gsave
.99 setgray
150 100 moveto
/Helvetica-Bold findfont 75 scalefont setfont
55 rotate
(Lattice Maker 2.3.1) show
grestore

Lattice Maker 2.3.1

What is Lattice Maker?

Lattice maker is designed to be used with Chem-3D and MacMolecule.It is an aid to help in the production of images of large super-structures and bulk structures of crystal lattices.

System Requirements.

Lattice Maker uses a Color Picker to set the colors of Atoms to be used in MacMolecule. For Lattice Maker to run Color QuickDraw must be available unless the machine is running system 6.0.7 or later. If this is the case then a B/W machine will be able to use a monochrome Color Picker, (a contradiction I know but useful all the same!). If you have a B/W machine and are using 6.0.5 or earlier you will still be able to use Lattice Maker but the color item in the Build Menu will be dimmed.

File Formats.

Lattice Maker requires it's input in the following format.

N_{Atoms}			
a	b	c	
x_{len} y_{len}	z_{len}		
x	y	z	type
...	...	...	...
...	...	...	...
x_n	y_n	z_n	$type_n$

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Where a,b,c are the lattice cell constants. These values are editable within the program.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 that specified by Chem-3D and you will still need to know these parameters if you are using MacMolecule and wish to define your own lattices. You will find a list of the types in the Appendix.

Lattice Maker will output in two formats. Either for Chem-3D or MacMolecule. Due to the added complexity if bonds were to be defined for such large structures they are omitted. This means that only space filling models are available in MacMolecule 1.5. This may be fixed in a later release of Lattice Maker.

If the program doesn't understand an atom type that it is given you can add this type to the program by using ResEdit, however this is very unlikely as Lattice Maker knows of all of the types in Chem 3-D (See Appendix for more details). If you do find one that is unknown then follow the instructions for customising types in a the next section.

Customising Types in Lattice Maker.

All the information about each atom type is stored as a $STR^{\#}$ resources made up of 6 strings in the following format.

1) 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 ionic diameter in Angstroms. Used by MacMolecule.

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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.

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.
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 use the Color Picker in the BUILD menu.

Known Limitations of Lattice Maker.

At the present time MacMolecule 1.5 only supports single characters to represent atom types. This make it difficult to represent a range of molecules without editing either Lattice Maker 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 chose 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.

When a file is being created no other operations are possible and unfortunately there is no Cancel during the build either! This means that if you start a very large file build and then decide to stop you will have problems.These will be fixed in a later release.

There is limited error checking for problems such as low disk space etc. So be aware that the file may not be created correctly , or Lattice Maker may crash if disk space gets low.
Future releases will add better error checking to make the program more robust.

When a color has been edited the new color is remembered for the duration of the program but is forgotten after it is Quit. This means that you must either edit the resource file to add you favourite colors or re-edit them each time in the program. This will also be fixed in a later release.

Disclaimer and Copyright Notices.

Peter J. Hardman.
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England.

I give you the user a licence to use this program free of charge on any machine either singly, or on a computer network . It may be freely distributed by any means, including electronic bulletin boards providing the following conditions are not broken.
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(3)All documentation and example files are include with the program.

I retain the rights to the program and as such you may **NOT**:
(1) Modify,translate, decompile of disassemble the program or alter the documentation (Except to translate text into another language).

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(2) Remove any Copyright or Proprietary notices, labels or marks in either the program or documentation.

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Any files that you create with this program may be used for any purpose. Please mention that the files were created using Lattice Maker © P.J.Hardman.

The software is provided on an as is basis, with no warranty of any kind. The author excepts no responsibility for damages arising from the use of this program under any circumstances.

Correspondence Comments and Questions

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

I welcome any comments about the program, it's limitations and possible future enhancements. Future releases will be made hopefully be made to SUMEX-AIM.STANFORD.EDU and possibly elsewhere.

Thanks for your support.

Have Fun.

Peter Hardman 1991.

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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 © Cambride 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

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Pb	824
Pt	784
Rb	371
Re	756
Rh	456
Ru	446
S bent	162

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Sb	516
Sc	213
Se	342
Si	144
Sn	504
Sr	382
Ta	736
Te	522
Ti	226
Tl	813
V	236
W	746
Y	393
Zn	303
Zr	404

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