

Obtaining PyRosetta

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1 Obtain a PyRosetta license

A. Go to:

<http://www.pyrosetta.org>

B. Click the “**Downloads**” link along the top of the page

C. Read about the licencing policy and click “**here**”

D. Skip to the PyRosetta section and click on “**PyRosetta**”

E. Read the PyRosetta licensing information

F. If you are an academic or non-profit user, click the “**License**” button
If you are not an academic user, please consult the [licensing information](#) on how to obtain a PyRosetta license

G. Read and Complete the Academic License form

H. Wait to receive a confirmation email regarding your license registration
You will receive a *username* and *password* for downloading PyRosetta

2 Download PyRosetta

A. Go to:

<http://www.pyrosetta.org>

B. Click the “**Downloads**” link along the top of the page

C. Select a [package](#) appropriate for your operating system and click on it

- D. Input the username and password you received in the email (step 1H)
- E. Wait for the .tar.bz2 file to finish downloading
- F. Decompress the downloaded file

```
tar -xvjf /your/path/to/PyRosetta/filename.tar.bz2
```

where *filename* is the name of the downloaded file
(probably something like `PyRosetta.MacOSX.Lion-r50085.64Bit.tar.bz2`)
note: this may be handled automatically during the download process

3 Setup PyRosetta

- A. Go to the downloaded directory

```
cd /your/path/to/PyRosetta
```

- B. Run `SetPyRosettaEnvironment.sh`

```
source SetPyRosettaEnvironment.sh
```

which sets up your paths to easily find the PyRosetta libraries

- C. (Optional) Add

```
source /your/path/to/PyRosetta/SetPyRosettaEnvironment.sh
```

to your “.bashrc” file

note: contents of the “.bashrc” are run when you start your BASH shell (the command prompt) so adding the above line to “.bashrc” will setup the PyRosetta paths everytime you start the session (so you don't have to think about it)

4 Troubleshooting

4.1 Do I have to use Ipython?

No. It makes searching the (very large) rosetta libraries easy with tab completion and more informative help messages (which can be setup in regular Python with sufficient knowledge/patience). Hence we recommend it, but use whatever interface you like.

4.2 What do the package names mean?

If an Operating System (OS) name (Windows, MacOSX, ScientificLinux, Ubuntu) appears in the package name, the package is built for use in that OS. The “-r40224” refers to the (svn) version of Rosetta this package was built with. The higher the revision, the newer the package (currently Rosetta is past r50000).

4.3 Wait, what is the Ubuntu package?

As this tutorial is being written, the only supported Ubuntu distribution is quite old (\approx 2yr). Hopefully, a current release will be available soon.

4.4 I get an error about some ELF class thing?

If you get an error message referring to some “wrong ELF class” then you are probably on a 32-bit machine trying to a 64-bit package. Unfortunately, there will be no errors for this mismatch until you try to import PyRosetta. Download and setup the appropriate package for your machine (try the package for the same OS that is 32-bit).

4.5 Is there a problem with my Python version?

PyRosetta is currently supported for use with Python 2.5 or later. Older releases may be fragile to your Python version. Currently, most OS default to using Python 2.7 or higher...which should work with PyRosetta.

4.6 But I think the problem is with my Python version?

If you are using Python 2.4 or earlier, you should upgrade to a newer version to use PyRosetta. If you think you are having a problem with a Python version newer than 2.5, download an older version of Python. Note: please do NOT replace your existing Python with the older version!!! This can lead to problems like OS failure. Instead just download the Python source, compile it, and use it with PyRosetta.