gsave
.99 setgray
150 100 moveto
/Helvetica-Bold findfont 75 scalefont setfont
55 rotate
(Lattice Maker 2.6.0) show
grestore

Information for New Users.

gsave
.99 setgray
150 100 moveto
/Helvetica-Bold findfont 75 scalefont setfont
55 rotate
(Lattice Maker 2.6.0) show
grestore

What is LatticeMaker?

LatticeMaker can be used with Ball & Stick,Chem-3D and MacMolecule to help in the production of images of large bulk structures or super-structures of crystal lattices.

System Requirements.

LatticeMaker uses colour pickers to set the colours of Atoms to be used in MacMolecule and Ball & Stick. For LatticeMaker to be fully functional Color QuickDraw and an 8-bit monitor must be present. If you have only have a B/W machine/monitor and are using 6.0.4 or later you will still be able to use LatticeMaker but all of the colour choices will be dimmed. LatticeMaker is System 7.0 friendly.

Installing LatticeMaker.

As you are reading this file you must already have unpacked all the files. The LatticeMaker Folder and Application can be anywhere on a hard-disk or floppy. However, for it to run you must place the LatticeMaker Preferences file into the system folder if you are using System 6.0.x or into the Preferences Folder in the System Folder if you are using System 7.0 or later. If the preference file is missing LatticeMaker will make one and place it in the correct location.

Place anywhere on disk

Place anywhere on disk. For example inside above folder.

Place in System Folder or Preferences Folder.

Menus and Dialogs.

This next section describes the main features of the menus and Dialogs that you will find in LatticeMaker.

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(Lattice Maker 2.6.0) show
grestore

The File **Menu.**

Use this menu to manipulate unit cell files. The Open… Item will let you select a unit cell to read into LatticeMaker. The format of these files is described later. The Close item becomes active if there is a file currently open and closes the file and removes all the windows. The Save Colours item becomes active if you have made changes to the colours of any of the atoms and have enabled the save colours preferences. (See the next section). The Quit item does the obvious and needs no explanation.

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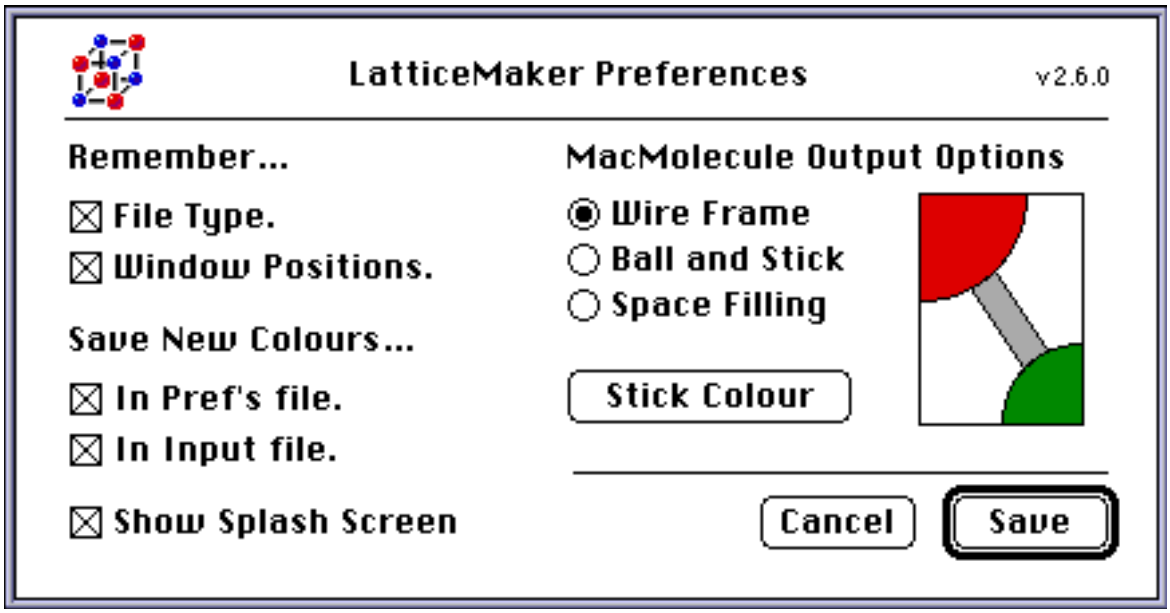
150 100 moveto
/Helvetica-Bold findfont 75 scalefont setfont
55 rotate
(Lattice Maker 2.6.0) show
grestore



Choosing the Preferences… item from the File menu brings up the dialog box shown. This allows you to choose which parameters you want LatticeMaker to remember when you quit the application. The file type item will remember the file type that you are currently using. If this is not enabled then LatticeMaker will use Ball and Stick Moldat as the default file type. The next item allows you to choose wether to remember where the windows are on the screen next time you run LatticeMaker. The next two options are used to specify where the new colours are saved. This allows the new colours to be saved in the Unit cell file but not in the Preferences file so that you may have the same atom with different colours in two or more Unit Cell files. The next time that you open an input file with stored colours, these colours are read instead of those stored in the Preferences file. If there are no stored colours then the Preferences file is used. The options on the right hand side are for those people who use MacMolecule. It allows you to choose the default type that LatticeMaker will create for files that are read into MacMolecule. You can choose the stick colour for the bonds in ball and stick mode by clicking stick colour. The current colour is shown graphically in the small window.

The Edit **Menu.**

This is a standard edit menu and has no function in LatticeMaker itself and is there purely for the support of DA's for those people who are still in the dark ages and using System 6!

The Build **Menu.**

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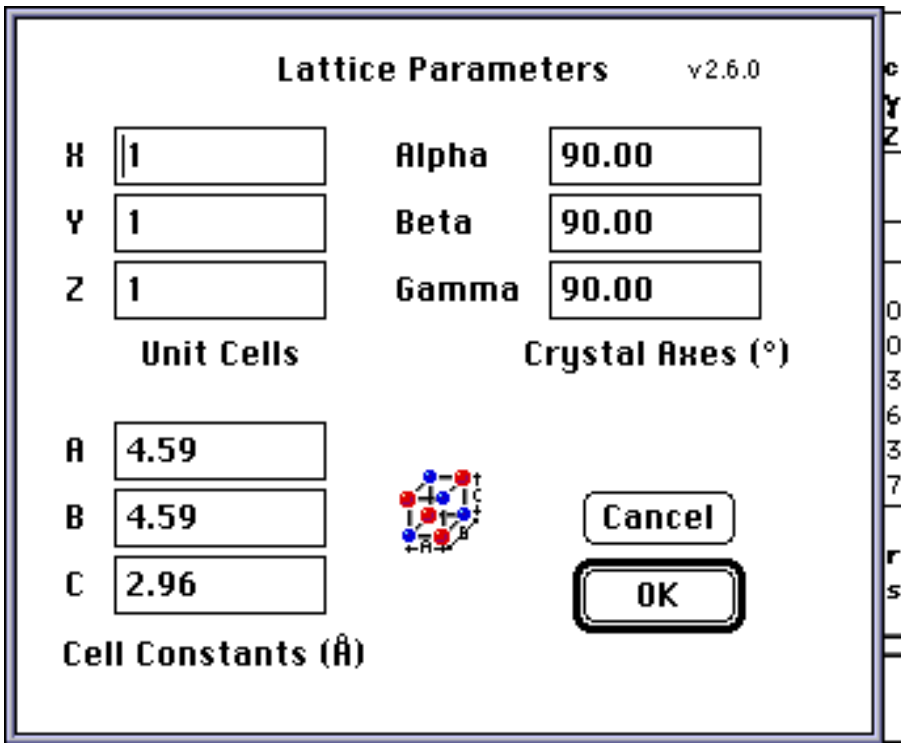
(Lattice Maker 2.6.0) show
grestore

This menu is used to control the size of the lattice and the type of output format that you wish to produce.Use the Size… item to select parameters which describe how the lattice will be built up and how big it will be.Use the Output File Type… items to define the type of output that you want LatticeMaker to produce. Currently four types are supported, but this may be extended subject to demand, and these are described later. The Bonds… item is used to choose how you want LatticeMaker to build bonds between the atoms in the Lattice. Use the Build… item to create the lattice when you are happy with all of your chosen parameters.

gsave
.99 setgray
150 100 moveto
/Helvetica-Bold findfont 75 scalefont setfont
55 rotate
(Lattice Maker 2.6.0) show
grestore

The Size… **Dialog.**



This dialog box is used to set up the size of the lattice that is produced by LatticeMaker and appears when the Size… item is chosen from the Build menu. The number of units cells that you want to build in each of the x,y and z directions, the unit cell parameters a,b, and c, and the angles between the crystal axes can all be set in this dialog. The angles between the axes are defined such that the a-axis of the crystal is parallel to the x-axis in cartesian space, and the ab plane or (001) crystal face is parallel to the xy cartesian plane.

The Output File Type… **Dialog**

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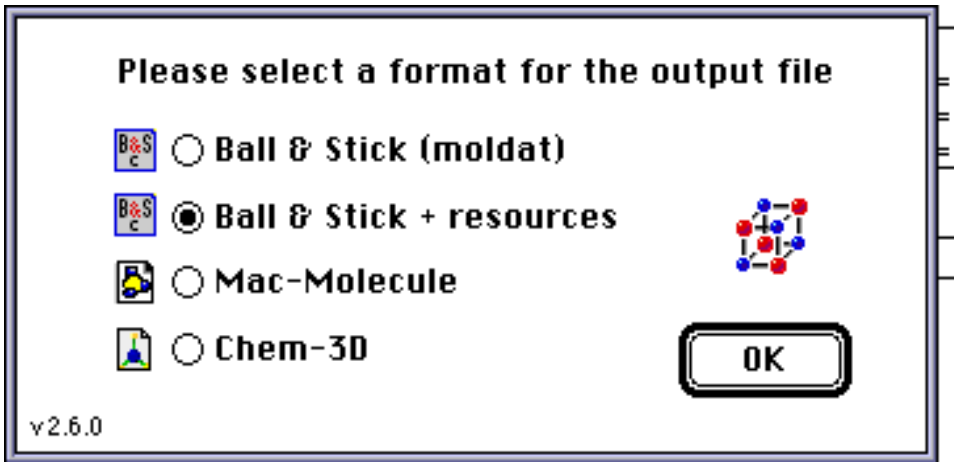
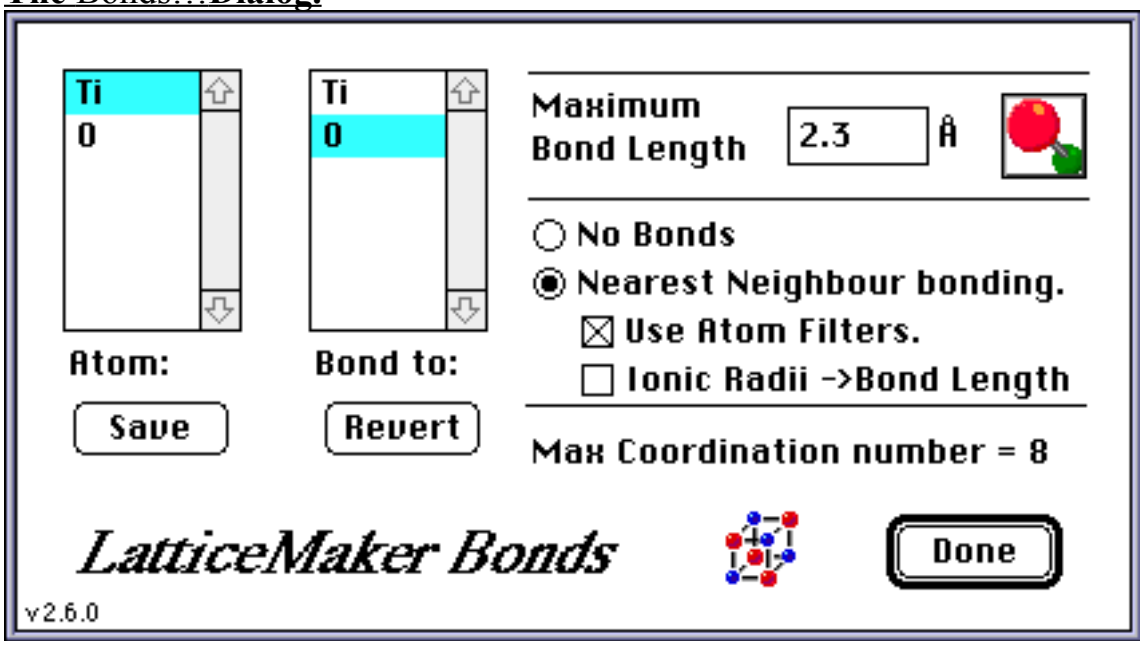
55 rotate
(Lattice Maker 2.6.0) show
grestore
```



This dialog allows you to choose one of the four types of output file. The only type that really needs explanation is Ball & Stick + resources. This output format adds specific resources to the output file so that when it is read into Ball & Stick all of the atom types will be set up and require no extra work defining new types. If Ball & Stick + resources or Mac-Molecule is the chosen type and an 8-bit colour monitor is present then a window showing the general appearance of the atoms will appear.

gsave
.99 setgray
150 100 moveto
/Helvetica-Bold findfont 75 scalefont setfont
55 rotate
(Lattice Maker 2.6.0) show
grestore

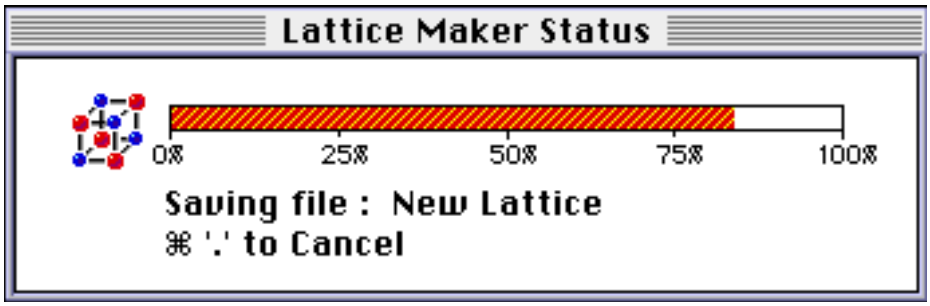
The Bonds…**Dialog.**



This version of LatticeMaker will optionally create bonds between atoms in the lattice. The methods used by LatticeMaker to create bonds are flexible enough to cope with most bonding situations. To add bonds to the lattice select **Nearest Neighbour bonding** and choose one of the following methods. For a lattice which contains only one atom type (for example Si) the simplest bonding scheme is to use nearest neighbour bonding, with a suitable distance selected in the maximum bond distance box. All atoms closer than or equal to this bond distance are bonded together. The maximum bond distance is limited to 10Å (as no real bonds would ever be this long). The maximum coordination number of each atom is currently fixed at 8 bonds. If the number of bonds exceeds 8 then any extra bonds are ignored. If you wish to build a lattice which contains more than one atom type where only hetro-nuclear bonds are allowed then the atom filters option allows the selection of allowed bonding combinations. Select the atoms which you wish to make bond to, from the left hand list. Then select from the right hand list (shift-clicking if necessary) the atoms you want to bond to. After you have made the selection press **Save** to remember your selection. Repeat this for all of your atoms. To make this option active you need to check the **Use Atom Filters** item. The final option which allows more control over bond formation is to use the ionic radii as a bond distance parameter. When this option is chosen the value in the bond length text box is ignored, and a value equal to the sum of the radii of the two atoms to be bonded is used as the bond distance. The radii of atoms can be changed by using the Ball and Stick colour picker or by editing the settings in the preferences file with ResEdit. (see later for details of customising resources)

```
gsave
.99 setgray
150 100 moveto
/Helvetica-Bold findfont 75 scalefont setfont
55 rotate
(Lattice Maker 2.6.0) show
grestore
```

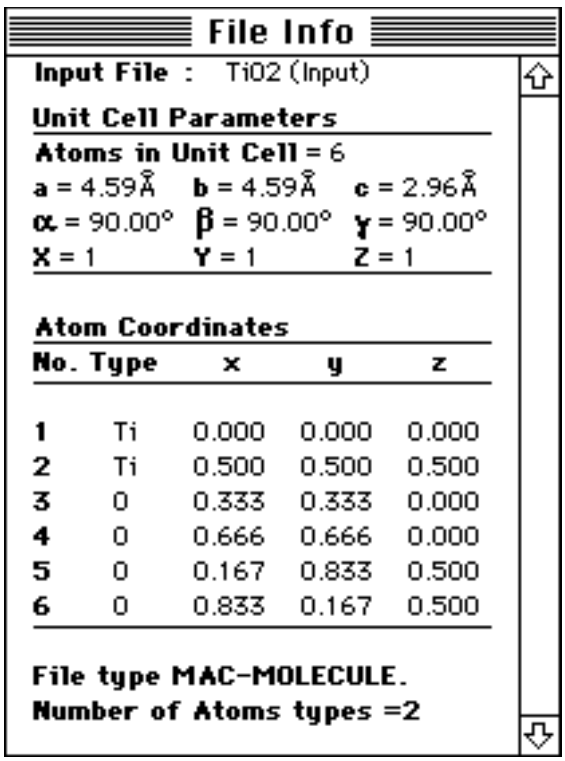
The Build… **Window.**



gsave
.99 setgray
150 100 moveto
/Helvetica-Bold findfont 75 scalefont setfont
55 rotate
(Lattice Maker 2.6.0) show
grestore

This window will appear while LatticeMaker is calculating and saving the file to disk. If you wish to stop the program before it is finished just press the ⌘ and '.' at the same time. If you are calculating a very large file it may take some time for LatticeMaker to respond.

The File Info Window.



This window shows the status of the current file and display information such as the cell constants a,b, and c and the number of cells in the x, y, and z directions. It also shows the positions of the atoms in the unit cell as they were read in from the unit cell file. At the bottom of the window is information about the current output File type and the number of different atom types that are present in the file. Currently LatticeMaker can handle up to 10 different types in each file.

This info Window scales as the number of atoms in the file changes so that it is always just the right size. If the list is too long to fit on the screen then the scroll bars will become active.

```
gsave
.99 setgray
150 100 moveto
/Helvetica-Bold findfont 75 scalefont setfont
55 rotate
(Lattice Maker 2.6.0) show
grestore
```

The Atom Colours Window.

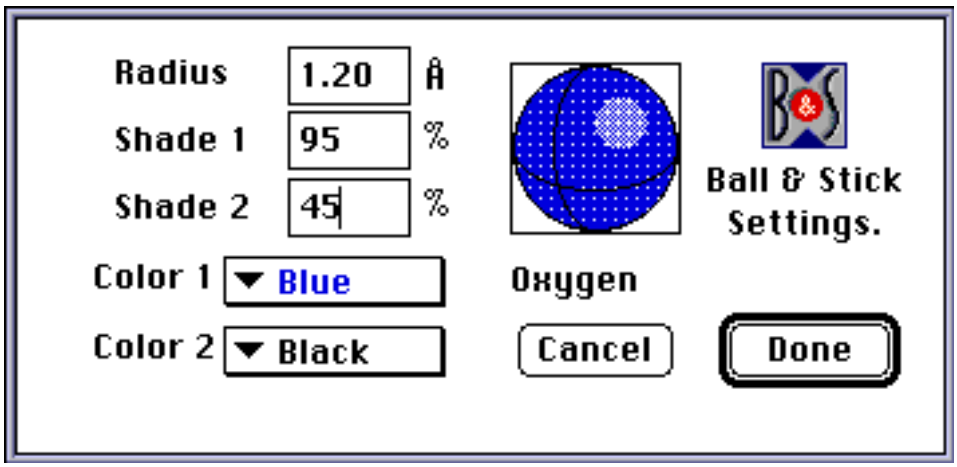
Mac-Molecule

Ball & Stick + resources

If either the Ball & Stick + resources or the Mac-Molecule file formats are chosen then one of the windows shown above will appear. This windows is updated to show the currently chosen colours. The Color menu that was present in older versions of LatticeMaker has been replaced by this Colour Window. Clicking in the balls will bring up either the standard colour picker or a custom picker if the file type is Ball & Stick + resources.

gsave
.99 setgray
150 100 moveto
/Helvetica-Bold findfont 75 scalefont setfont
55 rotate
(Lattice Maker 2.6.0) show
grestore

The Ball & Stick Colour Picker.



This picker allows you to do more than just set the colour of the ball but also the diameter of the atom as it will be drawn by Ball & Stick. The two PopUp menus choose the colours of the ball and the lines used to draw the outline and axes. This Dialog is of a similar type to that used by Ball & Stick but has been simplified here.

File Formats.

There has been a change in the file format since previous versions. LatticeMaker will still read in old files but will also support the new format which includes comments and lattice angles. The new format is shown below.

V2 This indicates that the file is version 2.
N_{Atoms}
a b c
x_{len} y_{len} z_{len}
alpha beta gamma

x	**y**	**z**	**type**
…	**…**	**…**	**…**
…	**…**	**…**	**…**
x_n	**y_n**	**z_n**	**$type_n$**

Where **a,b,c** are the unit cell lattice constants. These values are editable within the program. **alpha,beta and gamma** are the lattice angles between the axes. For an orthogonal system these axes are all 90°. **x_{len}, y_{len} & z_{len}** are the number of unit cells in each of the x-y and z directions. These are also fully editable within the program. x, y, & z are the unit cell coordinates of the atoms in the unit cell. The type is as specified by Chem-3D and you will need to know these

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gsave
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150 100 moveto
/Helvetica-Bold findfont 75 scalefont setfont
55 rotate
(Lattice Maker 2.6.0) show
grestore
```

parameters even if you are using Ball & Stick or MacMolecule or wish to define your own lattices. You will find a list of the types in the Appendix. LatticeMaker will output in four formats. Either Ball & Stick (moldat), Ball and Stick +resources, Chem-3D (cartesian) or MacMolecule (space-filing). See the example input files for example of how to use comments (this is text starting with a semicolon (;)).

If the program doesn't understand an atom type that it is specified, or you wish to have balls to represent multi-atom substituents, then you can add this new type to the program by using ResEdit, however most users should find this unnecessary as LatticeMaker knows of all of the element types defined in Chem 3-D (See Appendix for more details). If you do find an unknown atom or wish to add your own then follow the instructions for customising types in the next section.

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gsave
.99 setgray
150 100 moveto
/Helvetica-Bold findfont 75 scalefont setfont
55 rotate
(Lattice Maker 2.6.0) show
grestore
```

Customising Types in LatticeMaker.

All the information about each atom type is stored as a STR# resource in the LatticeMaker Preferences File. They are made up of 10 strings in the following format.

1). Ball & Stick or Chem-3D String eg. Ti, Si, or O.
2). MacMolecule Character. eg T,S(Limited to only one letter by MacMolecule)
3). String representing the atom radius in Angstroms. Used by MacMolecule and B&S.
4). String representing a Red value for the atom colour Used by MacMolecule.
5). String representing a Green value for the atom colour Used by MacMolecule.
6). String representing a Blue value for the atom colour Used by MacMolecule.
7). A number between 1 and 8 which represents the colour used for the Ball in B&S.
8). A number between 1 and 8 which represents the colour used for the lines in B&S.
9). A number between 0 and 100 which represents Shade 1 used by B&S.
10). A number between 0 and 100 which represents Shade 2 used by B&S.

The ID of the STR# resource is the same as the atom type, so to define a new type make a new STR# resource containing the relevant information for the new type.

******IMPORTANT NOTICE******

Any custom resources created for older versions of LatticeMaker (pre 2.5) will have to be updated to include the extra resources of they will fail to read in correctly and a file loading error will be produced.

Most of the RGB values for the atoms are set to zero in the resources but can easily be changed using ResEdit. The other way to set the colours of the atoms is to by clicking in the balls in the Atom Colour windows.

Known Limitations of LatticeMaker.

At the present time MacMolecule (currently v1.7) only supports single characters to represent atom types. This make it difficult to represent a range of molecules without editing either LatticeMaker or the output files. So for instance $CaCO_3$ could not be represented as Ca for Calcium, C for Carbon and O for Oxygen. We have to choose,for example, C for Calcium, X for Carbon, (as we cannot use C), and O for O.
Hopefully this limitation will be removed by a later version of MacMolecule. (Please!)

Although LatticeMaker will run without problems under System 7.0 it doesn't support things such as Apple Events or Publish and Subscribe (and probably won't as I cannot think of a use for them).

Possible additions to LatticeMaker will depend on the kind of response I get from users.
These may include:-
1). Full text editing support for creation an editing of Unit Cell files within the program.
(This may happen when I have figured out TextEdit.)
2). A built in Atom Editor to add new file types without having to resort to ResEdit (which is still very effective.)
3). Support for more input formats such as those from crystallographic databases.
This would incorporate symmetry operations to build lattices from the most unit cell descriptions (as are normally described in papers and journals).
4). What ever you might suggest.

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(Lattice Maker 2.6.0) show
grestore
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gsave
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150 100 moveto
/Helvetica-Bold findfont 75 scalefont setfont
55 rotate
(Lattice Maker 2.6.0) show
grestore
```

Additions Since Last Release.

v 2.5.0

Made Preferences more robust and flexible by having a Preferences file which stores all the colours and current preferences.

Added extra options to the Preferences Dialog to allow new colours to be saved in either the Preferences File or in the input file.

Opening a file now causes the input file resource fork to be searched for any STR# resources containing colour and other information before the Preferences file is searched. This means that colours can be stored more conveniently in the input file.

Enabled the Close item in the File menu and removed the New item which I thought I may use but have decided I probably won't!

Enabled the Save item and renamed to Save Colours. This will save the current colours assuming that there is a file open and that the relevant Preferences are set.

Added better support for Ball and Stick files by writing specific resources into the output file. In conjunction with this I have added a custom colour picker for Ball and Stick atom types.

Removed the colour menu item as the colour choice is now better served by the new interactive Atom colour windows.

v 2.5.1

Fixed a bug which caused LatticeMaker to report an error if an input file was used that didn't contain a valid resource information. This unfortunately made it impossible to create new files!

Added some cosmetic enhancements such as animated cursors during time consuming operations, and extra icons for some of the dialogs.

v2.6.0

Extended the input file format to include angles and comments.

Enhanced the Info window to reflect the addition of angles to the input file. Now

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(Lattice Maker 2.6.0) show
grestore
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has scroll bars if the number of atoms will not fit in a window that takes up the full height of the screen.This allows all of the coordinates to be checked to make sure they have read in correctly. (This window will be fully resizeable in a later version of LM)

Added bonds in the output file. The bond creation methods are very flexible and allow almost all possible bonding senarios.

Added an option to the prefs which allows the splash screen not to be showed at start up. and extended the prefs resource to include information about the MacMolecule bonds
colour and also the current output setting (either WF BS or SF).

Extended the output of MacMolecule format files to include a message at the end for
display in the text box of version 1.7 upwards of macmolecule. This message is stored as a TEXT resource so it can be edited by those willing to wield ResEdit.

Added Notifications. If LatticeMaker is switched into the background while doing some calculations then it will use the Notification Manager to alert the user if it is still in the background when the calcs have finished.

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(Lattice Maker 2.6.0) show
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```

Removed problems with strange cursors if another application was switched in and out. LatticeMaker now resets it's own cursor.

Despite the problems that it can cause LatticeMaker still works with both System 6.0 and 7.0. I will try to hold out for as long as possible before abandoning System 6.0!

Thanks

Thanks must go to all of the following.

Dr. Norbert Müller author of Ball and Stick for supplying me with a description of the Ball and Stick Moldat format and also for information about Ball and Stick resources. **Cherwell Scientific Publications Ltd** for the gratis copy of Ball and Stick. My Ph.D thesis is now full of wonderful models!
Dr. John Pilling for pointing out some of the bugs and providing the maths for the non-orthogonal calculations and also providing some of the unit cell files.
Also all those of you who have send messages of support and comments on the program and given me the incentive to continue.

Disclaimer and Copyright Notices.

Correspondence Comments and Questions

Any correspondence about LatticeMaker © 1992 should be sent to:-

Peter Hardman.

```
gsave
.99 setgray
150 100 moveto
/Helvetica-Bold findfont 75 scalefont setfont
55 rotate
(Lattice Maker 2.6.0) show
grestore
```


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email hpj%cxa.dl.ac.uk@nsfnet-relay(prefered).
or hardman%v2.cgu.mcc.ac.uk@nsfnet-relay.

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55 rotate
(Lattice Maker 2.6.0) show
grestore

I welcome any comments about the program, it's limitations and possible future enhancements. Future releases will be made available via (Info-Mac) sumex-aim.stanford.edu, MacSciTech (ra.nrl.navy.mil)

Thanks for your support.

Have Fun.

Peter Hardman 1992.

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(Lattice Maker 2.6.0) show
grestore
```

Appendix

This is a list of the atom types from Chem-3D that LatticeMaker recognises. This list is derived from Chem-3D plus 2.0.1 © Cambridge Scientific Computing 1986-89.

Ag	474
Al	133
As	333
At	851
Au	794
B	53
Ba	562
Be	42
Bi	833
Br	351
C sp	62
C sp2	63
C sp3	64
Ca	202
Cd	483
Cl	171
Co	276
Cr	246
Cs	551
Cu	294
F	91
Fe	266
Ga	314
Ge	324
H	11
Hg	803
I	531
In	493
Ir	776
K	191
La	573
Li	31
Mg	122
Mn	256
Mo	426
N	77
Na	111
Nb	416
Ni	284
O Bridging	89
O sp2	81
O sp2	88
O sp3	82
O Terahedral	84
Os	766
P	159
Pb	824
Pt	784
Rb	371
Re	756

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/Helvetica-Bold findfont 75 scalefont setfont
55 rotate
(Lattice Maker 2.6.0) show
grestore
```

Rh	456
Ru	446
S bent	162
Sb	516
Sc	213
Se	342
Si	144
Sn	504
Sr	382
Ta	736
Te	522
Ti	226
Tl	813

```
gsave
.99 setgray
150 100 moveto
/Helvetica-Bold findfont 75 scalefont setfont
55 rotate
(Lattice Maker 2.6.0) show
grestore
```

V	236
W	746
Y	393
Zn	303
Zr	404

For the more exotic atoms, or if you wish to use an atom to represent a molecule or substituent then create you own type and add the STR# resources.