



Version 2.1.4

Installing from Binary

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1 License information

PHOENIX-2.1.4 is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.

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Any use of results obtained using PHOENIX-2.1.4 in related or unrelated publications has to be properly acknowledged by reference to the name of the package, to the name of the developer(s), to the *NRIXS software* site <http://www.nrixs.com>, and optionally to the following paper: *W. Sturhahn, Hyperfine Interact. 125 (2000) 149-172*. This paper is included but cannot be distributed under the GNU General Public License agreement.

2 What is PHOENIX ?

The PHOENIX (PHOnon Excitation by Nuclear resonant Inelastic X-ray scattering) software is a scientific application to evaluate experimental data obtained using the technique of Nuclear Resonant Inelastic X-ray Scattering (NRIXS) which is also known as Nuclear Inelastic Scattering (NIS) and Nuclear Resonant Vibrational Spectroscopy (NRVS). The first version of the program was created in 1995 by W. Sturhahn shortly after the discovery of synchrotron radiation based inelastic nuclear resonant scattering. The PHOENIX program package is written in Fortran90. It was improved since then to handle various data input formats and provide useful diagnosis tools for high-quality data evaluation. A detailed treatment of sound velocity extraction was added in 2007, and a graphical display option was provided in 2009.

PHOENIX-2.1.4 supports all Mössbauer isotopes, the addition of raw data sets including normalization correction, the creation of an energy scale from angle and temperature data, a flexible procedure for the subtraction of the elastic peak, data normalization, detailed balance and moment calculation, a limited energy-range correction, the extraction of the partial phonon density-of-states using the Fourier-Log method, consistency checks, optional deconvolution, calculation of thermodynamic quantities, an extrapolation scheme to extract the Debye sound velocity as well as aggregate compressional and shear sound velocities.

The PHOENIX software package is mostly written in Fortran77 and Fortran90, and its programs have been used for data evaluation in numerous publications. PHOENIX has been installed on several UNIX-like operating systems: Sun's Solaris, Apple's Mac OS X, Redhat-Enterprise Linux, and Fedora Linux. Installation on MS-Windows type operating systems requires a Linux/Unix emulator software, e.g., cygwin, or better a virtual machine hosting a Linux-type guest-system, e.g., VirtualBox.

This binary distribution does not contain source code. The complete source code is available with the regular distribution. The binaries have been compiled using `gfortran` based on `gcc` version 5.2.0, please visit the gcc website.

3 Requirements

Before installation please verify the following list of requirements if runtime graphics are desired.

- alternative to provided graphics: Grace plotting tool available at <http://plasma-gate.weizmann.ac.il/Grace> ;
- Mac OS X: X11 if not distributed with Mac OS X. It is available at <http://xquartz.macosforge.org> .

4 How to install

PHOENIX is distributed as a compressed tar-ball named `PHOENIX-2.1.4-<type>.tar.gz` where `<type>` describes the operating system and architecture the binaries were built for. If this is an update from an earlier binary version of PHOENIX you may uninstall the earlier version as described in section 5. Even though this is not necessary it will avoid clutter. If you want to use both versions simultaneously you must install each version into a different location.

4.1 Extract files

Depending on the available system utilities you may have several options to extract the PHOENIX files. In many cases, a double-click on `PHOENIX-2.1.4-<type>.tar.gz` recovers the folder `PHOENIX-2.1.4`. If this fails find out the name of the directory into which you copied `PHOENIX-2.1.4-<type>.tar.gz` and open a terminal window. Then enter the following line commands.

```
> cd <name of directory>
> gzip -dc PHOENIX.2.1.4-<type>.tar.gz | tar xf -
> ls
... PHOENIX.2.1.4 ...
>
```

4.2 Configure and Install

Next, run the installation script to install the binaries. Several options can be specified to help a successful installation and functioning of the PHOENIX executables. For most cases, options should not be needed. Enter the following line commands to see the options.

```
> cd PHOENIX-2.1.4
> ./install --help
Usage: install [OPTION]...
Install PHOENIX

    --nographics      no graphics support
    --help             display this help and exit
    --prefix=<dir>    set <dir> as installation location
                    only used in 'make install'
                    preset location is <home directory>
    --spath=<list>    prepend directories to search path
                    <list> is a colon separated list of directories

Examples:
  install --spath=$HOME/etc    prepend $HOME/etc to search path
  install --prefix=/usr/local  install into directory /usr/local
>
```

Execute the script with appropriate options.

```
> ./install [OPTIONS...]
...
(messages)
...
>
```

The configuration script may be re-run with different options as needed. The last installation command is saved in the file 'installcmd'. The script produces various messages on the progress of the installation. The following files should have been created or overwritten: bin/padd, bin/pdsp, bin/phox, bin/psth, bin/psvl, bin/mpadd.

The installation step requires write access to the installation directory. By default the following files are copied into \$HOME/bin: mpadd, padd, padd-2.1.4, pdsp, pdsp-2.1.4, phox, phox-2.1.4, psth, psth-2.1.4, psvl, psvl-2.1.4. Support files are copied into \$HOME/share/PHOENIX-2.1.4.

The installed executables are only accessible by line command if DIR/bin is part of the 'path' setting in the login resource file in your home directory. This can be tested by typing 'echo \$PATH' or 'echo \$path' at a terminal prompt. If the directory DIR/bin is not part of the listing then the login resource file, usually something like '.bash_profile', '.profile', or '.login', must be edited to include DIR/bin in the 'path' setting. After that you have to logout and login again to update the 'path' settings.

4.2.1 Options

Here follows a description of the functionality of each option for the configure script.

nographics disable graphics support. By default the the built-in graphics tool is activated. This option disables this behavior. The PHOENIX executables still support the `xmgrace` visualization tool if found in the searchpath (see below).

prefix set the location for installation of the PHOENIX executables and their support files. By default the installation location is the installers home directory, i.e., the executables are copied into \$HOME/bin and the support files are copied into \$HOME/share/PHOENIX-2.1.4. If the prefix is set to another directory it is important to have appropriate permissions as installer, e.g., '-prefix=/usr/local' requires administrator or root privileges on Mac OS X or Linux systems, respectively.

spath prepend directories to the search path for essential support programs. By default the path contains the following directories: /bin, /usr/bin, /usr/local/bin, /opt/bin, /opt/local/bin, /usr/ccs/bin, /usr/ucb, /usr/openwin/bin, /usr/X11/bin. If the installation script fails to locate essential support programs in this path (reported upon execution of the script) directories have to be added. The correct syntax would be, for example, '-spath=/crazypath/dir1:~/dir2', where '~' symbolizes the user's home directory.

5 How to uninstall

The PHOENIX program package is uninstalled by the command

```
> cd PHOENIX-2.1.4
> ./uninstall
....
(messages)
....
>
```

This step removes all files that were installed during configuration. If a new version of PHOENIX is desired to be installed this step is optional. Different versions can co-exist and the version installed last takes priority in execution. Beware that modifications and local configurations saved into <install_dir>/share/PHOENIX-2.1.4 will be deleted by './uninstall'.

6 How to test

Examples are provided with the PHOENIX package. They are located in the 'PHOENIX-2.1.4/examples' directory and after 'make install' also in 'share/PHOENIX-2.1.4/examples' in the installation directory. Now change into an 'examples' directory (you need write access). If you don't have write access to the examples directory you should copy the content of an 'examples' directory to an accessible location. For example, enter something like

```
> cd ~/PHOENIX-2.1.4/examples/bccFe
> ls -px
Results/      in_padd      in_phox      in_psvl      mono.res      scan112.raw
scan115.raw  scan118.raw  scan119.raw
> padd --help
Usage: padd [OPTION]...
Run PHOENIX executable padd-2.1.4

    --geometry=<XxY+U+W> set the window geometry for
                        graphics display.
    --help              display this help and exit
    --infile=<file>     use <file> as input file
                        the default input file is 'in_kctl'
    --nographics        suppress visualization support
    --pipe=<fifo>       use <fifo> as pipe to output graphics data
    --vdelay=<val>     set visualization startup delay to <val>
    --version           display version number and exit
    --vtool=<exe>      use <exe> for data visualization

Examples:
  padd --infile=MyFile  use 'MyFile' as input file.
  padd --nographics     disable visualization.

> padd

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....
(messages)
....

-- CPU time :  user  0.11 s  system  0.01 s
-- PHOENIX module PADD finished

> ls -px
Fe_mon.csv  Fe_padd_ptl.txt  Fe_shf.csv
Fe_sum.csv  Results/         in_padd
in_phox     in_psvl          mono.res
scan112.raw scan115.raw      scan118.raw
scan119.raw
>
```

Several files were created during this addition of NRIXS spectra. Continue with commands 'phox' and 'psvl' to extract the DOS and sound velocities, respectively. Compare the content of output files with files provided in the 'Results' directory.