

iModel : An Interactive 3D Crystal Structure Visualization Program

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1. Program Installation and Updates

1.1 System Requirements

Windows 10 and above.

1.2 Download and Installation

The installation steps will be continually optimized with the program's further development and updates. For specific installation instructions, please refer to the readme document at the download address <https://github.com/iPowder/iModel>.

1.3 Update

Download the update content from the program's release page and follow the instructions in the update notes.

2. Program Interface

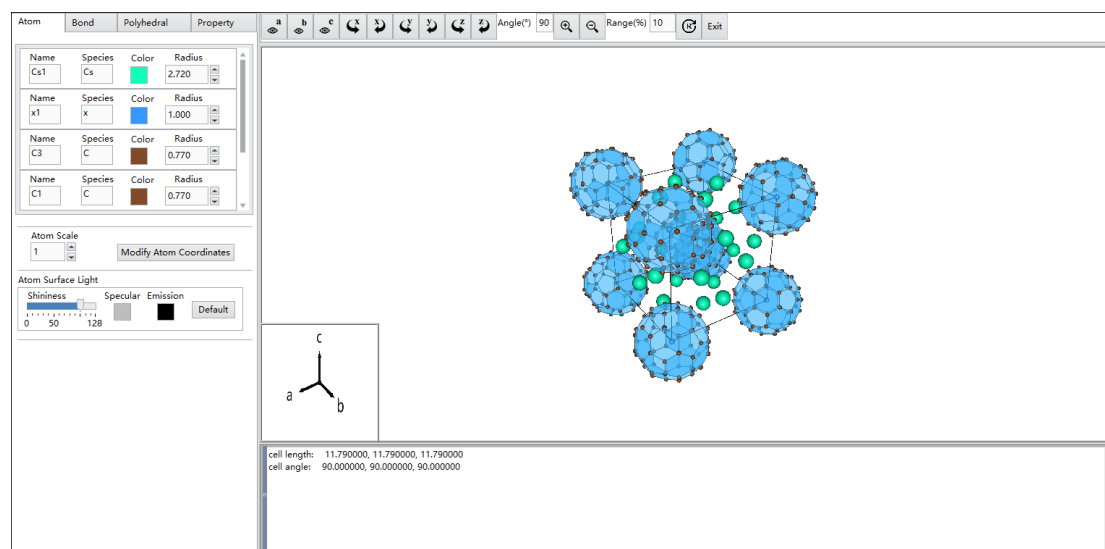


Figure 1: iModel program interface displaying the crystal structure of CSC_{10} .

The program interface is primarily divided into three windows, a toolbar, and a menu bar. The sizes of the three windows can be adjusted accordingly.

In Figure 1, the largest window is the structure model display window, where the display and manipulation of the crystal structure take place. Below this window is the structure information

output window, where crystal cell parameters, atomic coordinates upon mouse click, chemical bond names, and more will be displayed. The left window contains atoms, chemical bonds, polyhedral structures, and various other properties, along with related functional buttons.

The toolbar above the image is used to manipulate the structure model, enabling functions such as changing the viewing angle, rotating around a specific direction by a certain angle, zooming in and out, and resetting the image.

The menu bar includes three sections for file reading and writing, undo and redo operations, and help.

3. File Reading and Saving

3.1 Data File Reading and Writing

Click on the 'File-Open File' option in the menu bar to read crystal structure data files. Supported file formats include CIF, POSCAR/CONTCAR, CHGCAR, LOCPOT, vasprun.xml, CSSR, Netcdf, and pymatgen's JSON serialized structure files. Click on 'File-Save To File' in the menu bar to save the crystal structure as data files in formats such as CIF, POSCAR/CONTCAR, CHGCAR, etc. (refer to Table 1 for details).

Table 1: Data File Input and Output Formats

Input file formats		Input file formats		Output file formats	
1	*.cif	15	*.json	1	*.cif
2	*.mcif	16	*.xsf	2	*.mcif
3	*POSCAR	17	CTRL	3	*POSCAR
4	*CONTCAR	18	*prismatic	4	*.cssr
5	*.vasp	19	*.yaml	5	*.json
6	CHGCAR	20	*.yml	6	*.xsf
7	LOCPOT	21	*.in	7	*rndstr.in
8	vasprun	22	*.res	8	*lat.in
9	*.xml			9	*bestsq
10	*rndstr.in			10	*prismatic
11	*lat.in			11	*.yml
12	*bestsq			12	*.in
13	*.cssr			13	*.res
14	*.mson				

3.2 Save as Image File

Click on the File-Save As Image option in the menu bar to save the crystal structure as an image

file. Supported formats include jpg, jpeg, png, and bmp.

3.3 Project Files

You can save and load project files using the "Save As Project" and "Open Project" options in the menu bar, allowing you to pause and resume your work in the current state.

4. Structure Model Control

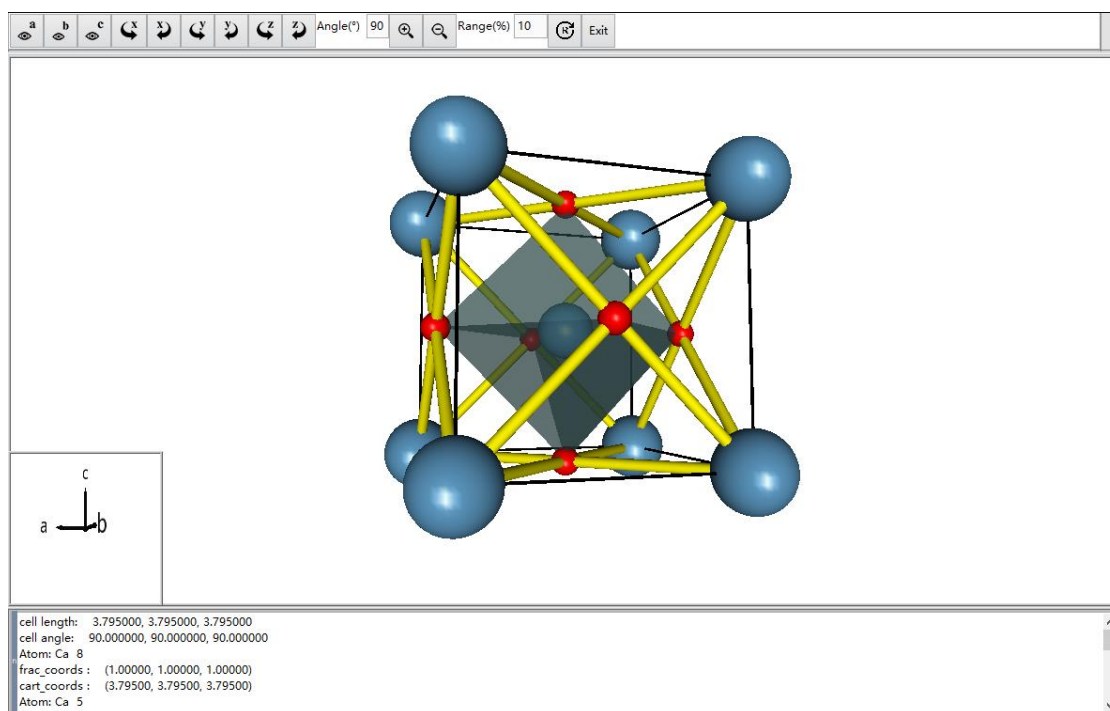


Figure 2: iModel program crystal structure display window showing the crystal structure of CaTiO_3 .

You can directly rotate the crystal structure by dragging with the left mouse button. The rotation center is the center of the display window, initially located at the origin (0,0,0).

Hold down the Shift key and simultaneously drag up or down with the left mouse button to zoom in or out on the crystal structure.

Hold down the Ctrl key and simultaneously drag with the left mouse button to freely move the structure model. After moving the structure model, the atomic coordinates remain unchanged; only the field of view is altered. Additionally, the rotation center will shift from the origin to the current center of the view.

Clicking on atoms, chemical bonds, or other objects in the structure with the left mouse button will display the selected object's name and coordinate-related properties in the structure information output window below.

Right-clicking on the structure display window with the mouse will bring up a prompt interface where you can view operation instructions and help.

5. Atom, Bond, Polyhedral, Property

5.1 Atom

The image shows a software window titled 'Atom Options Page' with four tabs: 'Atom', 'Bond', 'Polyhedral', and 'Property'. The 'Atom' tab is active. It contains a scrollable list of atom properties. The list has four columns: 'Name', 'Specie', 'Color', and 'Radius'. The first three rows are populated with 'Ca' (blue, radius 1.970), 'Ti' (light blue, radius 1.470), and 'O' (red, radius 0.740). The fourth row is empty with a grey color swatch and radius 0.000. Below the list is an 'Atom Scale' section with a slider set to 0.7 and a 'Modify Atom Coordinates' button. At the bottom is an 'Atom Surface Light' section with a 'Shininess' slider (0 to 128), 'Specular' and 'Emission' checkboxes (both unchecked), and a 'Default' button.

Name	Specie	Color	Radius
Ca	Ca	Blue	1.970
Ti	Ti	Light Blue	1.470
O	O	Red	0.740
		Grey	0.000

Atom Scale: 0.7 [Slider] [Modify Atom Coordinates]

Atom Surface Light: Shininess [Slider: 0 to 128] Specular [] Emission [] [Default]

Figure 3: Atom Options Page

At the top of the page, the names, species, colors, and radius sizes of all types of atoms in the current structure are displayed. Users can freely adjust them within a suitable range.

The Atom Scale controls the current size ratio of all atoms. The 'Modify Atom Coordinates' button is used for precise adjustment of each atom's parameters. Clicking it will open a window displaying parameters such as color and radius size for all atoms. Right-clicking on an atom allows for its deletion.

The Atom Surface Light section is used to adjust the three-dimensional lighting effects on the surface of atoms, including parameters for emission, reflection, and diffuse light. It also includes a reset button.

5.2 Bond

Atom	Bond	Polyhedral	Property
Bond Search Mode			
<input type="radio"/> All Bonds		X - X	Search
<input type="radio"/> A-X		Cs - X	
<input checked="" type="radio"/> A-B		C - C	
<hr/>			
<div><div>Radius 0.080</div><div>Opacity 1</div></div> <div><div>Atom Selection Atom1 Atom2 C C</div><div>Length Range Max Min 1.49 0</div></div>			
<hr/>			
<div><div>Radius 0.080</div><div>Opacity 1</div></div> <div><div>Atom Selection Atom1 Atom2 Cs Cs</div><div>Length Range Max Min 0 0</div></div>			
<hr/>			
<div><div>Radius 0.080</div><div>Opacity 1</div></div> <div><div>Atom Selection Atom1 Atom2 Cs Cs</div><div>Length Range Max Min 0 0</div></div>			
<hr/>			

Figure 4: Bond Options Page

In the Bond Search Mode option, you can adjust the chemical bond search mode, which includes three modes. In the A-B mode, only the chemical bonds composed of atoms A and B are searched. In the A-X mode, chemical bonds formed by atom A with all types of atoms are searched. The All Bonds mode searches for all potentially existing chemical bonds in the structure.

Then, the page displays the names, radii, colors, transparency, and bond length search range of chemical bonds in the current structure. Users can add new chemical bonds for display by entering the information in the gray area below. Additionally, you can right-click to delete selected chemical bonds

5.3 Polyhedral

The image shows a software window titled "Polyhedral" with four tabs: "Atom", "Bond", "Polyhedral", and "Property". The "Polyhedral" tab is active. It contains a list of four polyhedral objects. Each object has a "Color" field with a color swatch, an "Opacity" field with a numeric value and up/down arrows, and an "Atoms" field with a list of atoms. The first object has a cyan color, an opacity of 0.7, and a list of atoms containing "Central", "Ti", "Round", and "O". The other three objects have a gray color, an opacity of 0, and empty atom lists. Below the list is an "Atom Search Range" section with a dropdown menu set to "Additional".

Color	Opacity	Atoms
Cyan	0.7	Central Ti Round O
Gray	0	Central Round
Gray	0	Central Round
Gray	0	Central Round

Atom Search Range
Additional

Figure 5: Polyhedral Options Page

At the top of the Polyhedral page, users can click the Search button in the Search Polyhedra window to automatically search for polyhedral structures. In the A-B field to the left of the button, A stands for the Central Atom, and B stands for the Round Atom.

In the Atom Search Range option, under the Inside the cell mode, only the polyhedral structures present in the current single unit cell are searched. In the Additional mode, atoms around the current unit cell are included in the search range and added to the crystal structure, displaying polyhedral structures collectively.

Then, the page displays the color, transparency, central atom, and surrounding atoms for the polyhedral structures being searched in the current structure. Users can add new polyhedral structures for display by entering information in the gray area below or right-click to delete polyhedral objects.

5.4 Property

Atom	Bond	Polyhedral	Property
Unit Cell Lines			
Radius		Opacity	Color
0.03		1	
Axis			
Length	Radius	Color	Character Size
2	1		1
Background Color		Error Range	
		1E-5	
Unit Cell		Projection Mode	
<input checked="" type="radio"/> 1x1x1 <input type="radio"/> 2x2x2 <input type="radio"/> 3x3x3		Perspective	
Bond Color Mode			
Bicolor			

Figure 6: Property Options Page

Under this page, there are various options related to crystal structure properties. These include settings for the thickness, transparency, and color of cell indication lines, the length, thickness, color, and font size of coordinate axes, as well as the background color of the display window and the error range for program algorithm execution (such as atoms within the error range of atomic distances being considered as the same atom).

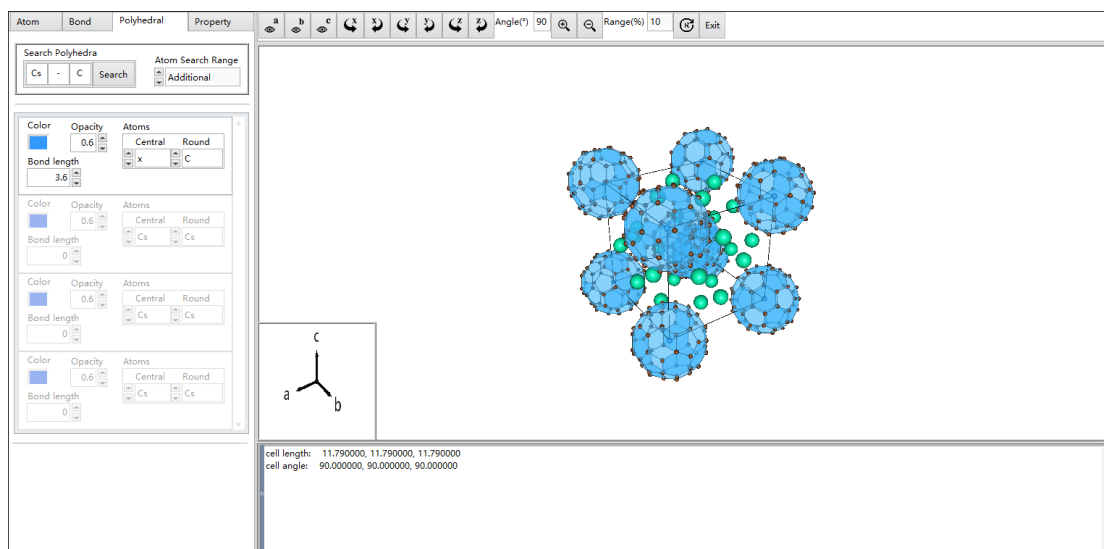
The 2x2x2 and 3x3x3 supercells can be displayed through the Unit Cell option, or revert to the initial single unit cell.

The Projection Mode is used to adjust the projection mode of the structure model and includes two options: Perspective Projection and Orthographic Projection.

The bond color display mode can be adjusted through the Bond Color Mode setting.

6. Example

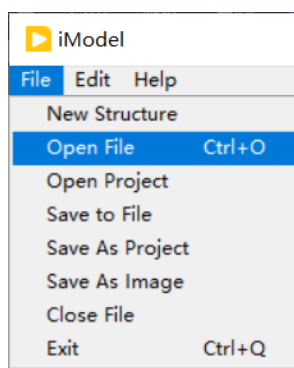
Structure of CSC_{10} with C_{60} polyhedron



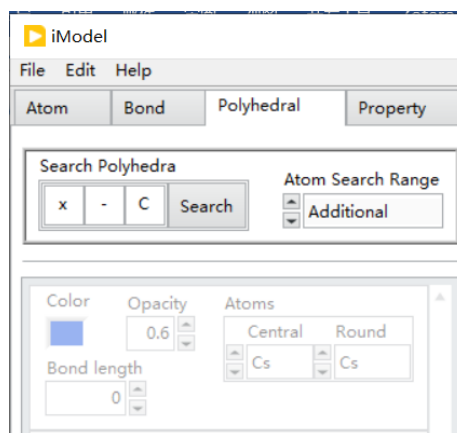
1. Open the CS10.cif file in the "example_files" folder of the program (using a text editor). At the bottom, add a line of data: "x1 H 0.0 0.0 0.0 1 0.0". This will add an H atom named 'x' (or any other name for different types of atoms) at the (0,0,0) position in the crystal structure.

```
loop_  
_atom_site_label  
_atom_site_type_symbol  
_atom_site_fract_x  
_atom_site_fract_y  
_atom_site_fract_z  
_atom_site_occupancy  
_atom_site_U_iso_or_equiv  
Cs1 Cs 0.2781 0 0.5 1 0.0  
C3 C 0.0611 0.1978 0.2212 1 0.0  
C1 C 0 0.2968 0.0611 1 0.0  
C2 C 0.1222 0.0989 0.259 1 0.0  
x1 H 0.0 0.0 0.0 1 0.0
```

2. Run the iModel program and click the menu "File-Open File" to open the CS10.cif file from the first step.



- Click the "Polyhydraulic" tab in the upper left corner to switch to the corresponding page. Click the drop-down box in "Search Polyhedra" and change the Central Atom and Round atom to x and C atoms. Then click the "Search button"



- In the various attributes of the new polyhedron below, increase the "Bond Length" to 3.6 or above (because the C60 polyhedron of CSC10 recorded in the data file, There is a certain error in the distance between the C atom and the central x atom. The program searches according to the minimum chemical bond length, so the search range of bond length needs to be increased).

