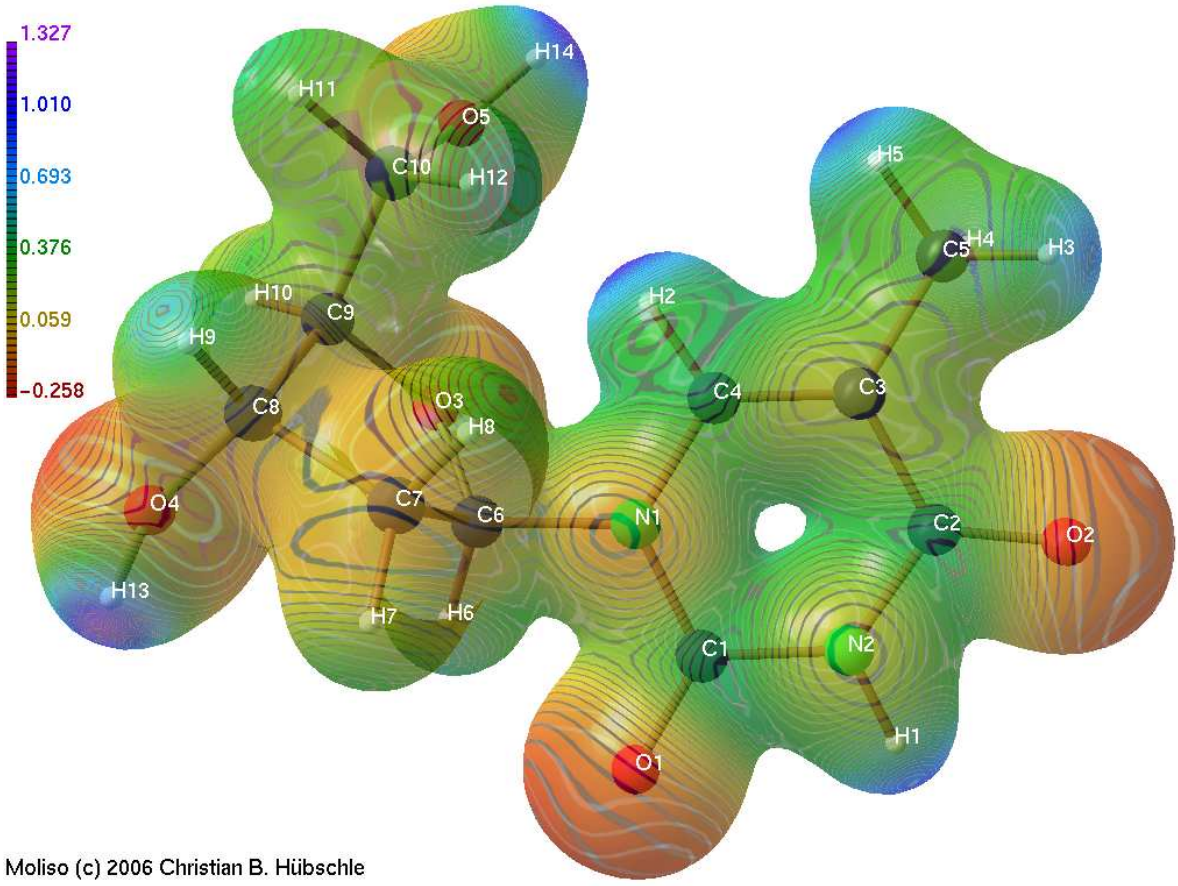
MolIso - A Program for Color Mapped Iso-surfaces

by Christian B. Hübschle

Version 2.0



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1 Purpose

This Program is intended for users of the XD program package [1] to display color mapped iso-surfaces created from several 3D property grid files. It is made to give the user an eye catching view into the physical properties of their investigated compounds. Recently GAUSSIAN-CUBE-files and CIF-files (for ADP's) were also implemented.

2 License


```
MolIso License
==============

moliso
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Reference:
Hbschle C.B. and Luger P. ,J. Appl.  Cryst.  (2006).  39, 901-904

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```

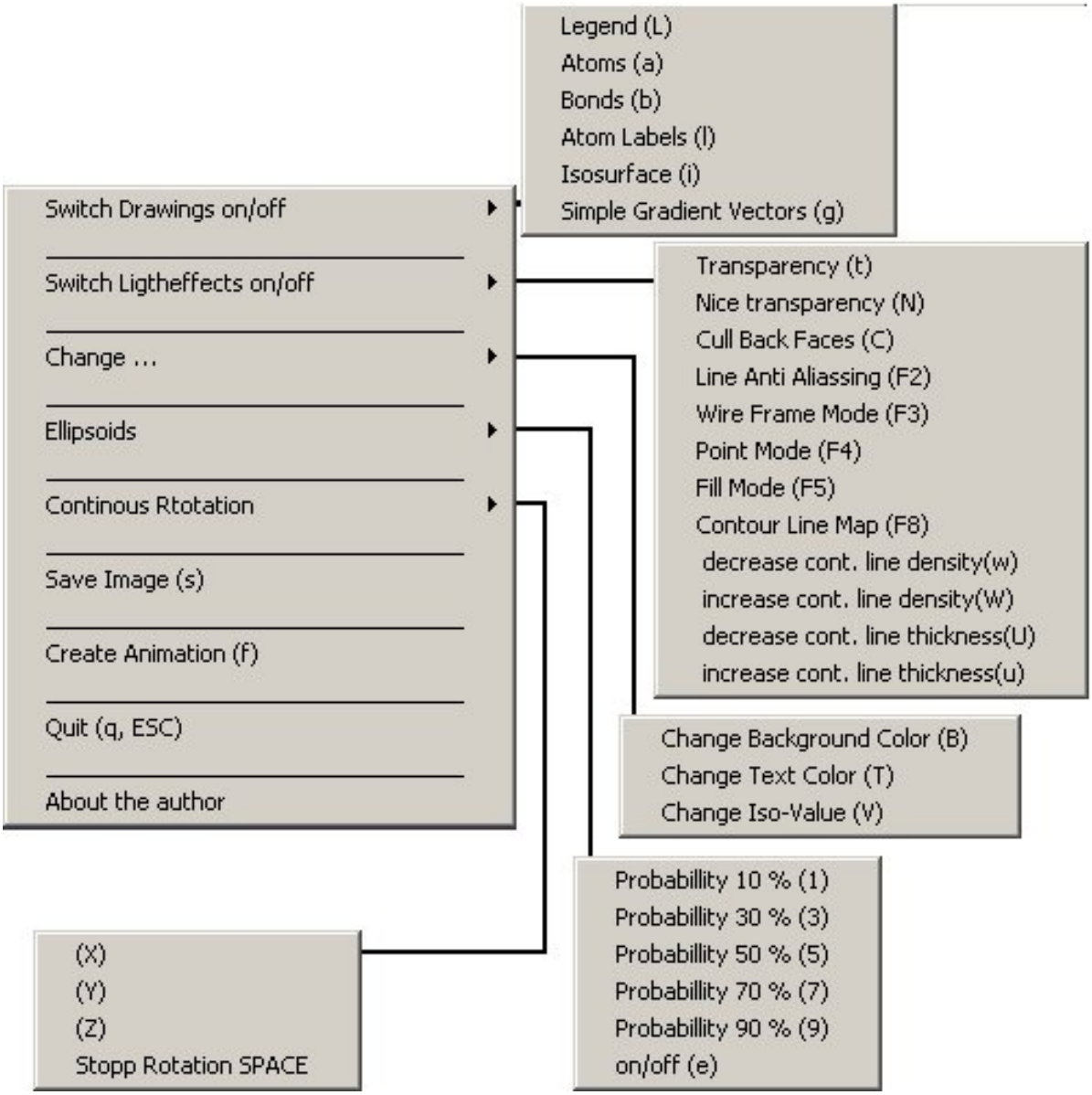
3 Installation

Before installation you have to think about some system requirements. The first requirement is that you need a not too outdated graphics accelerator card[1] build in your computer. And you need of course a driver for this graphic card as well which supports 3D acceleration. On a Linux-System you have to make sure that the GLUT library is installed correctly. On Linux you also have to install the IMAGEMAGICK package and the MJPEG-TOOLS package to access all functions of the program. On a Windows computer the installation is quite simple. Just double click on `moliso_setup.exe` and follow the instructions. If you have selected "example" a set of files will be copied in your `MyDocuments\moliso\Example\` directory. To view this example start MOLISO from your start menu and choose the `moliso.ini` file from the example directory.

4 Menu Structure

MOLISO has a pop-up menu which appears by pressing the right mouse button. The menu has the following structure: (shortcut keys are in parentheses (shortcut))

[1] A GeForce 2 is quite good enough, more graphics memory increases speed.

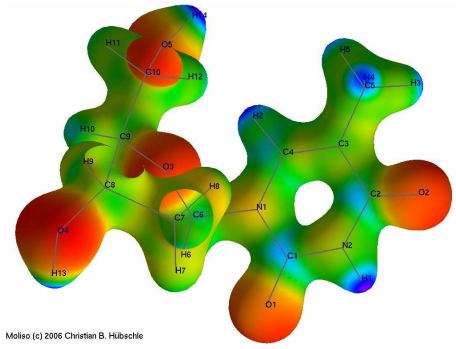


Most of the menu items should be self explaining, but feel free to play around to find out what the effects are. The menu may differ from the picture above, because the program is still under development. Some of the light effects need some more explanation.

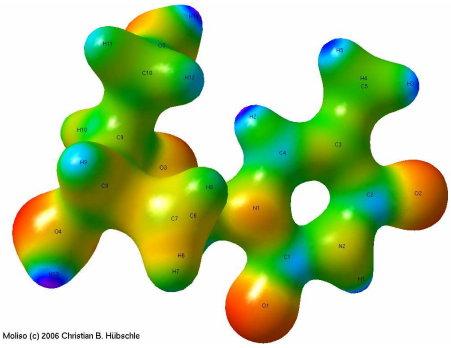
Nice transparency means that there are no drawing errors due to incorrect ordering of the drawn triangles of the iso-surface. These drawing errors show up as stripes in certain rotation positions. To prevent this the program stores 6 drawings of the iso-surface into the memory and shows up only the correct one in the actual rotational position.

Cull back faces: Computer graphic drawings normally consist of triangles or quadrilaterals. Theses faces are objects in 3D space, so they have a front and a back side. Normally when a closed body is drawn all "back faces" are occluded by the visible "front faces" of the body. So normally **cull back faces** is an option to prevent ren-

dering of “back faces” in the graphic accelerator card, and to speed up drawing. But in transparency mode the “back faces” are also visible. This can be used to simplify drawings for clarity. By pressing `F1` several times you come into a mode where the “front faces” instead of “back faces” are culled which gives you a sheer plan of your surface, like in the following picture.



sheer plan



front side

5 Keyboard Shortcuts

Additional to the shortcuts listed above in the menu structure there are some more keyboard shortcuts.

Key	Functionality
Arrow Keys	Rotate the drawings. Additional pressing of SHIFT or CONTROL leads to a de- or increase of speed.
PAGE-UP, PAGE-DOWN	Zoom in and out drawings. Additional pressing of SHIFT or CONTROL leads to a de- or increase of speed.
F1	Change some light-effects. Please watch the console. Press the F1 key several times to see all possible light effects
>	Export the 16 numbers of the orientation matrix
<	Import the 16 numbers of the orientation matrix
=	Change nearly all parameters (including orientation matrix) to the values, they had the last time you saved an image file in that directory.
k,K	In- or decrease viewing angle. The default viewing angle is 29 degrees.
w,W	In- or decrease contour line density. (F8 mode)
u,U	In- or decrease contour line width. (F8 mode)
p,E	Create a PDF vector graphics output file
r	Regularize the surface. Surface gets smoother but incorrecter each iteration
o	Free some memory. After that the value of iso-surface is not changeable anymore.
Q	Switch on/off quadrilaterals. (Effect only visible in F3 mode).
m	Switch on/off multicolor mapping. Iso-surface color changes to last color drawn (labels).

6 INI-File Keywords

Keyword	Possible Values	Explanation
Iso_Grid=	?	Absolute or relative path to the XD 3D grid file which contains the information for the iso-surface
Map_Grid=	?	Absolute or relative path to the XD 3D grid file which contains the information for the color map
Refl_Texture=	Can be empty.	Absolute or relative path to the ppm image file which contains the information for pseudo reflection effect (F6, F7)
Iso_Value=	Floating point number	The value of the iso-surface to be drawn
Gradient_Cutoff=	Floating point number	Lower border for drawing simple gradients
Grad_Atom=	4 Floating point numbers can be empty	Including sphere for simple gradients: first 3 numbers are Cartesian coordinates like in the grid file and the 4th number is the radius of the sphere.
XD_RES_PATH=	?	Absolute or relative path to the `xd.res` file. There must also be a `xd.mas` file present. (ignored if `Enable_Ellipsoids` is set to NO)
Transparency_Mode=	NICE/FAST	Fast leads to faster startup of the program but also to errors of the viewing when transparency is enabled.
Enable_Ellipsoids=	YES/NO	
Sphere_Detail=	1,2,...,N	Must be greater 0. Greater values lead to more surface points on spheres and ellipsoids.
Use_Stored_Surface=	Can be empty.	Use a previous saved surface instead of calculating it. Increases performance and decreases memory costs.
Store_Surface=	Can be empty.	Saved the surface for later use.
Regular_Iterations=	0,1,2,...,N	Regularize surface triangles N times. Surface looks smoother but gets more and more incorrect.
Background_Color= Text_Color=	4 Floating Numbers between 0.0 and 1.0 4 Floating Numbers between 0.0 and 1.0	red green blue alpha=transparency
Ellipsoid_Probability=	10/30/50/70/90	Ignored if `Enable_Ellipsoids` is set to NO
Mouse_Interaction=	0,1	Controls the message boxes for measuring distances and angles.

These are examples of `moliso.ini` files:

```
Iso_Grid=xd_rho.grd
Map_Grid=xd_esp.grd
Refl_Texture=1.ppm
Iso_Value=0.5
Gradient_Cutoff=0.005
Grad_Atom=0.0 0.0 0.0 1.0
Sphere_Detail=8
XD_RES_PATH=xd.res
Transparency_Mode=NICE
Enable_Ellipsoids=YES
Ellipsoid_Probability=50
```

```
Iso_Grid=gauss_density.cube
Map_Grid=gauss_potential.cube
Refl_Texture=
Iso_Value=0.07409
Gradient_Cutoff=0.005
Grad_Atom=
Sphere_Detail=2
XD_RES_PATH=my_own.cif
Transparency_Mode=FAST
Enable_Ellipsoids=YES
Ellipsoid_Probability=50
```

7 HowTo's

7.1 Creating Iso-surfaces in rho with the Electrostatic Potential Mapped on it

1. Open your `xd.mas` file in an editor of your choice and put an asterisk before esp in the line after the PROPERTY keyword.

2. Uncomment the `CUBE ato(1) ato(2) npts 20 stepsize 0.1` line and change ato(1) and ato(2) to two atom labels in-between the center of your compound is situated. Change npts to 100 for example and stepsize to a value that is smaller than X= (longest elongation of you compound)/npts.

3. Save your `xd.mas` file and run XDprop.

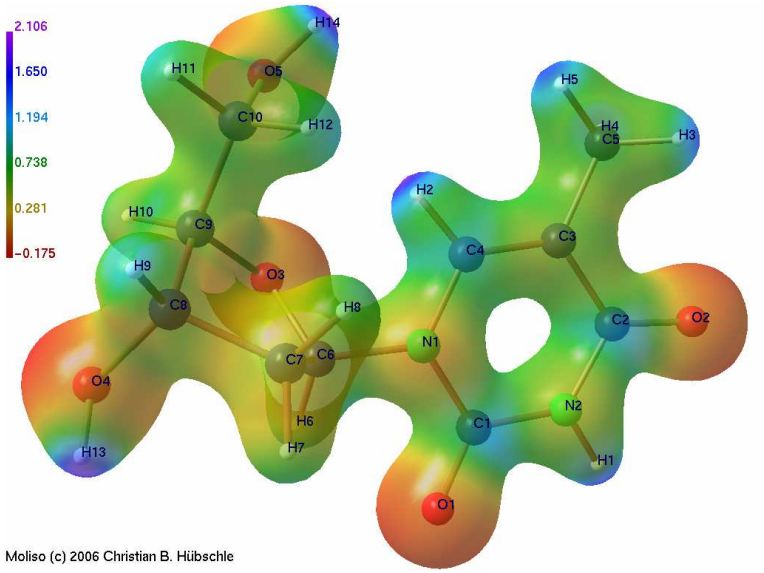
4. Repeat step 1-3 with rho instead of esp.

5. If you don't want to edit the `moliso.ini` file yourself, you can create an empty file called `moliso.ini` in the same directory where your `xd.mas,xd.res,` tt xd_esp.grd, `xd_rho.grd` files are.

6. On windows you can start now the MolIso program from your start menu. On Linux just type `moliso` on the console in your working directory and you are finished. After that you can rotate your molecule drawings by moving the mouse with the left mouse button pressed, move it by pressing the middle mouse button.

7. An open dialog appears on the screen. Change to the directory where your above xd files are and select the moliso.ini file.

8. After a more or less short loading time the color mapped iso-surface appears on the screen.



7.2 Moving the Molecule on the Screen

It is very easy to rotate the molecule just keep the left mouse button pressed and move it and the molecule rotates about the X and Y axes. You can also use the arrow keys to do that. Additional pressing of the SHIFT or CONTROL key de- or increases the rotation speed.

To move the molecule in X and Y axes direction just keep the middle mouse button pressed and move it around. You can also use the arrow keys on your keyboard by additionally pressing the ALT key to move the molecule that way.

To move the molecule in Z axes direction you can use the scroll wheel on your mouse or use the PAGE-UP and PAGE-DOWN keys on your keyboard. Again the speed can be controlled by additional pressing of SHIFT or CONTROL. MolIso uses a central perspective for the visualization, so this Z axes movement means zooming in or out of the molecule. You can change the viewing angle by pressing `k` or `K` (watch the console for the actual value) so that, in principal, it is possible to generate Schlegel diagrams of fullerenes or close to orthographic projection representations.

7.3 Creating Single Colored Iso-surfaces of a Single Property

Repeat steps 1-3 from above with your property. Edit `moliso.ini` so that the paths `Map_Grid=,Iso_Grid=` are directed to your 3D property grid file. Edit a new file in your directory called `Gradient.dat`. Insert two equal lines which contain 4 floating point numbers from 0 to 1. These are RGB and alpha values of your desired color. If you wish to have a blue iso-surface with 50% translucency for example you type in `0.0 0.0 1.0 0.5` two times. And then start MolIso to watch the result.

7.4 Creating Iso-surfaces with User defined Color Gradients

Create `Gradient.dat` as described above, but the lines don't have to be equal and there are up to seven lines allowed.

7.5 Fixing the Max and Min Value of the Color Gradient

If you have started MolIso in your directory before there exists a file `minmax.out` just copy or rename it to `minmax.in` and change the two values in an editor if you want.

7.6 Ex- and Importing the Orientation Matrix of the Drawings

The orientation matrix of the drawing contains information about the rotation, translation and scaling of all displayed components of the molecule. To reproduce a special view on the molecule drawings you need to ex- and import this orientation matrix which consists of 16 floating point numbers. By pressing the `>` key MolIso prints these 16 numbers to the console. The user can now use the mouse to copy these numbers to the clipboard. By pressing the `<` key the user can paste these 16 numbers with the mouse to the console. If you find this method too uncomfortable and complicated there is also an easier way to do it: Save an image of your molecule, the program writes automatically an `mconf.dat` file into the same directory. You only have to make sure that this file is in the same directory as your moliso.ini file. So you can import the orientation matrix from that file by pressing the `=` key on your keyboard.

7.7 Making Pictures with MolIso

Type `s` on your keyboard or choose the menu item "Save Image". On Windows a save dialog appears where you can choose the name and directory you want. On Windows only `.ppm` files are allowed. On Linux you can type in any image file type `convert` knows (see man convert) on the dialog.

7.8 Generating Vector Graphics with MolIso

This is an experimental option and the results do not always look as nice as the screen representation does, but the output is resolution independent and scalable to very huge representations. MolIso uses the gl2ps library from Christoph Geuzaine for producing the PDF-files. Please visit http://www.geuz.org/gl2ps/ for more information. To generate PDF-files with MolIso just type `p` or `E` on your keyboard. Specify a file name on the appearing dialog and wait until the program has computed the output file.

7.9 Generating Y-Rotation Movies with MolIso

The animation creation is a little bit different on Windows and Linux. On Windows you just have to choose 'Create Animation' from the menu or press the `f` key. Then you

can give the video clip file an appropriate name on the save dialog. After that you can choose the video codec you want to use and configure it. This depends on the codecs you have installed on your computer. After pressing 'OK' the molecule starts to rotate 360 degrees. Do not touch the mouse or the keyboard during this procedure! After the rotation stops you are done. And you can watch the created video clip with an appropriate viewer program. The size and the quality of your animation depends on the codec you choose.

On Linux you only have to make sure you have installed MJPEG TOOLS on your computer and press the `f` key. The molecule does a 360 rotation and creates an `rotation.avi` file in your working directory. This may take some time.

7.10 Using .CIF-files for ADP-Representation

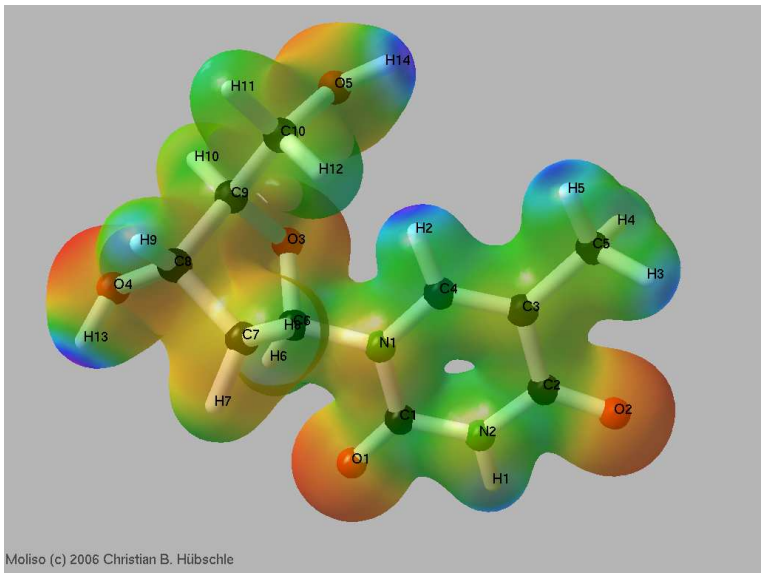
Normally Uij's are taken from the `xd.res / xd.mas` file. When using a .CIF-file instead it is necessary, that the order of the atoms in the .CUBE or .GRD-file is exactly the same as in the .CIF file. The program tries to find out the relative orientation of the grid-file in respect to the molecule in the cell. This is necessary because the orientation of the ellipsoids refer to the cell and normally not to the grid. When using GAUSSIAN-CUBE-files the values displayed in the legend are in au but the lengths are in Å.

7.11 Configure Atom and Bond Colors

To configure bonds and atoms in terms of color and radius/thickness you only need to provide a text file called `Atomcolors.dat` in the working directory. This file can consist of up to 17 lines plus comments.

```
!A Comment
!Atomic_number red green blue alpha radius
1 0.6 0.6 0.6 1.0 0.15
!this was for grey hydrogen atoms
6 0.0 0.0 0.0 1.0 0.27
!and this a real black carbon atoms
7 0.0 0.3 0.0 1.0 0.27
!dark green nitrogen atoms
8 0.5 0.0 0.0 1.0 0.27
!dark red oxygen atoms
0 0.6 0.6 0.6 1.0 0.15
!and bonds in the same thickness and color as the hydrogens
```

Atomic number of zero indicates bonds in this table. Radii of 0.0 lead to a pseudo space filling representation. The example above will lead to the following picture:



References

[1] T. Koritsánszky, T. Richter, P. Macci, C. Gatti, S. Howard, P. R. Mallinson,L. Farrugia, Z. W. Su and N. K. Hansen XD – A Computer Program Package for Multipole Refinement and Analysis of Electron Densities from Diffraction Data. Freie Universität Berlin, Berlin, **2003**.

[2] C. B. Hübschle and P. Luger *J. Appl. Crystallogr.* **2006**, *39*, 901–904.