storing results of electronic-state calculations using DVSCAT [7,8] into 3D electron densities, electrostatic potentials, and wave functions (up and down spins)
3	rho	Density file format of WIEN2k [10]
4	vnd	VEND script file (see Section10)
5	∗ed	VEND 3D data file (see below)
6	eb	Format of files storing energy eigenvalues resulting from band-structure calculations

The extensions may also be described in capital letters, but mixing lowercase and capital letters is inhibited.

Beware that the default extension appearing in the Open Dialog Box can be specified in the Preferences Dialog Box: {Default ext.}.

At the top part of ∗.den, *i.e.*, before the title line, we can put comment lines where the first column is '#' or '∗' in MEED [1], MEEDCAB and MEND [2], ENIGMA [3], and PRIMA [4, 5]. The unit of electron densities (number densities of electrons) recorded in these files is $Å^{-3}$.

A script, wien2venus.py, coded in Python (http://www.python.org/) by Masao Arai of AML/NIMS [11] makes it possible to export electron densities calculated with WIEN2k to a text file, ∗.rho, which is in turn input by VEND to display electron-density distribution in three dimensions. The unit of electron densities stored in this file is either $Å^{-3}$ or $(a.u.)^{-3}$,

where a.u. is the atomic unit for length, *i.e.*, 1 a.u. = a_0 = 5.2917721□10^{-11} m = 0.52917721 Å (a_0: Bohr radius). Both positive and negative densities may be included in ∗.rho; negative densities result from calculation of differences in electron densities.

VEND can display isosurfaces for electron densities (Density, Full, Total), spin densities (Alpha, Beta, Spin), electrostatic potentials (Potential), wave functions (Orbitals: HOMO, LUMO, or any other orbitals), and so forth calculated with Gaussian 98 with a keyword of 'Cube' [6]. Because electrostatic potentials and wave functions have both positive and negative values, their isosurfaces are represented with two different colors. Three-dimensional numerical data recorded in Cube files are drawn without any conversion; please ask Gaussian, Inc. (http://www.gaussian.com/index.htm) for units of physical quantities stored in Cube files.

VEND is also capable of displaying isosurfaces for electron densities, electrostatic potentials, and wave functions calculated with contrd [9] from files F09 and F39 output by DVSCAT [7,8]. Text files, CHG3D.TXT, POT3D. TXT, WXXX-3D.TXT, WXXXU-3D.TXT, and WXXXU-3D.TXT, created with the file converter, contrd, must be renamed ∗.scat. Three-dimensional numerical data recorded in these files are drawn without any conversion. Units for electron densities, electrostatic potentials, and wave functions are $(\text{a.u.})^{-3}$, H (Hartree, E_0), and $(\text{a.u.})^{-3/2}$, respectively. For details in these files, refer to VENUS\contrd\Readme_contrd.txt.

If electron densities in the unit of $Å^{-3}$ are desired, ∗.cube and ∗.scat should be converted into text files where 3D electron densities are repreented in $Å^{-3}$; writing a short program or script is enough to accomplish this purpose.

A VEND 3D data file store one of the following physical quantities converted from electron densities [12]:

□^{2}□($\boldsymbol{r}$): Laplacian of the electron density (∗.led)
$g(\boldsymbol{r})$: electronic kinetic energy density (∗.ked)
□($\boldsymbol{r}$): electronic potential energy density (∗.ped)
$h_e(\boldsymbol{r})$: electronic energy density (∗.ted)

with the format

Title	Title up to 80 characters
a, *b*, *c*, □, □, □	Lattice parameters with at least one space between two parameters (free format)
N1, N2, N3	Numbers of pixels along the *a*, *b*, and *c* axes, respectively, with at least one space between two integers (free format)

followed by elements of a three-dimensional array, D

(((D(I1, I2, I3), I3 = 1, N3), I2 = 1, N2), I1 = 1, N1)

with any number of data in each line and at least one space between two data (free format).

Files ∗.eb, which have practically the same format with ∗.rho, are used to visualize Fermi surfaces from results obtained with programs for band-structure calculations, *e.g.*, WIEN2k [10]. As a matter of convenience, a constant is added to all the energy eigenvalues in ∗.eb so as to make them greater or equal to zero. Therefore, the isosurface level has to be set with this padding in mind.

Masao Arai of NIMS will provide detailed information about ∗.eb in his Web page: http://www.nims.go.jp/cmsc/staff/arai/

A.2. Image-File Formats

BMP
EPS
JPEG
JPEG 2000 [13]
HDF5† [14]
PPM
RAW
SGI (RGB)
TGA
TIFF

† The output of an HDF5 file is supported only in the UNIX/Linux version.

Sizes and resolutions of images saved in the above formats can be altered with graphic programs and utilities such as Adobe Illustrator (Adobe Systems Incorporated), Paint Shop Pro (Jasc Software, Inc.), GraphicConverter (http://www.lemkesoft.com/), and IrfanView

(http://www.irfanview. com/).

Appendix B. Program Specifications

Maximum number of pixels for each direction	260
Maximum number of symmetry operations	48
Maximum number of pixels on isosurfaces	2 500 000
Maximum number of polygons	100 000

Appendix C. Files in the Programs Folder

VEND.exe	Executable binary file of VEND
preferences_VEND.ini	Default settings in VEND
palette.ini	File storing data for the color palettes

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[8] Y. Kowada, I. Tanaka, H. Nakamatsu, and M. Mizuno, "Hajimete no Denshi Jôtai Keisan," Sankyo Shuppan, Tokyo (1998) (in Japanese).

[9] This file converter was kindly written in Fortran for VEND by M. Mizuno, Department of Materials Science and Engineering, Osaka University.

[10] P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka, and J. Luitz, "WIEN2k, an Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties," ed. by K. Schwarz, Technische Universität Wien, Wien (2001); http://www.wien2k.at/

[11] This file converter was kindly coded in Python for VEND by M. Arai of AML/NIMS; http://www.nims.go.jp/cmsc/staff/arai/wien/venus.html

[12] V. G. Tsirelson, *Acta Crystallogr.*, *Sect. B*, **58**, 632 (2002).

[13] http://www.jpeg.org/JPEG2000.html

[14] http://hdf.ncsa.uiuc.edu/