wxDragon v1.8

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Contents

List of Figures

1. Introduction

1.1 Preamble

Sometimes in this work names of programs or companies are mentioned. This is done in a pure private matter, and is not commercially intended, without looking on rights they may be under. The single enduser may need to check for this if he wishes to further uses these names in his own buissness.

Also, at few points sites are mentioned. They are only intended to allow the user to get more and deeper informations about the products. I am in no way connected to these sides (well, beside my own and the wxDragon page maintained by me), and I don't take any responsibilities for them.

1.2 Intention

When starting writing wxDragon, in the old times, when it still was MacDragon, the nearly totaly absence of programs which immediately can read the output from quantum chemistry programs such as Gaussian striked me to death. The user, in this case also me, had to extract the coordinates with an editor, modify them in some way or the other, and then use a program for displaying it, which was not designed to be used for this kind of thing. In my cases, I had to convert the output of Gaussian to an input file for either Schakal or Xmol. Schakal is a program used by crystallographs, nevertheless the output was nice, but only in HPGL, so it had to be converted to postscript or something else in order to get it printed on a normal printer. Xmol, at this time, run only on such strange machines like SGI and IBM, both too expensive for the end user, and printing was not realized then (or I didn't find it). And, besides the geometries, all other informations like charges, energies and so on, had to be extracted by hand. Fearfull stories from the past!

1.3 What can be done

wxDragon is here to change that all. It can reads several different file formats and sometimes can extract additional informations. The recognized file formats are

Abinit [1, 2], ADF [3], ASW [4], BIND [5], CIF, CPMD [6], DL_POLY [7], EXCITING [8], FPLO [9–13], Gamess-UK [14], Gamess-US [15], Gaussian 92-03 [16, 17], Ghemical [18], ICSD [19], JANA [20], LMTO-ASA [21], MDL-MOL[22], MolStruct [23], MPQC [24], Crystal [25], PDB [26], Schakal [27], Siesta [28], Turbomol [29], VASP [30, 31], Wien2K [32], XMol [33].

1.4 Requirements

For the moment wxDragon is known to work under the following OS:

- Windows NT 4.0/2000/XP/VISTA/7
- Linux (many different flavours)
- Sun with SunOS 5, discontinued.
- FreeBSD 4
- MacOS 9.1, discontinued.
- MacOS X, from 10.4 upwards

In principle wxDragon should work on any machine where the wxWidgets toolkit, including the wxGLCanvas, can be compiled succesfully. For a list of supported machines see **http://www.wxwidgets.org**. A working OpenGL library on the machine is, besides the wxWidgets toolkit, the only true restriction.

1.5 The Icon

The icon representing wxDragon is modeled after a mask from the traditional chinese opera, of which I seem to be a fan, sort of. Also, my bad chinese may also worked this way (thanks to Prof. Ming Fong Kuo). The mask also is program for wxDragon: the visitor sees some nice colors and things, but the things behind the mask may look the other way round. What Do You Believe In?

1.6 The License

Preliminary wxDragon Licensing Information

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wxDragon is SHAREWARE.

One may use wxDragon for a trial period - for the moment this period is not specified, but when using wxDragon becomes substantial for your work i think it will be time to pay. If you want to pay the shareware fee, please get in contact with me first, the email adress is

info@wxdragon.de

Copyright Notice

If you redistribute the unregistered version of wxDragon, the entire contents of this distribution must be distributed, the binary, and the complete contents of the docs directory.

Note that distributing wxDragon 'bundled' in with any product is considered to be a 'commercial purpose'. In this case please contact me for special pricing.

wxDragon doesn't claim to be suitable for anything. Just test it....

The author may be contacted via:

- eMail:

  info@wxdragon.de

1.7 The Future

Who knows...

Before we start, there is something important: sometimes you will stumble over the letters *NWY*. This is a special feature, short for *Not Working, Yet*. So please stay tuned, and if you really want to work especially with this feature, drop me a note.

1.8 Installation

After endless criticism about the complicated installation process I changed the procedure. It should be very easy now to install wxDragon;

- Windows: Download the glut-lib for Windows and put the glut32.dll into the WINDOWS/system32 folder. Then just double-click wxDragon.exe. That's it.
- MacOS X: Unpack the package and put the application wxDragon into your Applications folger. Double-click it.
- Linux/Unix: put the wxDragon file somewhere into your path and start it. If some libraries are missing (re)install them.

2. A Quick Overview

2.1 The principal Things

At startup the user may see the following window:

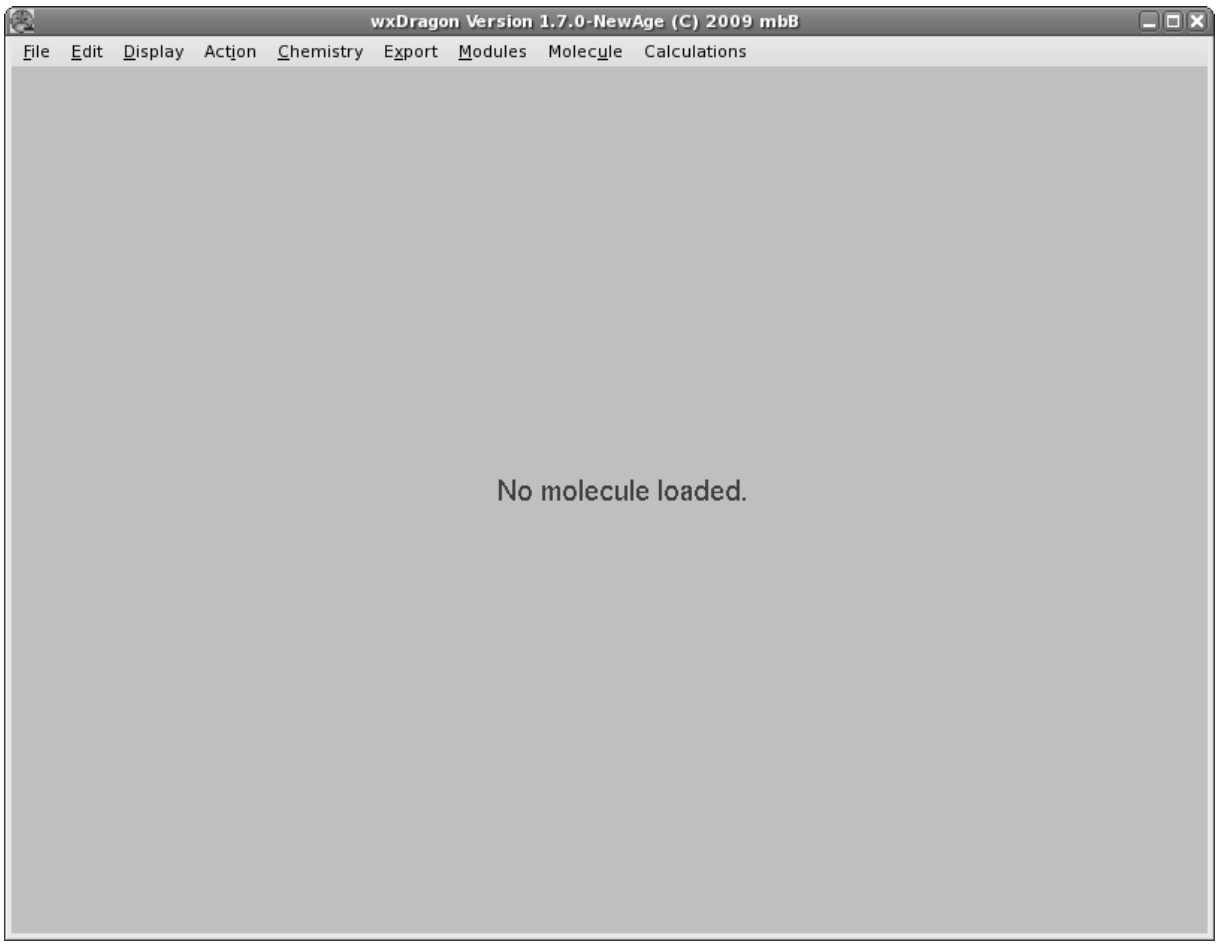

Figure 2.1: Startup window of wxDragon

It consist of 2 regions: the menubar on top of the drawing area. Both parts will be briefly described in the following sections.

2.1.1 The Menubar

Within the Menubar the items are grouped together mostly by the topic. In the Display menu one can find options regarding the style and way things are being plotted in the

drawing area. A detailed description about all items follow in the menu chapters starting at chapter 4.

2.1.2 The Drawing Area

Below the menubar the actual drawing area is placed. Most of the output, like geomtries, energies or temperatures, are given here. If no molecule is loaded, this fact is printed in the middle of the drawing area.

2.2 The Mouse

When the mouse pointer is within the actual drawing area, the three mouse buttons trigger different actions. In cases where no 3 mouse buttons are available, the middle button is replaced with the SHIFT key, which must be pressed together with the left button. If only one mouse button is available, the right button is replaced by the combination of the ctrl-key together with the left mouse button. The number of mouse buttons can be set in the preference dialog, *System* section.

2.2.1 The Right Button

When pressing the right mouse button within the drawing area, a menu will popup containing some important shortcuts. A description of all option is given in section 23.1.

2.2.2 The Middle Button

The middle button is for selecting and deselecting of atoms, bonds, planes or triangles. When the mouse pointer is within a certain range of an object, and the middle button is pressed, the atom becomes selected. This object will then become the new selected object one, objects which were selected before will step down one step (when an atom is selected: the old atom one becomes two, two becomes three, three becomes four, and four is being deselected), otherwise the old selected object is deselected. If the object is already selected, it will be deselcted, and in case of atoms, all older selected atoms will step up one step. Be aware that there is sequence in which the elements are tested: first the atoms, then the bonds, and later on the planes. So it may be possible that when ones click on a plane, a underlying bond or atom may be selected and the respective popupmenu may be presented. In this case please vary your clicking position until you get the planes dialog.

Above selection mode for atoms is only true for normal operations. If one chooses the *Selection Mode* from the canvas menu (see chapter 23.1) all atoms which are selected stay selected until they get deselected or an respective action in the planes dialog (see chapter 13) was used.

2.2.3 The Left Button

If the left mouse button is pressed, and hold pressed while the mouse is moved, the molecule shown is rotated according to the mousemovement. If the CONTROL key is pressed together with the mouse movement, the molecule can be moved in x and y (in screen coordinates).

2.2.4 Different Mouses

To emulate a missing middle button on a 2 or 1 button mouse, press the left/only button together with the SHIFT key. To emulate a missing right button, press the button and the CTRL key simultanously.

The number of buttons available can be controlled over the *Preferences*-dialog, in the section *System*. Here, the number of mouse buttons can be set and saved, so that after every startup of wxDragon the number of mouse buttons is set according to the saved one. This dialog can be reached with klicks on only the left mouse button, so it should work with every mouse under all operating systems.

The shift or the CTRL key will not always work. One should try all special keys in order to determine which one emulates the missing mouse-keys.

2.3 The wxDragon Files

At start wxDragon would like to write at least 2 files to the storage device: a file named *defaults_pref* where all saveable settings in wxDragon are written to. One can change the settings easily through the *Preferences* menu to be found in the *Edit* menu. The second file is named *dragon_atoms_pref* and contains the settings for the atoms like radii and colors.

All files will be written to the directories *$HOME/.wxdragon* (Unix and Mac) or to *$APPLICATION_DATA* (Windows). Please let this happen, otherwise wxDragon will complain about it.

2.4 Files to be Read

wxDragon distinguish between 2 different kind of files: the normal input and output files of the various programs, and the files where some kind of simple data are stored, like BAND, DOS,or COHP files, which are of the kind PROPERTY in wxDragon.

Since the format of the first ones, the real in- and output-files can be determined mostly automatic, they can be read in by the simple *Open* menu. Sometimes the filename or the file-ending is important, but mostly the type are recognized and opened.

Many property-files dont contain an easy-to-recognize keyword so that the user have to determine the format of the file he wants to open with the right open-command, found in the *Load Props* menu.

Having a shell from which ones open wxDragon, one can give the filenames to be opened right behind the wxDragon commando, for example *wxDragon OUTCAR POSCAR* will open the files OUTCAR and POSCAR directly. If one wishes to open property files, the commandline would be more like *wxDragon -p DOS -p COPL*. The ordering of the filenames will be kept. In order to allow automatic recognition by wxDragon in some cases the filenames must follow some naming rules as describe in chapter 4 on page 9.

3. Getting Started

3.1 VASP

3.1.1 The Start

You want to do a VASP calculation but you have nothing. How to start?

You can build a crystal as described in subsection 3.2 and modify it to your needs. Then go to the *Export* menu und select VASP. You can export the POSCAR and also let wxDragon generate the right POTCAR for it. Details are given in section 9.3.24 on page 31. The INCAR and KPOINTS file must be generated by hand, but simple starting files for them can be made using the VASP module from the *Modules* menu (see section 10.10 on page 37).

3.1.2 Afterwards

You have successfully run a simulation with VASP. What to do next?

Start wxDragon and open the OUTCAR file with it. The structure should appear in the window. If the calculation was an optimization you can open the Trajectory-Dialog (to find in the *Display* menu) and look at the optimization process step by step, or within an animation. The energy of the actual step can be displayed on bottom of the window. This can be enabled within the *Misc.Display Options* Menu under the *Display* menu. The energy will be updated for every step.

If the OUTCAR contains the result of a force calculation the resulting vibrations can be shown using the Vibration-Dialog, also found in the *Display* menu. For more details see chapter 12.2.

Opening the *MD-Module* dialog (under the *Modules* menu) will give you some more options. First, it shows the lattice parameters of the found cell, and the temperature and energy, if found. If you want to multiply the cell shown, this can be down in the second half of the dialog by giving new values for A,B, and C Mult and do a *Make*.

If you want to calculate the pair (or radial) distribution funtion of the optimization use the *RDF* button, the button *MSD* calculates the means square displacement of the run for a selected atomtype. After the calculation a new property dialog will open, where one can control the printing of the values calculated (see chapter 17.3 for more details).

If in the same directory as the OUTCAR some potential files like the ELFCAR, CHGCAR, CHG or such ones are present you can press the *Module* button to open the surface control dialog. For more details afterwards see chapter 15.

At the bottom of the dialog you will be able to control the displaying of the cell (*SHOW cell* will hide and show the cell, *Toggle Cell* will toggle the cell shown throu 3 different settings, which can be seen only if one has changed the multiplicity of the cell)

or even convert the result of your calculations into a crystal. See chapter 16.3 for more details.

3.2 Crystals

You want build a crystal? Open wxDragon and choose the *New Crystal* menu found in the *Modules* menu (or try to press CTRL-C). A new dialog will open where one can input all necessary data, for more details see chpater 16.

When the crystal is generated, one can play with it: show different planes in the unitcell using the Planes-dialog (see chapter 13), or find some polyhedrals using the respective dialog (see chapter 14).

After pressing the *Find Spacegroup* button (do it even if you dont really want to find a new spacegroup) one can visualize some of the symmetryelements found, see chapter 16.4 for details.

3.3 Gaussian

See the results of a gaussian calculation. Open the log file in wxDragon. If the run was an optimization, one can use the Trajectory dialog, found in the *Display* menu, to look at the optimization process step by step (see chapter 12.1 for more details).

If the run contained a vibrational analysis, the Vibrations dialog (found int the *Display* menu) can be used to animate the vibrations, see chapter 12.2. Or one can display the forces leading to the vibration using arrows on the atoms.

If the outfiles contains a recognized orbital analysis, the resulting orbitals can be shown using the Orbital dialog, see chapter 12.3.

And, if one wishes to start a new calculation using Gaussian, the Gaussian-Module (see section 10.7) can be used to generate a new input file.

4. File Menu

4.1 Open

Popup an fileselection dialog, in which a file could be choosen for opening. If wxDragon recognizes the format of the selected file, it will process the file and extract all information it is able to read out of the file. About the required files of the programsystems which can be read, please see chapter 18.

4.2 Close

The actual active molecule is deleted, all related dialogs are closed. If there are more molecules loaded, the molecule before the closed one (according to the list in the Molecule Menu) is diplsayed.

4.3 Load Props

Open of properties must be done in this special submenu since here the abilities of autorecognizing which file format is given is very limited. Please choose the property file format accordingly.

4.3.1 LMTO DOS

Reads in the DOS file generated by the program LMTO-ASA [21] with an *lmdos* run. Be aware that the DOS file is a binary file, so only DOS files generated on the same kind of machine as the one wxDragon is runnning on can be read correctly. After an succesfull opening, the property dialog and a new displaying window opens. For a further description of the possibilities therein please read section 17.2.1 on page 54.

If you get strange results one can try to open the DOS as an 64 bit dos, use the resprective menu option or the *-p64* switch.

4.3.2 LMTO COHP

Reads the COPL file generated by the program LMTO-ASA [21] with an *lmcohp* run. This file is an simple ascii file, so no problems are to be expected between different kind of computers. After an succesfull opening, the property dialog and a new displaying window opens. For a further description of the possibilities therein please read section 17.2.2 on page 54.

4.3.3 LMTO BAND

Reads the BNDS file generated by the program LMTO-ASA [21] with an *lmband* run. This file is an simple ascii file, so no problems are to be expected between different kind of computers. After an succesfull opening, the property dialog and a new displaying window opens. For a further description of the possibilities therein please read section 17.2.3 on page 54.

4.3.4 FPLO DOS

Reads the +dos.XXXXX file generated by the program FPLO [9]. This file is an simple ascii file, so no problems are to be expected between different kind of computers. After an succesfull opening, the property dialog and a new displaying window opens. For a further description of the possibilities therein please read section 17.2.3 on page 54. NWY.

4.3.5 FPLO BAND

Reads the +band file generated by the program FPLO [9]. This file is an simple ascii file, so no problems are to be expected between different kind of computers. After an succesfull opening, the property dialog and a new displaying window opens. For a further description of the possibilities therein please read section 17.2.3 on page 54.

4.3.6 VASP DOS

Reads in the DOSCAR file generated by the program VASP [30, 31]. After an succesfull opening, the property dialog and a new displaying window opens. For a further description of the possibilities therein please read section 17.2.1 on page 54.

4.3.7 VASP EIGENVAL

Reads in the EIGENVAL file generated by the program VASP [30, 31] which contains the bandstructure. After an succesfull opening, the property dialog and a new displaying window opens. For a further description of the possibilities therein please read section 17.2.3 on page 54.

4.3.8 WIEN DOS

Reads in the DOS file generated by the program WIEN [34] with an *lapw5* run (usually named *.outputt). After an succesfull opening, the property dialog and a new displaying window opens. For a further description of the possibilities therein please read section 17.2.1 on page 54.

4.3.9 Crystal BAND

Opens the bandstructure from a Crystal [25] calculation.

4.3.10 Crystal DOS

Opens the DOS from a Crystal [25] calculation.

4.3.11 BIND Band

Opens the bandstructure from a BIND [5] calculation.

4.3.12 BIND DOS

Opens the DOS from a BIND [5] calculation.

4.3.13 BIND COOP

Opens the COOP from a BIND [5] calculation.

4.3.14 EXCITING Band

Opens the bandstructure from a EXCITING [8] calculation.

4.3.15 EXCITING PDOS

Opens the DOS from a EXCITING [8] calculation.

4.3.16 ABINIT Band

Opens the bandstructure from a ABINIT [1] calculation.

4.3.17 ABINIT DOS

Opens the DOS from a ABINIT [1] calculation.

4.3.18 SIESTA Band

Opens the bandstructure from a SIESTA [28] calculation.

4.3.19 Simple XY

Reads in a file in the simple format, where the numbers are stored in rows. After an succesfull opening, the property dialog and a new displaying window opens. For a further description of the possibilities therein please read section 17.2.6 on page 55.

4.4 Save

The active molecule is saved, together with some display information, e.g. which atom is hidden, and which bonds are shown. Also the current rotation state is saved. When this file is opened again, the molecule is shown in the same state as it was when it was saved. This is handled within the wxDragon Internal file format, which is described on page 61 in section 18.3.5.

4.5 Save CML

The active molecule is saved in the chemical markup language format (or, at least, what I think is), together with some display information, e.g. which atom is hidden, and which bonds are shown. Also the current rotation state is saved. When this file is opened again, the molecule is shown in the same state as it was when it was saved.

4.6 Print

Print the active molecule into a postscript file. An option dialog appears which allows some tuning. First of, the quality of the picture can be choosen between **BlackWhite**, giving a simple Black and White picture, **Low**, resulting in a slightly better picture than the first one, and **High**, which prints a high quality color picture. On the left side, some modifications can be switched on or off.

- *Perspective*: Prints the picture with a slightly perspective in it for a good 3D impression
- *Shaded Balls*: a light source is included, giving the atoms a more realistic ball effect
- *Filled Bonds*: draws the bond as filled cylinders and not only with two lines
- *Reduced Radii*: lessens the radii of the atoms by the factor of 2, clearifying the picture with many atoms somewhat
- *Crosses*: draws a horizontal and vertical line in order to enhance the 3D effect
- *Pattern*: fills the atoms in the Black and White description with a pattern, which varies between the different atom types
- *Fill Isosurface*: print the isosurface as filled triangles, otherwise they are printed as wireframes.

After the selections are done, press the Print button and a file selection dialog will appear in order to select or type the name of the resulting postscript file. Printing may take a while, especially when printing isosurfaces. To inform on the progress made a progressbar appear for the generation of the objects. After this is finished, another progressbar show up to inform on the progress of the file-writing. Some computer are faster in step 1, some in step 2.

Another important point can be set in in the preferences, using the print tab. There, the number of bins, into which bonds or the triangles of surfaces are divided. A good number may be 2–4. Be aware that a higher numer here may result in real long printing times, which may look even like a crash of wxDragon, so please be patient.

4.7 About

A dialog with the version and the license info appears and may be read. If you find wxDragon usefull, please pay your shareware fee. With it you will get access to unrestricted version of wxDragon as well as preferred attention in case of bugs or suggestions for improvement or extensions.

4.8 Quit

Close all molecules and quit wxDragon. The end of your session with wxDragon.

5. Edit Menu

5.1 Undo

Several actions within wxDragon can be undone, if the user wishes to make it not happen. These actions are

- Showing and hiding of Bonds between atoms
- Showing and hiding of lines between atoms, like distance lines, angular description lines, or simple connection lines
- Showing,hiding, and alterations of atoms

5.2 Copy

NWY.

5.3 Preferences

Opens a dialog in which the user can set desired opening values to some options. A detailed description can be found in chapter 19 on page 62.

5.4 Atom Preferences

Opens a dialog in which the user can set values for the atoms, such as radius, prefered bond angle, or the color of the type. A detailed description can be found in chapter 19.2 on page 63.

6. Display Menu

This menu allows to control the appearence of the molecule as it can be seen in the drawing area. The first 4 items allows the user to choose the general display style of the molecules resp. atoms. The third section affects anything around the atoms and bonds, like atomic labels, energies, and so on.

In the next section 3 vital dialogs for animation and special features like animation of MD runs, vibrations, or the visualization of orbitals can be found. At the bottom, some special features concerning the drawing area are located.

6.1 Hide Atoms

Disables the drawing of all atoms. It does not affect the individual drawing state of the single atoms.

6.2 Lines

For the moment, this is not a real stick only model, the atoms will become very small balls, so the bonds will become more important. The atoms will be shrinked to 10% of their normal radius as given in the atom preferences.

6.3 Ball&Stick

The atoms will be displayed as balls with half of the normal radius. This seems to me a quite suitable ratio, since then the structure are quite filled, but still parts in the background can be seen.

6.4 Mod. Ball&Stick

The same as the normal Ball&Stick mode, but here the atoms are scaled to 80% of their normal radius. In cases that the file supplies atomic radii, they will be available here.

6.5 Spacefill

Here, the atoms will be shown in their full radius, as defined in the atomic preferences. For a start, in the preferences for all atoms the covalent radius is given (according to some book of mine, the *which* is long forgotten)

6.6 Real Atom

The feeling of real atoms is given here: a small atomic core, surrounded by a larger electron sphere. And, who knows, perhaps someday real electrons may be flying around.

6.7 Center

Should allow to center the molecule if it will be made work in the future after the user has moved.

6.8 Atom Display Options

A wide range of option can be found here. The will be described very briefly:

- **Symbols** if activated, the atomic symbols of the atoms are shown. If a special label could be read from the input file, they will be shown. In order to turn single labels off or on see section 7.10.7.
- **Number** if activated, each atom will marked with a number, according to their position within wxDragon, and this is mostly as the were read in from the input file.In order to turn single numbers off or on see section 7.10.7.
- **Ignore Hydrogen** if activated, no hydrogen atoms are shown. May be usefull to somebody who usually uses many useless Hydrogens.
- **Show H Symbol** if activated, not only the atomic symbols of the heavy atoms are shown, but also on Hydrogens.
- **Show H Number** same as for **Show H Symbol**, but for the atom number.
- **No Bonds** if activated, no bonds or line are shown at all. This is only a weak switch, which may be overwritten by some special dialogs like the MStep dialog (see section 6.11).
- **Colored Bonds** if activated, the bonds between atoms will no longer be simple grey (or whatever color you choosed), but is printend in the colors of the two atoms they connect.
- **Show X Atom** if activated, and in the input file some X Atoms (no real atoms, just points in the space) were present, they will be shown also.
- **Show Atomkey** if activated an atomkey explaining the actual atom colors. The position of the key can be determined in the preferences dialog, see 19.
- **Track Atoms** if activated, the old atom positions will not be cleared and therefore one can track the path the atoms will take.
- **Show Coord.Sys** toggles the displaying of the coordinate system in the right top corner. Somebody may wish to ignore it.
- **Show Coord.Sys in Zero** if activated, the coordinate system is show in the origin of the shown cell.

6.9 Misc Display Options

- **Distance** if activated, and some distance are defined (see section 7.10.8), a line between the two correnspondingatoms is drawn, and the distance in Å is shown in the middle of the line.
- **Angle** if activated, and some angles are defined (see section 7.10.9), lines between the central atom and the both outlying atoms are drawn. Additionally, at 2/3 of these bond lines, a connecting line is drawn between the lines, and in the middle of it the angle in $\cdots$ is given.
- **Dihedral** same as for **Angle**, but here the dihedral angle is shown. For defining of an dihedral angle see section 7.10.10
- **Charge1** if activated, and in the input file charges of the atoms were found, those charges can be shown at the corresponding atom. If the name of the charge is known, the item name **Charge1** will be replaced with this name. In order to turn single charges off or on see section 7.10.11.
- **Charge2** same as for **Charge1**, will be used if 2 different charges can be found in the input file.
- **Mag.Mom.1** if activated, and the file read in contained some recognized informations about magnetic moments, those are shown next to the atoms which carry them.
- **Mag.Mom.2** same as for **Mag.Mom.1**, will be used if 2 different sets of magnetic moments can be found in the file.
- **Show Mag.Mom. Arrow** Shows the magnetic moment not as pure numbers, but like arrows, with direction of the moment, the length of the arrow is scaled according to the magnetic moment.
- **Dipole** NWY.
- **Quadrupol** NWY.
- **Energy1** same as for **Charge1**, but for an energy found in the input file.
- **Energy2** same as for **Charge2**, but for an second energy found in the input file.
- **Temperature** same as for **Energy**, but for a temperature found in the input file.
- **Show Force** if activated, and informations about forces on the atoms can be found in the file read in, they can be shown here using arrows.

6.10 Display Style

- **Label Units** if set, the units of the shown distances, angles and similiar things are shown together with the value.
- **Static Size** NWY

- **Relocate Labels** NWY
- **Don't hide Labels** NWY
- **Label Lines** NWY
- **1A Order** determines how the atomic labes are printed: first the atomic symbol and then the number, or (if the item is selected) first the number and afterwards the symbol.
- **Restore Orig.Pos** restores the position of zero movement and zero rotation for the molecule, just as it was immediately after the opening of the molecule. May be usefull to find back into the molecule after a lot of rotations.

6.11 Trajectory

The trajectory item consists of a submenu, containing 3 items. The latter two are simple: go to the first/last step. The first item opens a dialog for further control. The dialog is described in detail in section 12.1 on page 40.

6.12 Vibrations

With this item vibrations found in the input file can be animated in the drawing area. For deatils please see section 12.2 on page 42.

6.13 Orbitals

In case of some inputfiles, orbitals can be displayed. About the details please see section 12.3 on page 43.

6.14 Viewing

6.14.1 View-Control

A small dialog pops up. Using the first slider one can zoom into the molecule. The second slider (*View Distance*) changes the distance of the virtual spectator to the screen, so it may look like zooming, but some things may behave different.

The third slider controls the size of the shown coordinate system, just in case you want it smaller or bigger.

The next 2 text inputs let one control the size of the drawing canvas. This can be done also by simple dragging the window to the size one wishes, but here it can be controled in steps of pixels. And dont forget to press the *Set Size* button when the input is finished.

The following choice let one look directly along some given crystallographic axis (be aware that up to now only a small subset is working, sorry).

The last option, *Shift Origin into Cellcenter*, shifts the origin, the point (0,0,0), into the center of the crystallographic cell. Comes handy sometimes.

6.14.2 Second Window

Opens or closes a second window with a second view. In the resulting two windows two different views of the same molecule as well as two different molecules can be viewed.

6.14.3 Link/Unlink Movement

When two viewing windows are opened the movement of the two shown molecules can be linked together. So, when rotating a molecule in the first window, the molecule in the second window is also rotated by the same amount as the first molecule.

6.14.4 Background Color

Here the background color can be choosen freely. Have a nice try. The original color is something around 140 for all colors. After selecting the desired color, simple press **Add to custom colors** and then **OK** to change the background color.

6.14.5 Show Arrow

If forces on atoms were found in the input file, they can be displayed using the apprearing dialog. The length of the arrows can be scaled using the slider, so that even smaller forces can be seen.

7. Action Menu

7.1 Stop Action

Stop the Handle-Action (see 7.10) and switch back to the normal selection rules when clicking atoms. This should be done when one is finished with the desired action, just to be sure that nothing unwanted happens.

7.2 Show Selection

Toggle the displaying of the selected atoms, which will be painted in a slightly darker color than the original one (which, of course, is a little hairy to see when the color is black...).

7.3 Clear Selection

Clears all selected atoms.

7.4 Meassure Win

Opens a window which displays the distances, angles and dihedrals between the selected atoms, see picture 7.1. Be aware that the latest selected atom will become atom 1 while the number of all the other selected are increased by one and the fourth atom is deselected.

7.5 Clean Display

Clears the display from all items which dont belong there in order e.g. to make a picture. So, the atomkey and the coordinate system will be hidden. Just a shortcut.

7.6 Move Mode

In the normal mode the position of the whole molecule shown can be shifted around the canvas by pressing the CTRL key and then moving the mouse while the left button is pressed.

When *Move Mode* is activated now one can, while the CTRL key is pressed, click on an atom and move this around the display (of course, keep the left mouse button down).

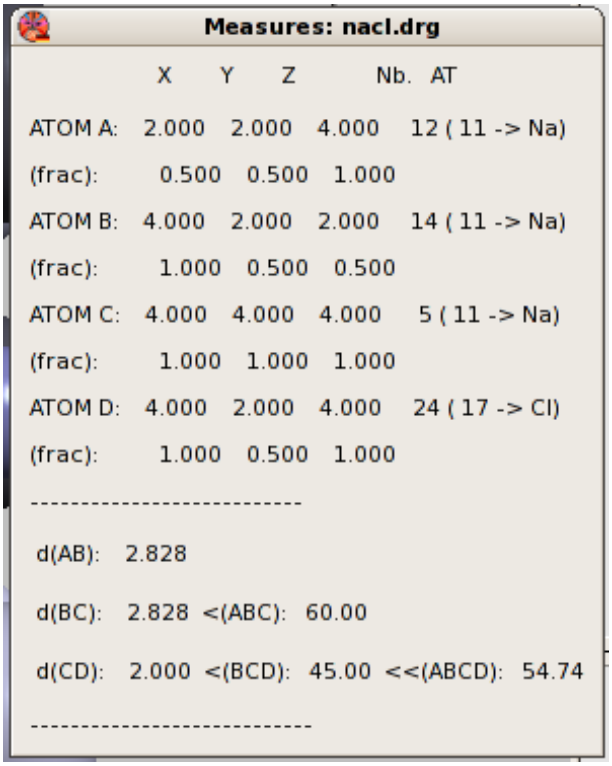

Figure 7.1: The Meassure Window

But: a more civilized way to move an atom around would be to double click on an atom and modify the atomic position or, better, modify the displacement setting according to ones wishes.

7.7 Define New Unitcell

Real experimental feature. Don't use it right now.

7.8 Take New Unitcell

NWY.

7.9 Clear Unitcell

NWY.

7.10 Handle

Handle allows the user to selectively switch the displaying options. By selecting an atom the selected options is toggled. Select the desired toggle option and then select the needed one, two, three or four atoms, respectively.

7.10.1 Handle Atom

Handles the selected atom according to the setting in the *Selection* Menu, see 7.11. As default this usually means hiding the atom.

7.10.2 Handle Bond

After selecting two atoms a bond is drawn between them. The bond is removed if the bond already exists.

7.10.3 Handle Triangle

After selecting three atoms a triangle is drawn between them. The triangle is removed, if it already exists.

7.10.4 Handle Plane

After selecting four atoms a plane is drawn between them. The plane is removed, if it already exists.

7.10.5 Atomkey

In the upcoming dialog one can control which atomtypes will be shown in the atomkey (which will be shown only if the setting in the *Display* menu is activated.

7.10.6 Track Atom

NWY.

7.10.7 Handle Atomlabel

Toggles the drawing of the Atomlabel, if the general setting in the *Display* menu is activated.

7.10.8 Handle Distance

After selecting two atoms a line is drawn between them and the length is drawn beside it. The line is removed if it already exists. The general setting in the *Display* menu must be activated.

7.10.9 Handle Angle

After selecting three atoms a line is drawn in the angle between them and the angle is drawn beside it in °. If the menu option *Label Units* (see 6.10) is set, the unit is append. The line is removed if it already exists. The general setting in the *Display* menu must be activated.

7.10.10 Handle Dihedral

After selecting four atoms a line is drawn to show the dihedral between them and the angle is drawn beside it. The line is removed if it already exists. The general setting in the *Display* menu must be activated.

7.10.11 Handle Charge 1 or 2

Toggles the drawing of the charge value, if the general setting in the *Display* menu is activated.

7.10.12 Handle Mag.Mom. 1 or 2

Toggles the drawing of the magnetic moment, if the general setting in the *Display* menu is activated.

7.10.13 Handle Mag.Mom. Arrow

NWY.

7.10.14 Handle Colour-Atom

NWY.

7.10.15 Set Atomlabel

Lets the user set the label for the selected atom. After this happened, no longer will be the atomsymbol be printed, but the new text.

7.10.16 Text

With this option one can add text to every point of the drawing canvas. After clicking on the starting position a dialog will appear where the text can be typed. The text will be fixed at this position and not affected by rotation. Deleting the new text ist hard at the moment, but will be possible later by selecting the text again. Sorry, for now: save the molecule and delete the corresponding line in the file and open the molecule again.

7.11 Selection Mode

Determines the action to be taken if *Handle Atom* is selected and an atom is marked. Possible choices are hiding the atoms or choosing different representations of the atom (line, ball and stick, spacefilll).

7.12 Goodies

7.12.1 Show all Atoms

Sets the visibility of all atoms to true. All atoms are displayed.

7.12.2 Hide all Labels

Hide all labels so that individual atom labels can be switched on. May be sometimes better than hiding all unwanted labels.

7.12.3 Hide all Charges 1 or 2

Same as in *Hide Labels* for the charges of type 1 or 2.

7.12.4 Calculate Bonds

This menu allows the calculation of bonds between a single, selected atom or an atomsort and another sort of atoms. The minumum and maximum distance in which to draw a bond (or, if selected, a small line instead) must be specified. Bonds can be drawn or removed likewise. Some other options like the thickness, type or the color can be set directly. wxDragon distinguishes between dynamic and static bonds. While static bonds are always drawn, dynamic bonds will be recalculated every step in a dynamic run (like a MD-Sim) and if the distance is to large, the bond will not be shown.

7.12.5 Modify Atoms

Atoms can be modified according to their atom sort. The displaystyle of them can varied in many cases. Just play a bit with the dialog. One important option is the posibility to shift the selected atom in the origin, making his coordinates (0,0,0). May be handy sometime when one wishes to have an atom in the center of the definition.

7.12.6 Polyhedral

Here it gets insteresting. When displaying a crystal, here one can switch on or off the displaying of polyhedrals. A center atom (or all or none) can be specified together with the edge atom type, and wxDragon tries to find all possible matches, starting from higher polyhedrons, going to lower symetry if no higher one where found. A combobox allows to select a specific polyhedron to look for, the center atom (or all or none) and the corner atomtypes must be choosen. Note: one can choose more than one corner atomtype to allow for mixed polyhedrals.

The color can be choosen to be the default one (as set in the preferences), or the color of the edge atoms, or set new with the color button.

Another important option is the *Make Selected* button. First toggle the selection mode to the continuesly selection mode (in the canvas-popupmenu with the right mouse button at the bottom) and select as many atoms as you deem to be the polyhedral one wishes to see and then press the *Make Selected* button. If wxDragon recognizes the polyhedrals, it will be make the necessary planes by itself.

7.12.7 Planes

With this dialog one can visualize the various crystallographic planes within a crystal. A simple dialog will pop up and allows for easy control of the planes. One can make a single plane, or add new ones to allready existing ones. Or remove them selectivly.

The normal of the plane is shown in order to symbolize the positive surface direction. When the *Generate Surface* button is pressed, all atoms over the plane (positive direction) or under the plane (negative direction) are hidden in order to generate a surface.

8. Chemistry Menu

The topics of this menu are still in development, so they are not yet available.

8.1 Spectra

NWY.

8.2 Diffraction

The submenu X-Ray is working partially. It calculates the diffractogramm for the given crystal. Be aware that at the moment there may be to much peaks, since the special positions aren't used. Work in progress!

8.3 Symmetry

NWY.

9. Export Menu

9.1 Pictures

The actual drawing in the drawing area of wxDragon can be saved to a picture file. The following formats are possible:

- BMP
- JPEG
- PNG
- PNM
- PCX
- TIFF

A picture with the size of the actual drawing area is generated, and the user is prompted for a filename and location in order to save it. Up to now on some plattforms some formats may be disabled, depending on the support made by wxWidgets. Also on some plattforms there seems to be a (memory related) bug if the picture is too large. Just make the drawing window of wxDragon somewhat smaller, this should help.

I prefer the jpeg format, since the quality is good, the size is rather small, and it can be easily converted to a level-2 postscript file with the utility **jpeg2ps** [35].

9.2 Movies

9.2.1 PovRay Movie

This Optionis deemed very nice and smart. It lets you generate - over some external steps - an movie. So, let's see, how it can be done. Of course, some special knowledge will be needed, but I will tell you the stupid way I do these things. First go into the *Preferences* within the *Edit* menu and set the path for the povray things accordingly to your local machine. How and what to do is described in section 19 on page 62. Then after selecting the *Movie* item, a dialog appear. It consist of a text editing window where the header for the program POVRAY can be edited according to the needs of ones molecule. Don't worry, one does not have to be perfect immediately. For a start, simple check the Checkbox *APPLY* and then press *OK*. The dialog will vanish for a few milliseconds. That's it? No. In the background your computer will using povray to render the picture, and when finished it will be displayed using your favoured display program. Look at what you get and decide what must or should be changed in what way. Do the necessary

changes in the movie dialog, close your viewing program for the povray output, and restart the iteration process again by pressing *OK*.

When the output from the povray run is satisfying, just uncheck the *APPLY* checkbox and press *OK* again. In your current working directory for every step wxDragon has stored about your molecule it will generate a file named *movie.xxx.pov*, where the xxx is the number of the step. So, these files now must be rendered individually with POVRAY, using any desired resolution and other options. Take a look at the POVRAY documentation. I generate PPM files. When finished, the program mpeg_encode gives me, properly installed and configured, a nice mpeg movie which can be played by all plattforms and browsers. Try it. And if you have a better idea on how to make a movie (MPEG or some other stuff?), just drop me a description on what is needed and, in general, how it can be done.

9.2.2 MPEG Movie

NWY.

9.2.3 Quicktime Movie

On the Apple (and on some unix plattforms -if requested by the user), a normal quicktime movie can be generated out of the box. In the normal wxDragon release this feature produces a short movie of the first and the last trajectory step, just to show that its possible. Registered user who payed the shareware fee get access to a version of wxDragon where a full movie over all (selected) steps can be generated.

The user can choose the first and the last step for the movie, as well as the quality of the encoder used, and the frame rate (in fps). A file name must be given under which the movie will be generated.

Due to not yet resolved problems the user must resize the wxDragon window in order to get correct pictures in the movie. Which may be true also because of the size of the resulting movie.... While the movie is generated, don't touch anything, just let your computer alone (since up to now the pictures are read directly from the screen, and no other window should interfere with it, otherwise you will see it afterwards in the movie.

If the loaded file contains a vibration node, a vibration movie can be generated also. The user can choose the desired vibrationnode and the times of its repeating.

9.2.4 AVI Movie

On Windows plattforms, a normal AVI movie can be generated out of the box. In the normal wxDraogn release this feature produces a short movie of the first and the last trajectory step, just to show that its possible. Registered user who payed the shareware fee get access to a version of wxDragon, where a full movie over all (selected) steps can be generated.

The user can choose the first and the last step for the movie, as well as the quality of the encoder used, and the frame rate (in fps). A file name must be given under which the movie will be generated.

While the movie is generated, don't touch anything, just let your computer alone (since up to now the pictures are read directly from the screen, and no other window should interfere with it, otherwise you will see it afterwards in the movie).

If the loaded file contains a vibration node, a vibration movie can be generated also. The user can choose the desired vibrationnode and the times of its repeating.

9.2.5 Animated GIF

NWY.

9.3 Export

Depending on the nature of the molecule opened by wxDragon, they can be exported in several different file formats. In most cases an dialog appear where the generated output can be checked and altered somewhat, and then the user can choose between ignore it (*Close*) and *Save it to file*.

9.3.1 Andrei-Mult

Up to now only an Aachen-Internal.

9.3.2 Abinit

Produces output which could be used in an abinit-input file to do a calculation. Will contain the cell definition and the atomic positions with an hint on the ordering.

9.3.3 ADF

Produces output which could be used in an adf-input file to do a calculation. Just the atomic positions.

9.3.4 aixCCAD

Some format I used to use.

9.3.5 CIF

Produces output which could be mistaken as an CIF-file. All input given which is needed for a basic CIF-file.

9.3.6 Cinema4D

NWY.

9.3.7 Conquest

Produces output which could be used in an conquest-input file to do a calculation. The cell definition and the atomic positions.

9.3.8 CML

Produces output which could be mistaken as an CML-file. At least wxDragon will read it in again.

9.3.9 CPMD

Produces output which could be used in an CPMD-input file to do a calculation. The cell definition and the atomic positions. For the option of the popup dialog please see the VASP section (9.3.24).

9.3.10 CrystalMaker

NWY.

9.3.11 Crystal

NWY.

9.3.12 DL-Poly

Produces output which could be used in an DL-Poly-input file to do a calculation. For the option of the popup dialog please see the VASP section (9.3.24).

9.3.13 Excite

Produces output which could be used in an excite-input file to do a calculation.

9.3.14 FPLO

Produces output which could be used in an FPLO-input file to do start a new fedit-run.

9.3.15 Gamess-UK

9.3.16 Ghemical

Produces output which could be mistaken as an ghemical-file.

9.3.17 LMTO-ASA

Generates out of **crystallographic** data an INIT file which can be immediately used for calculations with the LMTO-ASA program ([21]).

9.3.18 MacMolecule

Some relict from the old days - NWY.

9.3.19 PDB Format

Generates a file containing the atoms and their coordinates using the PDB data format [26]. Can be done from all different type of molecules. Warning: very smiple file, it may not be conform with the standard pdb file. Working on it.

9.3.20 PovRay

Assembles a file which can be used to render the molecule with the program POVRAY [36] to give high quality pictures in any resolution one may wish to get. Can be done from all different type of molecules. The file generated by wxDragon is only a starting point, one still has to rework the camera, light and display section in order to get exactly what one want.

9.3.21 Schakal

Generates out of **Crystallographic** data an file which can be immediately used with the program SCHAKAL [27].

9.3.22 Siesta

Produces output which could be used in an Siesta-fdf-input file to do a calculation.

9.3.23 Simple XYZ

Results in a simple list containing the atom types and their x,y, and z coordinates. Works for all types of molecules.

9.3.24 VASP

Try to generate a POSCAR file which can be used immediately in a VASP calculation. If wished, and if in the preferences the corresponding path variable was set accordingly, the needed POTCAR can also be generated using the standard atomic potentials, which name consist only the simple atomic symbol. Works for all kind of molecules.

One can choose to export all positions or hide the atoms which are generated throu the periodic boundaries. If one wishes that this will be done using the (more often more accurate) crystallographic coordinates. The output can be in cartesian coordinates or in the direct ones.

If a random displacment is wished, one can give the maximum displacement value in the first text field. If one wishes a fixed displacement for all atoms, the respective x,y, and z values can be given here.

If one wishes to preserve the atom ordering as shown in wxDragon with the numbers the atoms carry, this can be selected here also. In order to generate a VASP-5 compatible POSCAR, the next checkbox may help. And finally, one can control the number of digits in the POSCAR file.

When you find that not all atoms that should have are exported one can play with the accuracy number. Increas it to make the search for possible atoms more relaxed and see what happens. Decrease it to make the search more restrictive, so some atoms may even vanish.

9.3.25 Viewkel

Makes a file which can be read in by the program VIEWKEL [5].

9.3.26 Wien2K

Generates a ṡtruct file which can be used in a Wien2k [32] calculation as a starting point where one dont have to use the web-interface.

9.3.27 XMol XYZ

This file can be read in by the program XMOL [33]. I used to play with it in the old days.

9.4 GOM – Generic Output Module

After quite a few output modules written the realization came that there must be a easier way to generate output. The idea of a flexible way to describe the desired output format was born - the Generic Output Module, short GOM. Those files can be loaded in wxDragon (and also in the shell with the option *-gom filename.gom*), but also those files can be put in the plugin-folder with the ApplicationData\wxdragon folder under windows or the $HOME/.wxdragon folder under Mac OSX and Linux. The GOM-files in there are loaded automatically at startup and are available at the Export-menu in the GenericOutput submenu.

9.4.1 Format description

The format of the GOM-files is the following:

- Line1: Name of the Module. This name will appear in the GenericOutput-menu for selection. Please try to avoid special characters or spaces. No guaranty that they will work
- Line 2: Here the option "m(X)" can be given determining what step should be used to generate the output. "X" can be "a", meaning all succesive step, "l" for the last step. "X" can also be a simple number or a range of number like "1-5", but the numbering doesnt make too much sense, because one never can be sure that those step are read in in the opened file.
- Lines 3-X: output options.

The available output options are grouped in several section. There is a general section containing options for string output and formatting:

- s(): outputs the characters inbetween the () as a string. Be aware that if you are using brackets in your string, the closing one will terminate your string, but the closing bracket will be printed. So, if you want to print something like "Text (for example) to use", one has to do it with two s() commandos: s(Text (for example))s(to use).
- _(): a space is printed here

- v(): no space is printed here
- f(X"%ggg"): the string in the brackets is used for exporting numbers. The first character denotes the number typ: f for floating numbers, i for integers, and l for long floats (like the crystallographic settings). The rest of the string gives the export string. The style is like in the printf commando in C. Don't forget the quotation marks, e.g. "%10.5f" prints the number in a 10 digits long space with 5 digits after the decimal point.
- i(X) sets the condition when this module can be applied. A "c" in the brackets tells wxDragon that this file can be applied onto crystals. A "m" allows for molecular systems, and a "s" enables simulations (like Molecular Dynamics). If no i() is given all 3 possibilities are enabled, combiations of i() settings are also possible like i(cs), the ordering of the characters is not important.
- # denotes a comment, the rest of the line will be ignored.

The crystallographic sections contains options for selecting lattice settings in many different ways:

- c(x),c(y),c(z),c(a),c(b),c(g): prints the lattice vectors a,b, or c, or the angles alpha, beta, and gamma.
- c(xyzabg): prints the all lattice setting from a to gamma with spaces inbetween.
- c(m1): prints the cell vectors in matrix form, all in 1 line
- c(m3): prints the cell vectors in matrix form in 3 linesi
- c(spc): prints the spacegroup in the Hermann-Mauguin notation
- c(ispc): prints he spacegroup number
- c(orig): prints the origin

The atomic data can be printed with the following options:

- a(xyz): prints the cartesian coordinates of the atoms in one line.
- a(fxyz): prints the fractional coordinates of the atoms in one line.
- a(l): prints the atomic label
- a(t): prints the atomic number (the ordering number)
- a(#): prints the number of the atom in the molecule
- a(fx),a(fy),a(fz): prints the fractional coordinate x (or y, or z).
- a(x),a(y),a(z): prints the cartesian coordinate x (or y, or z).
- a(l#): prints the number of atomic type for the actual atom
-

Properties of the molecule or the atoms can be printed with the e() option:

- e(fxyz): prints the forces on the atoms
- e(mxyz): prints the magnetic moment in arrow notation
- e(m1): prints the magnetic moment 1 on the atoms.
- e(m2): prints the magnetic moment 2 on the atoms.
- e(c1): prints the charge 1 of the atoms.
- e(c2): prints the charge 2 of the atoms.

Some overall informations about the molecule can be printed with the n() option:

- n(nat): total number of atoms printed.
- n(at): number of atoms, sorted for atomic types found
- n(lat): atomic labels, sorted for atomic types found
- n(at,): number of atoms, sorted for atomic types found, separated by a ","
- n(lat,): atomic labels, sorted for atomic types found, separated by a ","
- n("lat"): atomic labels, sorted for atomic types found, each label is printed with "" around it.
- n("lat",): atomic labels, sorted for atomic types found, each label is printed with "" around it, separated by a ",".

There can be many options within one line, but be aware that as soon one a() option is found this results in the output for all atoms, so the results of your line may not what you expect. For example a line like "a(fxyz)c(m3)" wont print the lattice matrix, because those options are contrary to each other.

9.4.2 Examplefile

An example file may look like:

```
DFTB+Input
m(1)
i(c)
f(f"%.10f")
f(l"%.10f")
s(Geometry = {)
_()s(Periodic = Yes)
_()s(LatticeVectors [Angstrom] = {)
c(m3)
_()_()s(})
s(TypeNames = {)n("lat")s(})
s(TypesAndCoordinates [relative] = {)
a(l#) ()a(fxyz)
_()s(})
s(})
```

Applying this to a simple rocksalt structure with the lattice parameter 4.0 produce the following output when selecting the "DFTB+Input" submenu entry:

```
Geometry = {
  Periodic = Yes
  LatticeVectors [Angstrom] = {
4.0000000000 0.0000000000 0.0000000000
0.0000000000 4.0000000000 0.0000000000
0.0000000000 0.0000000000 4.0000000000
   }
TypeNames = {"Na" "Cl"}
TypesAndCoordinates [relative] = {
1 0.0000000000 0.0000000000 0.0000000000
1 0.5000000000 0.5000000000 0.0000000000
1 0.5000000000 0.0000000000 0.5000000000
1 0.0000000000 0.5000000000 0.5000000000
2 0.5000000000 0.5000000000 0.5000000000
2 0.0000000000 0.0000000000 0.5000000000
2 0.0000000000 0.5000000000 0.0000000000
2 0.5000000000 0.0000000000 0.0000000000
  }
}
```

10. Modules Menu

10.1 New Molecule

A support dialog will appear to build a molecule using the z-matrix. Be aware that the main action happens in the display window. First choose the type of the new atom in the dialog, then double click into the window. Select a new atomtype, and the double click on the first atom. One will get asked for the distance to this atom. Select a new atomtype (or not) and double click on the atom, to which one wishes to give the distance, give the distance, then double click the atom, to which the angle will be given, and enter the angle in the popup dialog. And finally, if one have more then 3 atoms already on screen, one can double click the atom to which the dihedral will be inputet. If one wishes to correct an already finished line, just double click on the coresponding line in the z-matrix, and one will be able to correct the distance, angle, and dihedral. Press Accept when finished.

10.2 New Z-Matrix

Here the Z-Matrix will be build by hand, all atoms and values have to given in the right field. First, give the first atom type and press Accept. Then gve the next atom type in the first text input. Since there is only one atom already there to which the distance can be given, there is no choice here than to give the distance in the next text field and press accept. Then put in the next atom type and press the TAB key to proceed to the next field. Here, one must give the atomtype and the number of it according to the z-matrix build at the bottom of the dialog (like *C1*), then give the distance to it. Only when some valid value is given in the distance field the next field is enabled, where the atom and number of the angle-atom can be given, and the angle is added in the next field. For the next and all following atom, this procedere is extended to the dihedral atom also. After pressing Accept the molecule is build online in the display.

If one wishes to delete or correct an already given line just double click on it in the z-matrix table. The above fields will be filled with the selected values and one can select Delete in order to remove the line completely (which is of course only possible if no later line depends on the atom one wishes to delete) or change the values and press Accept again to use the changed values. Pressing Clear will abort the changes.

10.3 New Crystal

A new crystal can be generated using this module. About the details, please see section chapter 16 on page 51. After the crystal is generated as one like it, the data can be exported to different file types, as described in the export section chapter 9 on page 27.

10.4 Crystal-Module, MD-Module, QC-Module

If the active molecule is of a crystallographic file type, the data of the crystal can be modifiedusing this dialog. The dialog is described in section 16 on page 51. If the active molecule is an MD-Sim, the MD-Sim dialog will appear, see 21 on page 67. If the active molecule is an simple molecule, the z-matrix editing dialog will popup and one will be able, to edit the existing molecule, see section 10.2 above.

10.5 Property

NWY.

10.6 aixCCAD

NWY.

10.7 Gaussian

A dialog appears with some basic options to switch in order to generate a basic input file for Gaussian. For somebody used to gaussview these options will look too simple, but for some students they are enough, I think, containig all basic options. After building the input file one can save it to a file. Editing direct in the text control below the option is also possible, but be aware that these changes will be deleted when an option is changed in the input fields on the top half of the dialog. After building the input file one can save it to a file.

10.8 Gamess-US

A dialog appears with some basic options to switch in order to generate a basic input file for Gamess-US. For somebody used to more advanced interfaces these options will be a too simple starting point, but for some students they are enough, I think, containig all basic options. After building the input file one can save it to a file. Editing direct in the text control below the option is also possible, but be aware that these changes will be deleted when an option is changed in the input fields on the top half of the dialog. After building the input file one can save it to a file.

10.9 LMTO

NWY.

10.10 VASP

Let one construct a simple INCAR file, in case one doesn't know what one is doing. Nothing to be proud of. One can select the options wanted and then press *Save INCAR* to save the INCAR file.

The button *Save ALL* is more for absolute startes because it generates all 4 file needed for a VASP calculation. The INCAR depends on the setting given in the dialog, the KPOINTS file uses the input from the KPoint-Line textcontrol, the POSCAR is generated using some default assumptions, and the POTCAR is made using the settings from the Preferences dialog. Be aware that thos files are really just simple files which should be edited to ones need before running.

10.11 Phononcalculation

NWY.

11. Molecule Menu

11.1 Molecule Info

Here, a window pops open with the data of the current active molecule. In it the file type is given, and informations about found properties such as the number of atoms, vibrations, energies and charges. Just to be sure wxDragon is talking about the same output file as you think it should be.

11.2 The Rest

The name of every new opened input file is appened at the end of this menu. The active molecule is marked in front of the name, and the user can switch to any other molecule/property by selecting the respective name in the menu. In order to distinguish between different files with the same name, the complete path is given.

12. The Animation Dialogs

12.1 Multistep Dialog

12.1.1 Intention

Many calculations contains not only informations of a single geometry, but rather a series of coordinates, like in geometry or energy optimizations or, more important, molecular dynamics simulations. wxDragon allows the user to visualize the steps continously, so that a *movie* of the steps can be seen. Of course this dialog can also be used if more than one step is found in the file read in. The actual number of steps found can also be seen in the *Molecule Info* dialog.

12.1.2 What can be done

In picture 12.1 the Multistep dialog is shown. On top of the dialog a slider can be found representing the actual shown step. By dragging the slider, a desired display step can be found manually. The second slider controls the number of frames per second which should be shown when an automated run through all display steps is started. High numbers (*High* depends highly on the used hardware) may be somewhat optimistic, but with the evolution of faster graphic cards and CPU's, soon it will be important. Next the Play and Stop buttons allow the automatic run through all steps found at the given slider speed.

The two buttons in the middle stops an eventual running mstep show, and switch to the first or the last step, respective. The following two buttons allows the user to navigate step by step forward or backward by one step.

The first checkbox in the lower half of the dialog inflicts the display options of the actual step on all other. What does this mean? Well, the user can make e.g. some atoms disappear, and make some distance lines, and when the run is started, these options stay through all steps, so that for instance a special distance can be followed.

If the second chekbox is checked, the first step found in the inputfile will not be used in the cyclic show of the steps. This may be used in cases where the first step is an calibration step, where the atoms are located on some funny places, before the second step is correct, or the second step is a mere repeat of the first one.

The next checkbox lets the user switch bonds on and off directly, without going over the menu items. If the "Don't Flip" button is checked, the atoms will not be flip to the other side of the shown box – no periodic boundary condition is applied, even if the original output file contains the flipped coordinates.

By using the "Make Movie" box, wxDragon will generate a series of pictures (the format can be choosen) and will save them automagically under the name "mstep_movie.xxx.yyy",

where xxx is the step number and yyy the format. Afterwards one can use his favourite programm to make a movie out of all the single files.

The last button, *Close*, propably doesn't need an explanation.

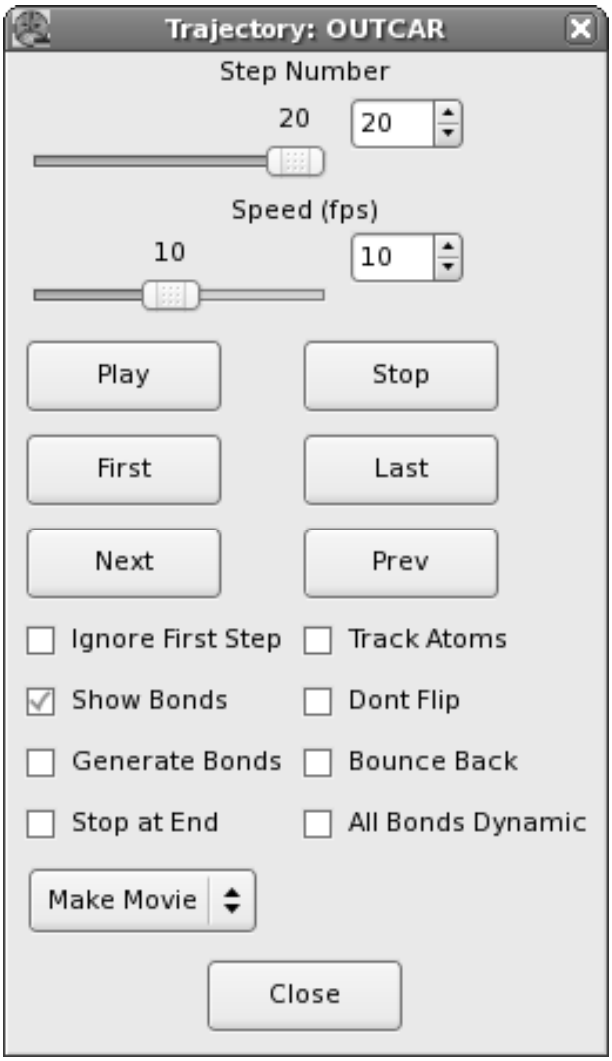

Figure 12.1: The Multistep Dialog

If one wishes to make an avi movie out of the trajectory one should use the AVI option in the *Export* menu, see 9.2.4 on page 28. There one can choose between an animation of a trajectory and a vibration (if available).

12.2 Vibration Dialog

12.2.1 Intention

In freqency calculations, the resulting force matrix is very ofter very complex, and the pure numbers in the output file can not be interpreted easily. And even the visualization of the forces using vectors on the atoms is often also too complex. An anamition of the vibration, on the other hand, allows an understanding at the first glance, and it is very intuitive. This can be done with wxDragon.

12.2.2 What can be done

In picture 12.2 the Vibration dialog is shown.

Figure 12.2: The Vibration Dialog

The first slider lets one choose the vibration at which to look at, if more than 1 vibration is found. The next slider controls the speed of the animation and is given in frames per second. Of course, the real speed depends not only on your hardware, but also on how big your molecule is, so this is only a hint at how fast it would be. The *Play* and *Stop* button doesn't need an explanation. The next slider is there just for show and counts the steps of an vibration (should be 20 for all). The counter on the right let the user choose the exact step of the animated vibrations. This details of this position can be viewed in the meassure win (see section 7.4 on page 20), or even exported into some file format using the Export menu (see section 9 on page 27). In the text field below it some additionally information about the vibration like its frequency is given, if found, and the intensity. With the *Prev* and *Next* button one can cycle throu the vibrations. The next slider and the following textinput field let one choose the scale the amplitude of the vibration, from a small wiggle to a large movement. Just play with it!

If the choice *Make Movie* is set to some other options than itself wxDragon saves a picture of each step of the simulation, about like mentioned in the Multistep section (12.1 on page 40), only the picture files will be named different.

If one wishes to make an avi or quicktime movie from the vibration, please use the AVI or Quicktime option in the *Export* menu, see 9.2.4 on page 28. There one can choose between an animation of a trajectory and a vibration (if available).

12.3 Orbital Dialog

12.3.1 Intention

Allthough the orbital information given in some quantum chemical program systems can still be interpreted sometimes directly from the output file, in many cases some parts may be overlooked, or the whole system is too complex at all. In these cases, wxDragon may of help.

12.3.2 What can be done

In picture 12.3 the Orbital dialog is shown.

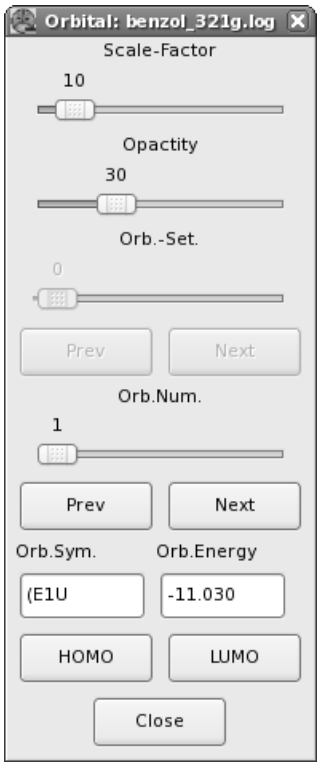

Figure 12.3: The Orbital Dialog.

On top is a checkbox to let the user choose between a simple display method (s-orbitals are spheres, p-orbitals are 2 smaller spheres and so on), the size depends on the coefficients, or a more sophisticated one, where a real surface is drawn. The first slider controls the scaling of the orbitals on the screen. If the orbital coefficients are a little small for the actual orbital, the orbitals can be boosted to be better seen. The next slider controls the opacity of the orbitals drawn in order to allow some insights behind the front orbitals.

The next set of controls is disabled for now. The next enabled set allows to cycle through all found orbitals. In the two text field below some found values are given for the actual orbital, like orbital symmetry or energy.

The following two buttons (HOMO and LUMO) should be self descriptive, also the last button.

13. Planes Dialog

13.1 Intention

In order to understand a crystal better, here some planes throu the crystal can be plotted.

13.2 What can be done

In picture 13.1 the planes dialog is shown.

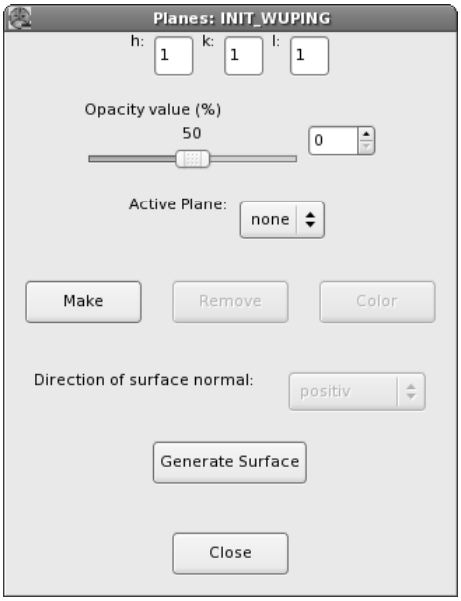

Figure 13.1: The Planes Dialog.

On top of the dialog the h,k,and l value of the plane can be set. In the slider below the opacity of the plane can be contolled. The next choice lets one controll the plane used for the next operations. The *Make* button makes the plane according to the hkl values. The *Remove* and the *Color* button removes the active plane or sets a different color for it.

The next two controls can be used to generate surfaces. First the direction of the surface normal (which is indicated with an arrow) is set to be used with the next button. Pressing *Generate Surface* will hide all atoms above (direction of surface normal: positive) or below (direction: negative) the active plane.

13.3 The Triangle Dialog

When a plane or a triangle is selected by the mouse, a popupdialog appears. There the triangle can be deleted, the color can be changed using the dialog which pops up, or the printing of the normal vector can be controled. This is meant for single triangles or cubeplanes. If one wishes to do more of this, use the planes dialog.

14. Polyhedral Dialog

14.1 Intention

Here the unit cell can be filled with various different polyhedrals like tetrahedrals, octahedrals, or cubes using a simple dialog.

14.2 What can be done

In picture 14.1 the polyhedral dialog is shown. First of all one has to select the center atom type, or choose ALL or none at all. Then the corner atom type must be specified. Be aware that one or more center or corner atom types can be given, so that the resulting polyhedral can contain more than one atom type. The tolerance value gives one some control on how exact the polyhedral must be positioned.

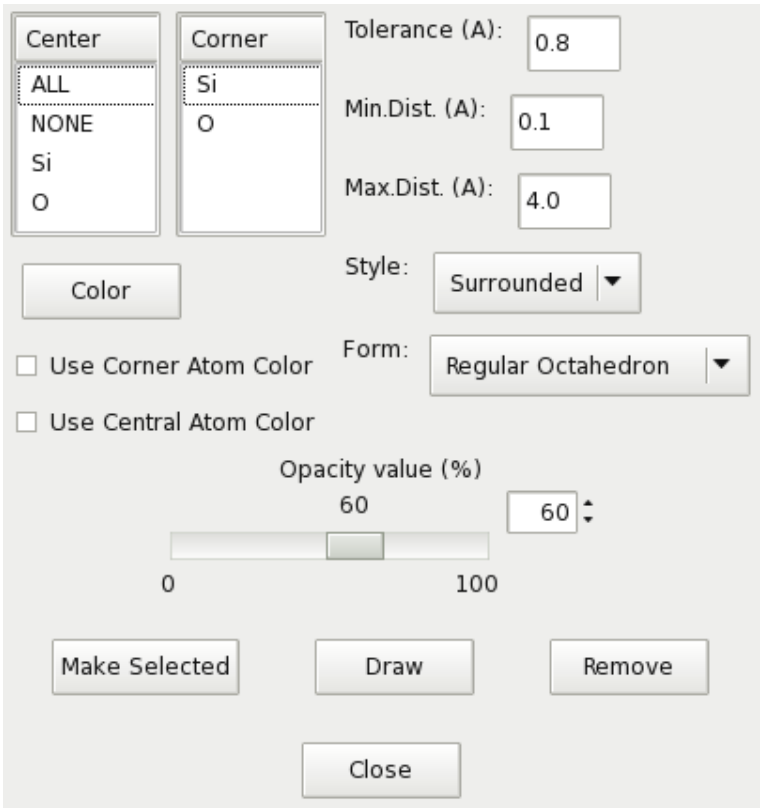

Figure 14.1: The Polyhedral Dialog.

The style choice gives one the option to choose between a simple polyhedron (*normal*,

polyhedrons surrounded with a line (*Surrounded*), or no plane, just the surrounding line (*outlined*). The Color button is there to choose a different color for the polyhedron, but one also can determine that the corner or the center atom can give the color to the polyhedron. The desired form of the polyhedron can be choosen in the Form choice. Should be pretty descriptive. The opacity value of the planes can be set next, ranging from pretty invisible (0 percent) to full (100 percent). Then press the Draw or Remove button, depending on what you want to do - add a new polyhedron, or remove the defined one.

A nice feature may the the button *Make Selected*. Switch to selection mode (in the popupmenu in the drawing canvas) and select a few atoms which should belong to the new polyhedral and press the button. wxDragon tries to make sense of your selection and generate an appropriate polyhedral. Usefull if one wishes not all polyhedrals of some kind can be seen but only a few one.

15. Isosurface Dialog

15.1 Intention

Simple structures or orbitals were good - in the old times. Nowadays everybody is interested in the actual density distribution of some property, like the electrons. Those informations are too hard to retrive by just looking at the denisty matrices, so, why not let wxDragon do the hard work for you?

15.2 What can be done

When a file is loaded, where some sort of surface can be viewed, open the menu "Modules", click on one of the three central modules (crystal, quantum chemical, mdsim). This will open a new dialog. Within he new dialog, in all cases there will be one choice together with an button "Module". Choose the surface to display within all choices offered, and press the button. The Isosurface dialog will open, as shown in picture 15.1, offering a range of possibilities.

- **Show Isosurface** Toggles the display of the isosurface
- **Isosurface value** Controls the iso-value for the surface to show, from 0 to the highest value found
- **Opacity value** Changes the opacity of the isosurface from 0 (not visible) to 100 (surface is no longer transparent)
- **Show Slice** Toggles the display of the slice
- **HighQual** Don't use the fast but fuzzy, rough slice, but the high resolution one. This is rather slow, so use it with care. The rough one may sometimes display a little disturbing pictures, but thats mostly due to the rough rasterization of the slice
- **Azimuthal slice angle** Controls the azimuthal angle, from 0 to 360
- **Polar slice angle** Controls the polar angle, ftom 0 to 180
- **Slice offset** Controls the sliceoffset from the center of the box
- **Minimum/Maximum Iso Value** determine the minimal and maximal value for displaying the isosurface or the slice. The sclie ony shows values between those two, the isosurface value is relative to the two borders. The actual values are shown in the two textcontrols below the sliders.

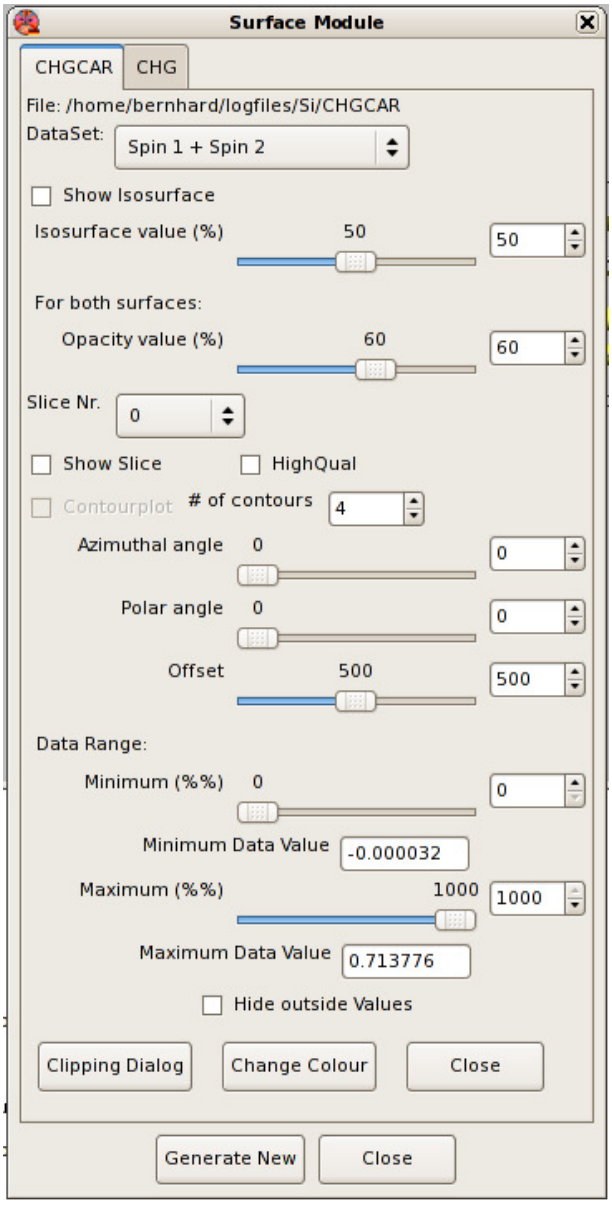

Figure 15.1: The Isosurface Dialog.

- **Close** Closes the Isosurface dialog

When displaying the values as a slice, one would be advised to first use only the low quality version to positioning the slice and only for the final look use the high quality setting, because this is a little slow.

wxDragon tries to make sense of the values read in from the respective file, but at the end the user must know what these values mean, or? In case of VASP the values are of Electrons per Volume like described in the manual.

16. Crystal Dialog

The Crystal Dialog is the central interface for the crystal part of wxDragon.

16.1 Intention

This dialog enables the generation of crystals starting from the crystallographic data. Additionally, the number of unit cells shown can be varied, not only in steps of 1.

16.2 What can be done

The upper part of the crystal dialog provides an interface to easily generate or manipulate crystals. The space group symbol or the corresponding number must be given before the next textfield is accessible. This can be either he origin field, if the spacegroup incorporates the choice, or the field for the first lattice parameter. The number of necessary fields of lattice parameters depends on the given spacegroup, and are activated only when needed.

When in doubt, if the notation of the spacegroup you entered is correct, use the number, this allways is the method with the smallest error.

When all necessary parameters are given, the field for entering the atomic positions is activated. Here the atomic positions in a form like *Symbol xpos ypos zpos* should be given. The positions should be given in fractional coordinates as simple floating numbers or in symbolic values like *1/2*. By selecting an already accepted line the line will be printed in the selection field. There the line can be edited or deleted. If one wishes to simply discard the line, just delete it with backspace.

In the upper part of the dialog, the fields for changing the properties of the shown unit cell: the range of the shown atoms can be determined. Floating numbers are possible to select a supercell from e.g. -0.3 to 2.3.

When someone doesn't know the spacegroup of a cell, but the atomic positions (*Lagen*), one can choose the spacegroup 1, give the values for a,b,c, alpha, beta, and gamma, and then enter all the atomic positions within the unit cell. By pressing the **Find Spacegroup** button, wxDragon tries to find a higher spacegroup suitbale for the choosen configuration.

If the found spacegroup seems right to the user, he can press the **Generate Crystal** button in order to generate a new crystal with the found values.

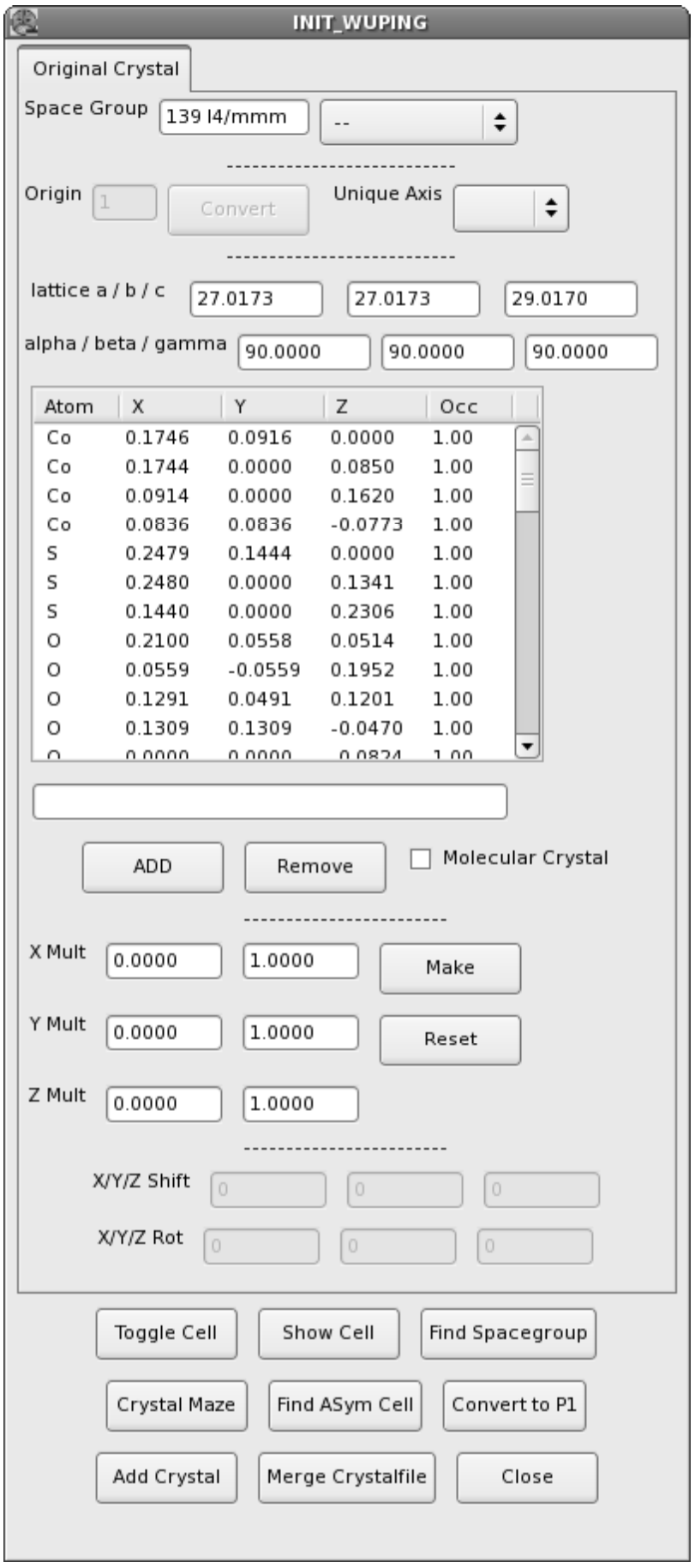

Figure 16.1: The Crystal Dialog.

16.3 Convert to Crystal

Convert to crystal is rather close related to the *Find Spacegroup* option, so please see the next section (16.4) for details.

16.4 Find Spacegroup

This dialog 16.2 should enable the user to find the spacegroup asoziated with the actual atomic positions and the cell.

The accuracy lets one set the accuracy of the search algorithm. When no or not the hoped for spacegroup was found, play with the accuracy, reduce or increase it and search again. If the starting molecule or crystal has two or more atom types which should be handled in the search as only one type the button *Equalize Atoms* can be used. Use *Reset Atoms* to reset these settings. Finally press the *Symmetry-based Search* to find the spacegroup. In the text field *Found Values* the new values for the found spacegroup are given for your information, and the spacegroup found is given in the top right.

In the text field on the right, *Symmetry Elements found*, the symmetry elements tested and found are given. The user can double click on one of them and they get visualized in the molecule. Rotation axes are printed as arrows, mirror planes are plotted as a simple plane, and mirror-glide-planes are plotted as a plane with an arrow in it to give the orientation of the shift.

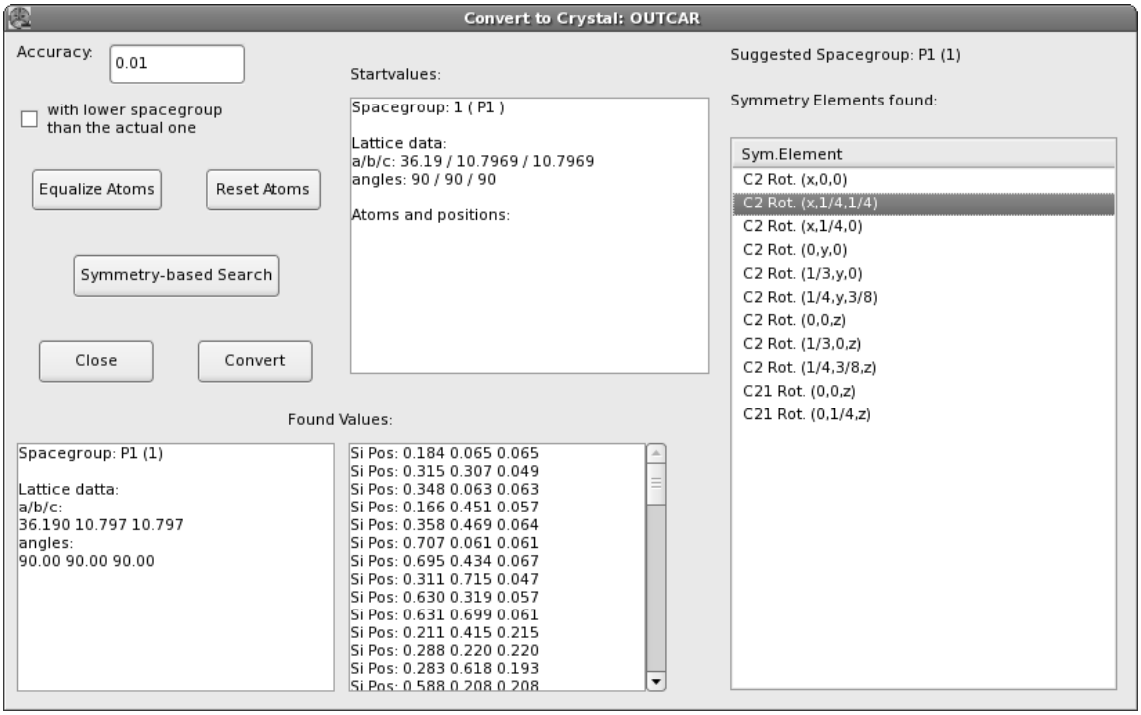

Figure 16.2: The Convert to Crystal Dialog.

17. Properties

17.1 Intention

wxDragon provides an interface to analyze some properties out of the solid state area. Without complicated and time consuming actions it should be possible to look at different kinds of curves without above mentioned actions.

17.2 What can be done

17.2.1 LMTO-DOS

Fully support for LMTO-DOS is included. Be aware that the DOS-file of LMTO is a binary file, so it can be viewed with wxDragon only if they run on the same plattform as the calculation.

The property can be analyzed using several options, which are presented in the dialog. See the description below in section 17.3 on page 55. The file DOS provides atoms, the second quantum number l (representing the orbitals s, p, and d), and the spin, if found.

17.2.2 LMTO-COHP

Fully support for LMTO-COHP is included. No restrictions apply in this case.

The property can be analyzed using several options, which are presented in the dialog. See the description below 55. The file COPL provides all classes for which the COHP's were defined, and spins, if used.

17.2.3 LMTO-BAND

Fully support for LMTO-BANDS is included. No restrictions apply in this case.

The property can be analyzed using several options, which are presented in the dialog. See the description below 55. Open the file BNDS, which provides the Points in the Brillouinzone and the corresponding bands.

17.2.4 VASP-DOS

Basic support, not very far.... Read the DOSCAR file, even if more than one dataset it available. The datasets (usually the total DOS and then some projections) are shown in two different property panels.

17.2.5 WIEN-DOS

Basic support, not very far.... Reads the *.outputt files.

17.2.6 Simple XY

A single x,y1,y2,y3,y4...file can be read in also.

17.3 The Dialog

In figure 17.1 the property dialog is shown. in figure 17.2 the plotting window is shown, where two properties are opened.

The control dialog contains three regions. The first one is the topmost area. Here some settings for all properties can be done, like changing the size of the drawing canvas for a single property. With the *Flip Axis* checkbox one can change the drawing direction of the DOS and COPS (chemists like to draw them with the energy upwards, physicists like to draw the energy to the right). With the next choice the properties can be exported in a few different formats. Do what suits your needs. Or close the Property dialog. The button "Save Settings" lets one save the actual settings, so that this saved file can be opened as a script file to automatically set all options when opening another property afterwards. The the script section (chapter 22 on page 69) for more details.

The rest of the dialog contains a control set for each property opened, organized in the notebook style. The first one draws into the leftmost region in the drawing windows, the second one to the right of the first one, and so on.

Each panel is divided into 2 regions. The first one is the one in the middle of the dialog. Here one can control the general printing options, for example the X and Y ranges, the labels printed on the canvas, or which parts of the frame should be shown. If the property has an fermi level, the options to print a line at the fermi level, or print the whole thing relative to the fermi level, may be important. Also the choice to select the energy which one wants to use in the diagramm. The buttons with the *Fit* names allow for an easy fitting of the ranges to the data loaded. The *Redraw* button should be used for that purpose, and the *Reset Range* one for this purpose.

For the second or more property one can even choose to use the ranges from the first property, in order to compare them more easily. If one has two or more properties of the same kind (for example 3 DOS curves) one can merge them together into one file, so that all their informations can be shown in one diagramm. If the curve shown looks way too rough for your beautiful eyes, use the Smooth-option with the choice directly under it to set the smoothing strength. **1** means quite strong smoothing, while more than 1 reduces the smoothing effect more and more. The *Show Grid (2)* draws a grey grid in order to make reading the curve more easily for the ticmarks of x and y resp. x2 and y2.

The second half of each panel contains the actual data set found. This may vary with the properties loaded. The main part will be the Classes, but if spin information is found for more than one spin, both will be shown in the Spin field, and if some additional information is found (like the magnetic quantum number l) they are shown in the 3 field. By simply pressing the *Show* button, all classes, spins and l values will be added and shown. If one wishes to show only selected values, the user can select the desired values, even multiple selection can be handled with the SHIFT key (select from to) or with the CTRL key (select the one under the mouse). The five options below the selection fields

Figure 17.1: The Property Dialog

can be used to make the picture a little bit nicer. The *Fill* checkbox fills the curve under the curve with solid black (or color). The button with a color name on it draws the curve in the respective color. If one wishes to have an integral draw also, use the third box. The next box can be used to draw a dashed line instead of a full one. And the last option can be used to flip the curve in the other direction of the main axis (may be nice to have the DOS of one spin drawn to the left, and the other spin in to the right).

Between the classes and the Show button the values of the curve and the integral curve are given according to the value in the treshold text field in the above section. The values are calculated for each data section and given there.

17.3.1 The Drawing Window

Concerning the Drawing–Window a few things need to be said here. If more than one property is displayed they are plotted next to each other.

If one select a rectangle with the mouse, the drawing gets zoomed to this region. To reset the range press the *Redraw* button.

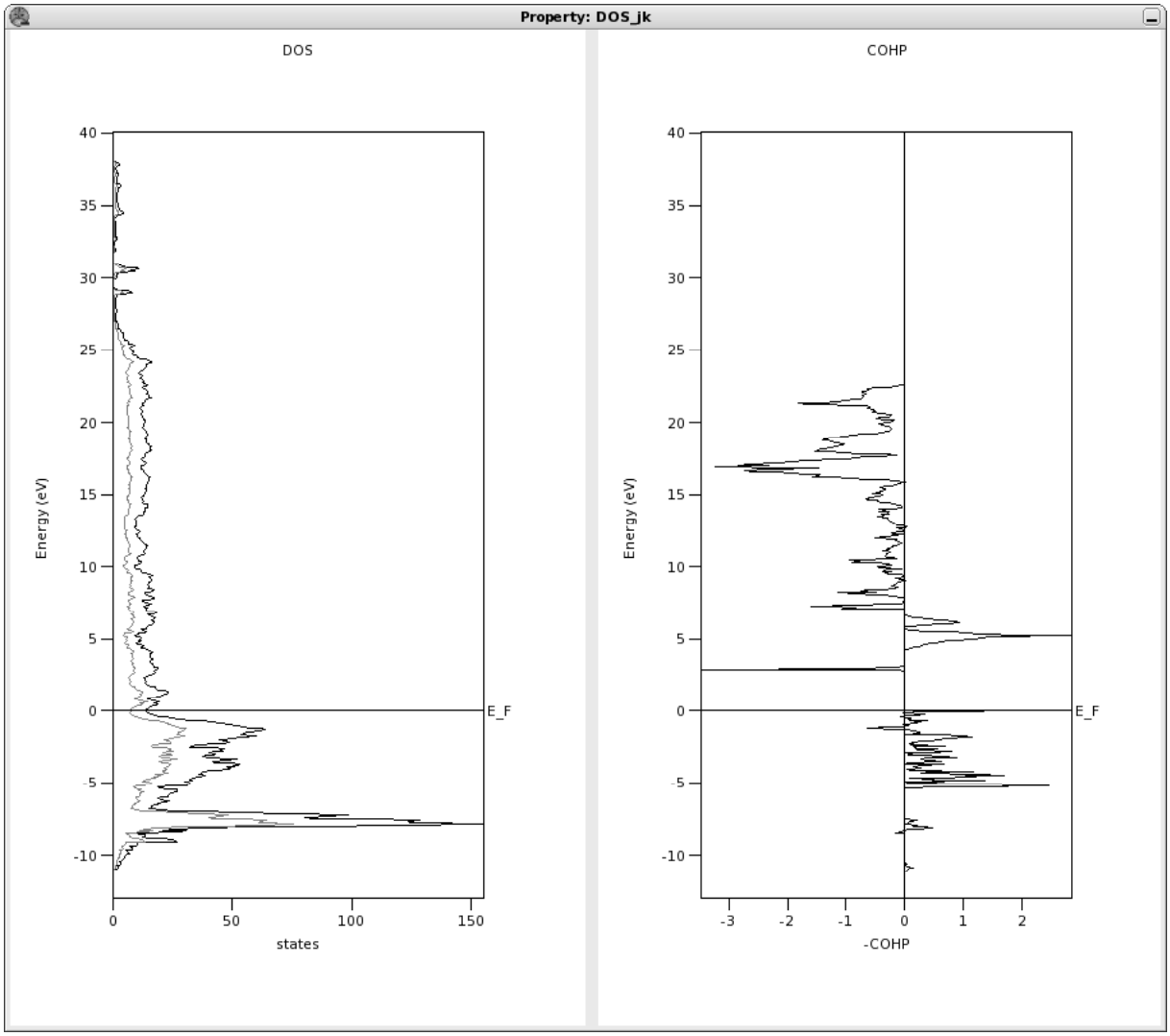

Figure 17.2: The Property Window

18. Recognized Filetypes

wxDragon is no wizard, it sure needs some keywords within the files it reads in order to determine the type of the file, and the program which produced it. Here the determination scheme will be briefly described.

18.1 Outputfiles

18.1.1 Gaussian

The output files of the various Gaussian version will be detected according to the newest string describing the verion, e.g. if "Gaussian 94" is found, but no "Gaussian98", then it propably is the 94 version of the program who generated the output.

wxDragon can read in:

- atomic geomtries
- geometries out of an energy minimization
- vibrations
- orbitals
- SCF and MP2 energies
- charges

18.1.2 Gamess-UK

If the file contains the string "G A M E S S - U K" everything else is straight forward.

18.1.3 Gamess-US

If the file contains the string "G A M E S S - U S" everything else is straight forward.

18.1.4 Turbomol

Again, only the string "TURBOMOLE" must be found.

wxDragon can read:

- atomic geomtries
- vibrations
- charges

18.1.5 Bind

The output from the bind program out of the YaeHMOP packet can be read, the geometries and the molecular orbitals can be read.

18.1.6 VASP

In the first line of the file the keyword "vasp." must be found. Otherwise a file can be given to wxDragon, where the first line contains "VASP", the second line the name of the corresponding POSCAR file, and the third line the name of the desired OUTCAR file.

Opening the vasprun.xml file is possible, the name must not always be *vasprun*, so one may choose to save the old vasprun.xml file in another name. wxDragon tries to read as much as possible from a vasprun.xml file, even the bandstructure or DOS properties. The properties can be accessed afterwards using the MD-Sim Module dialog.

When in the same directory files named "ELFCAR" and/or "CHGCAR" and/or "LOCPOT" are present, those file will be read in and wxDragon allows then the visualization of the resulting isosurfaces.

wxDragon can read:

- atomic geomtries
- geometries out of an MD run
- temperature
- magnetic moments
- charges
- forces
- total energy

If a "CHG" file is found, the charge densities included in this file are asigned to every tenth step (in accordance to the vasp-manual). When isosurfaces are shown, and a trajectory run is animated, the isosurface will change accordingly. This case is named "ANIM CHARGE"...

18.1.7 ADF

First, the string "Amsterdam Density Functional (ADF)" must be found. In order to distinguish between the old version 1. and the newer one, a following "1." within the line were the ADF keyword was found must be present.

wxDragon can read:

- atomic geomtries
- geometries out of an energy minimization
- vibrations
- charges

18.1.8 CPMD

The output from the Car-Parinello Program CPMD is detected by the keywords "PROGRAM CPMD" and should be read in. At least, thats what was done the last time I had an CPMD file to test. This file got lost a long time ago, so don't bet on the ability of wxDragon to much.

18.2 Inputfiles

Inputfiles are mostly quite short, and very ofter short of real unique keywords, so here problems may be rise. Don't get angry, give it a new try.

18.2.1 LMTO

For LMTO, wxDragon recognizes two files: the INIT file (where in the first line the keyword "SPCGRP=" can be found) and the CTRL file (where in the second line the keyword "LMASA" canbe found). The files will be treated accordingly to the found type.

18.2.2 VASP

It the filename contains "POSCAR" or "CONTACR", this file will be read, together with the file "POTCAR", which must be located in the same directory. The POSCAR/-CONTAR files can have ending to their liking, like POSCAR.firstrun. wxDragon then will first look for a POTCAR named POTCAR.firstrun, and if this is not present, it will look for the simple POTCAR.

18.2.3 Schakal

If the first line contains "TITL", it will be assumed that this may be Schakal input file.

18.3 Special Files

18.3.1 Jana

The keyword "JANA" in the first line should be present, and the version information "2000" in order to clarify the exact type.

18.3.2 PDB

If the file ends with a ".pdb", wxDragon assums the PDB data file format and will try to read the file. Be aware that for now wxDragon will read very simple pdb-files with only simple atom definitions in them.

18.3.3 Wien2k

wxDragon can read simple ".struct" files, as well as the "*.outputt" file from a DOS calculation. Work is in progress.

18.3.4 FPLO

wxDragon can read the input file "=.in" as well as the "out" file from calculation. Work is in progress.

18.3.5 The wxDragon Internal File Format

This is a special format for wxDragon, where not only the actual atom positions are stored, but also the current display mode including visibility, rotation state, label on/off and so on. If a trajectory if available, the steps will be saved as well.

The advantage may be, that all usefull (for wxDragon) information is stored in a file, which useually is much smaller than the original output file - which then can be compressed and stored away.

19. Preferences

19.1 General Preferences

When changing something in the following preferences, the user can apply the changes immediately, or save them to file, so that they get loaded the next time wxDragon is started. Or the user can close the dialog without saving any changes. The options are available as an menu on the top of the dialog.

19.1.1 Display

The user can set here the default display options he wishes to be active if he just opened a file.

19.1.2 Crystal

Here the options for opening crystals can be set so that not a full unit cell is generated but only the read in molecular fragment is show.

19.1.3 Applications

For some used (helpper-)applications the path to the executable or some additional pathes for them can be set here. Or the size of the povray-preview window. Also the path to the standard POTCARs for VASP files.

19.1.4 Print

Sets the default for the printing dialog. Like printing with a slight *perspective* (does not relate to the one displayed!), if the atoms should be printed as *shaded balls* and not only simple circles. Or if the bonds should be filled (*filled bonds*) or represented by the two outlines. Should the atoms printed in the actual selected display style (spacefill, lines,...) or should the radius be reduced by default (*Reduced Radii*). Should the atoms become a cross on them in order to improve the 3D look of them (*Crosses*), should they be filled with different *pattern* according to their type? Some options only work in low quaility mode or black and white, some only in the high one. Just play with it. The next checkbox is about isosurfaces, wheter they should be drawn only as the outline of the triangles or filled with the surface color.

In the following radio box the default print quality can be set.

Page Setup doesn't work up to now.

Two textcontrols determine the the number of fragments, into which bonds, triangles, atoms and all other triangles or planes (from surfaces, planes) are divided into when printing. A good number seems to be 3.

The number of iterations when calculating the overlap of 2 triangles or planes can be set in the next control. 4 seems to be a good choice.

Be aware that with these setting (3 fragments and 4 iterations) printing of a few atoms and bonds with a surface or slice will take around 10-30 seconds, but with larger numbers of fragments and/or iterations this time may increase vastly. Also the size of the resulting postscript file will increase.

In the last two controls the fontstyle and -size used in the postscript output can be set.

19.1.5 Modules

Up to now, nothing should appear hear.

19.1.6 Accuracy

The number of digits after the decimal point can be set here for energies, temperature and for the rest (default). Some people (*ab initio* ones) may want 10, some people (empiric one) may be happy with only 2. Choose what suites you best. And a scaling factor for automatic bond generation ¿ between atoms using their radii can be set.

19.1.7 Color

Set the color of bonds, the background, and for surfaces (positive and ¿ negative value). When klicking the button, a respective color dialog appear, so that a new color can be set. If the standard font colour black is not good for displaying purposes, here the default font colour can be changed here also to some nice colour.

19.1.8 System

The number of the available mouse buttons can be set here. The missing buttons are replaced by the shift key (middle button) and the cntrl key (right button). The default size of the drawing window when starting wxDragon can be set next by selecting one from the few defaults sizes. The number of threads is not working right now, so let it be. The checkbox labeled *Small Dialogs* let the user control the size of some important dialogs (like the crystal module). Use this box if you have a small display and some parts of the module dialogs are displayed out of sight.

19.2 Atom Preferences

Here various default values for the atoms can be set, see picture 19.1. The default radius, angle and mass used, and the full name (may be used in some output). Also the color of the atomtype can be set. After double clicking an atom in the top list, the values can be changed below. After changing the desired values, the user can discard the changes or accept them. Without accepting them, nothing will change in the list above.

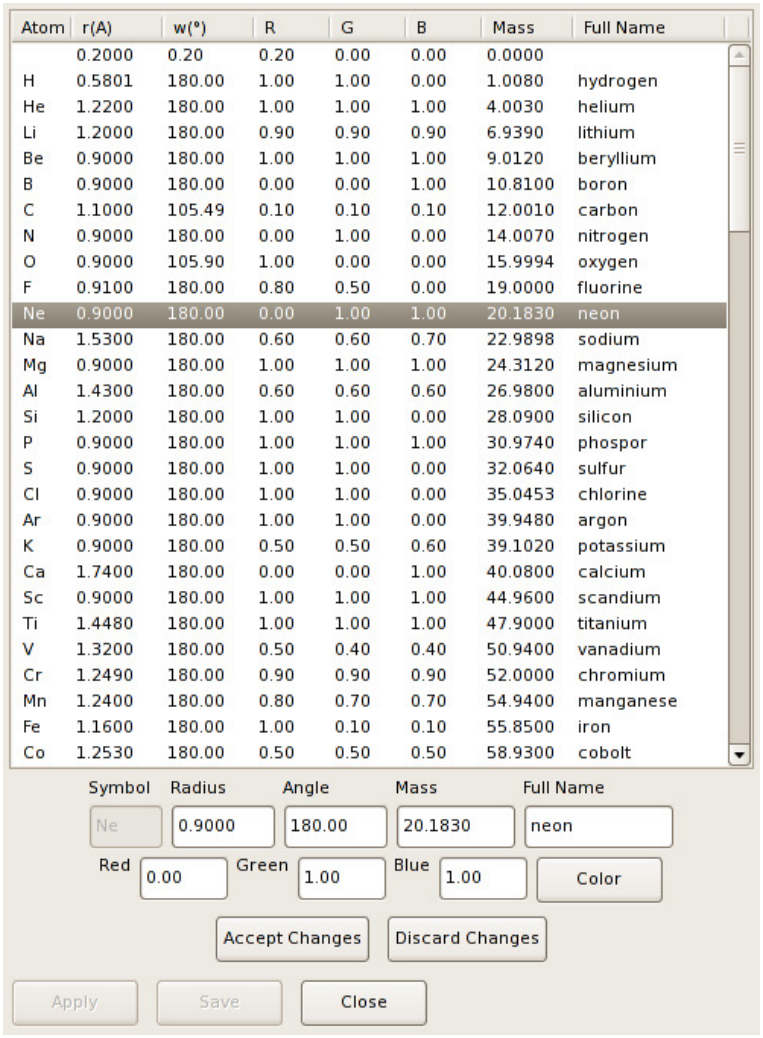

Figure 19.1: The Preferences Dialog

The user can apply the accepted changes immediately, but this will only be temporary until wxDragon closes. Additional the changes can be saved so that the values will stay after an restart of the program. By simply closing the dialog all changes made will be discarded. The overall changes can only be applied or ¿ saved when no actual atom is selected.

20. Howto Make a New Molecule

20.1 Intention

This section can be used to build up new molecules from ground, or, when the dialog gets opened throuh the QC-Module, the existing molecule can be modified or extended.

20.2 What can be done

There are two different ways to build the molecule. The first one is completly based on a dialog as shown in fig. 20.1. The description of this is given in 10.2 on page 36. Be aware that the atomtype and the number of the atom is needed to identify the right atom.

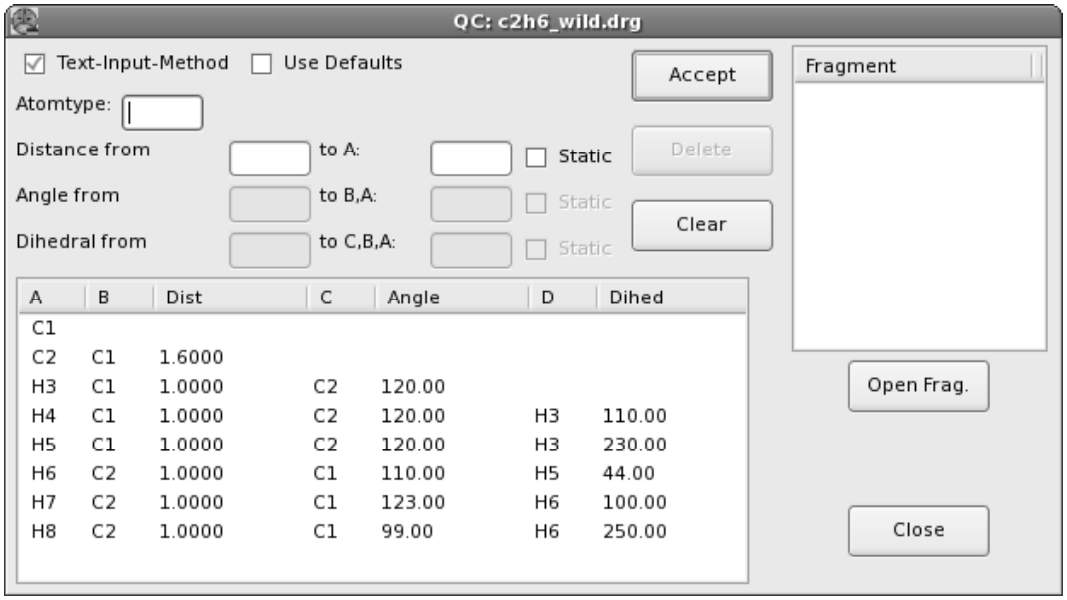

Figure 20.1: The ZMatrix Dialog.

The second way to build the molecule has the dialog shown in fig. 20.2 only for support or correction. The actual building is done in the drawing area.

Just set the desired atomtype in the field of the dialog, and click into the drawing area. The first atom will be set. For the second atom, set the desired atom type (if it is the same as the previous one, one do not need to set it again) and click on the first atom. A small dialog will pop up to ask for the distance to the first atom. For the third atom the procedure is the same at first, but after the distance selection, one must click on a second atom to define the angle, which must be given in the popup dialog then. For

the fourth and all afterwards atoms one also must click then on a third atom to define the dihedral and give the actual value in the dialog.

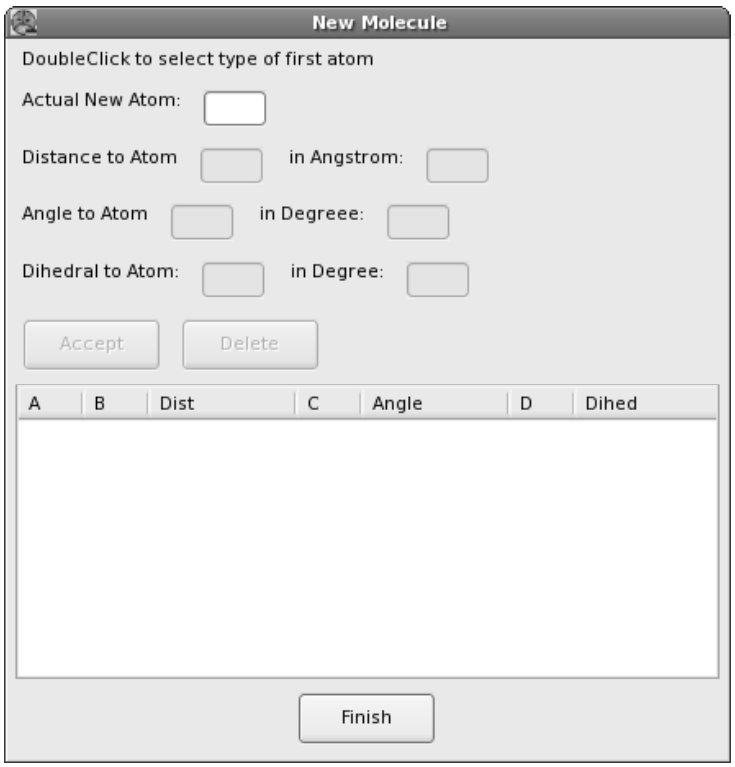

Figure 20.2: The New Molecule Dialog.

Of course if the selected atom for the distance or angle seems to be wrong, deselect it and select a new one. If the last atom needed is selected, the cycle will restart again. If corrections must be done afterwards, select the line with the desired values in the dialog.

20.3 Howto Make a New Crystal

Please see chapter 16 for details.

21. The MD-Sim Module

At the top of this dialog (fig. 21.1) the lattice parameters are repeated, and the temperature, kinectic and potential energy of the simulation, if found, is given. If two or more simulation step are found, the user has then the option to calculate the radial distribution function (or pair correlation function) can be calculated. An extra dialog will open, where the user can choose the atom pair, the first and last step, and the range at which to look. When calculated, a new property dialog will open to let one controll the plotting, see 17.3 at page 55. Similiar to the RDF also the mean square displacement (MSD) can be calculated. If the steps found came with an energy, the plotting of the energy over the steps can be controlled with the third button in this section.

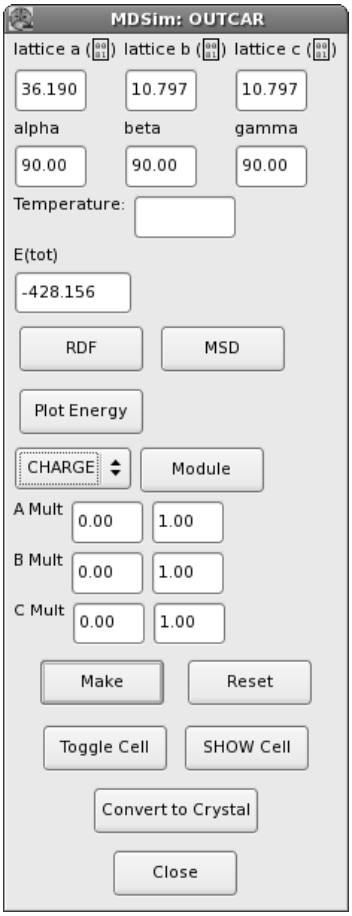

Figure 21.1: The MD-Sim Module Dialog.

The next section lets the user expand or restrict the found simulation box. The expansion of the cell still stays also when surfaces, slices or planes are drawn, those properties

will get expanded. This may come handy if something important is happening at the border of the simulation box. When the cell is multiplied, the showing of the cell can be controlled. The last important button lets the user convert the found MD cell into an crystal. When pressing this button, the dialog *Find Symmetry* is opened, fro more details see 16.4 on page 53.

22. Script

wxDragon has the ability to be controlled by a simple script language. It can produce automated output with it, ensure that the molecule opened is shown in a predefined rotation angle and zoom factor. With properties the selection can be set, printed, and exported.

A script file can be loaded with the command line option "-s". The relative order of this doesn't matter, the commandos in the script file are applied to all already loaded molecules and also will be applied to all latter loaded ones. In the script file one can set the target file format to which the script is applied (like VASP OUTCAR, LMTO DOS, or all Crystals). More than one script file can be loaded, so don't put everything into just one.

22.1 Generating Scripts

Some dialogs offer the possibility to save the actual settings in the script format. They can immedeately be used as script files without further editing them.

- Display-Menu-¿Viewing-¿View-Control: with the "Save Settings" option a small file will be generated containing the actual zoom, shift and rotation setting.
- Property-Control: use the "Save Settings" button to save the actual settings for all controls in the dialog

23. Misc. Issues

23.1 The GL-Canvas Menu

When pressing the right mouse button within the drawing area, a context menu will appear. Depending on the object hit it will contain:

23.1.1 The background

The display style of the OpenGL objects can be toggled between the solid and the wireframe style, where only the edges of the triangles were plotted. This allows e.g. an easier look at atoms behind some front atoms. The third item switches the angular momentum on or off. If it is on, and the molecule is rotated a bit with the mouse, this movement will continue, even when the mouse button is already released. The fourth item toggles the display between the rough, but fast, Lowres display style, where e.g. atoms are plotted using only a few triangles, and between the HighRes modus, where the atoms are (nearly) real spheres. It may looks better, but it also will be slower (depending heavy on the graphic engine one is using). The next two items allows the navigation between the loaded molecules, the next or the previous molecule within the list as it appears in the Molecule Menu (and as the molecules are loaded). The last two items toggle the between the perspective and the orthonormal view of the molecules.

23.1.2 Atom

23.1.3 Bond

23.1.4 Triangle

The possible choice here are to change the color of the triangle (a dialog will pop up) or to delete the triangle.

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