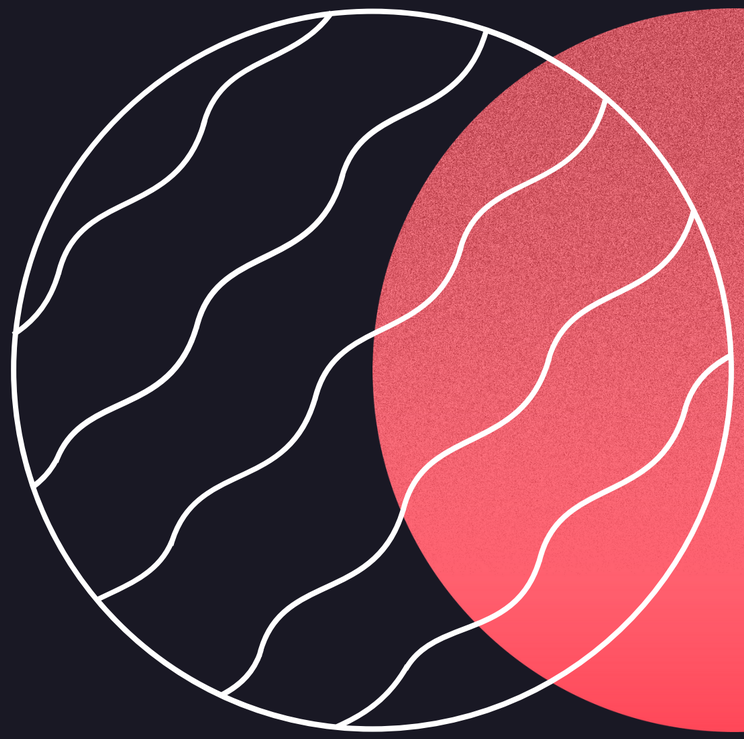
PyLadies Amsterdam



# Python in Astrochemical Research

Amanda M. Alvarado
February 24, 2021

# ABOUT ME

- Puerto Rico
- BSc Chemistry, UPR-Mayaguez
- MSc Student Physical Chemistry, UPR-Rio Piedras
- Research in Astrochemistry

# WHAT IS ASTROCHEMISTRY?

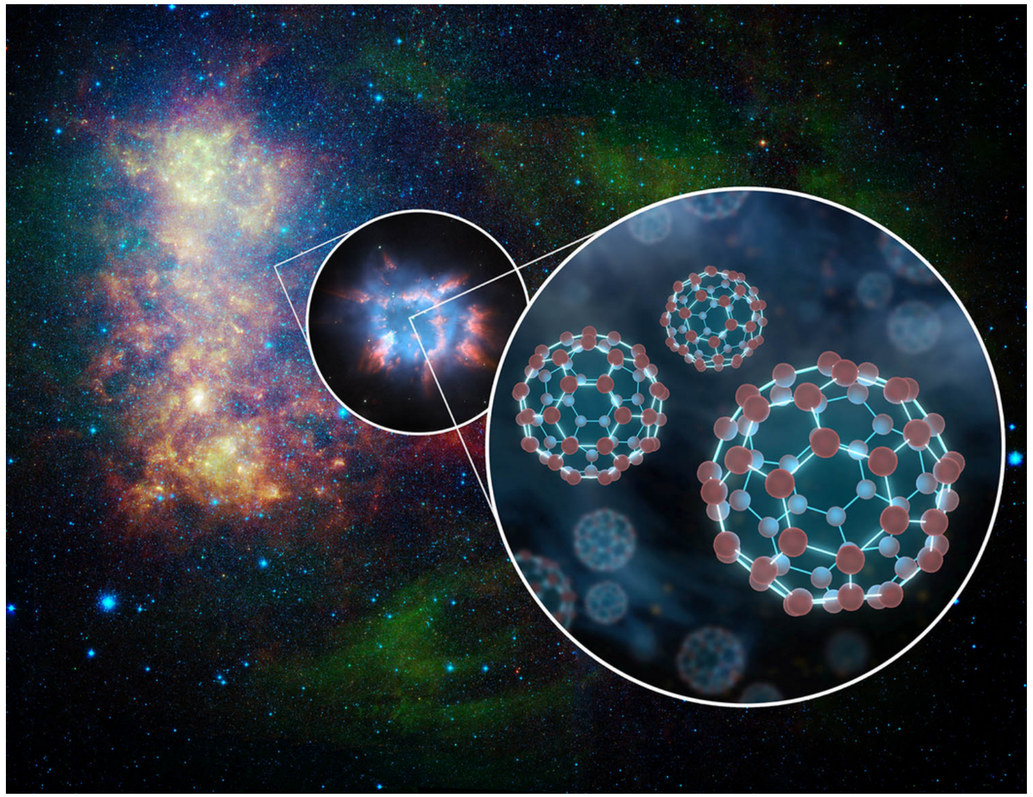


Figure by T.Pyle; credit NASA/JPL-Caltech

Astrochemistry is the study of the formation, destruction and excitation of molecules in astronomical environment and their influence on astronomical objects.

It aims to answer questions such as:

*How, when, and where are the molecules produced?*

*How complex is their chemistry?*

*How do they cycle through the phases of stellar evolution?*

*Can they become part of planetary systems and form the building blocks of life?*

# RESEARCH WORK

## What do I study?

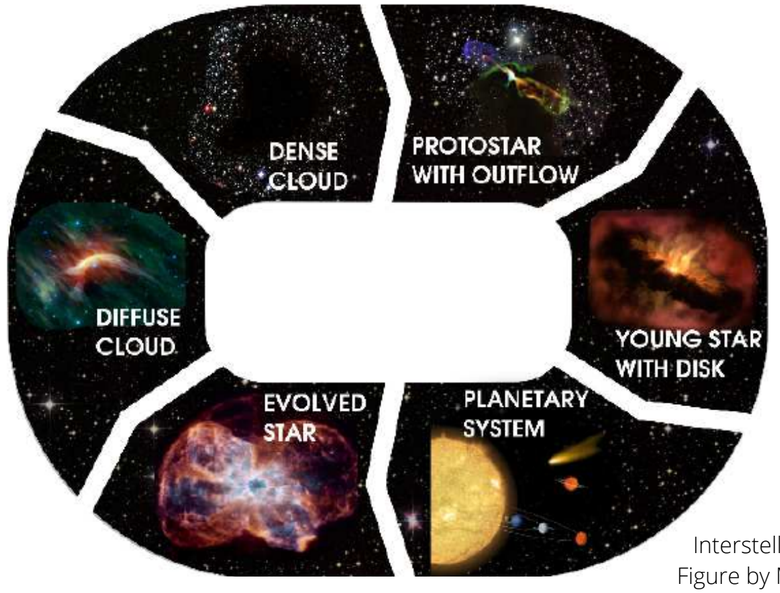
My research focuses on studying the evolution of water molecules in star forming regions.

## What results I wish to obtain?

Abundance of water molecules in the region of study (Molecular Cloud-NGC1333) and the physical and chemical conditions they are found in.

## Why is my work relevant?

Water is a fundamental molecule in the Universe, it facilitates chemical reactions that are essential to the evolution of life.

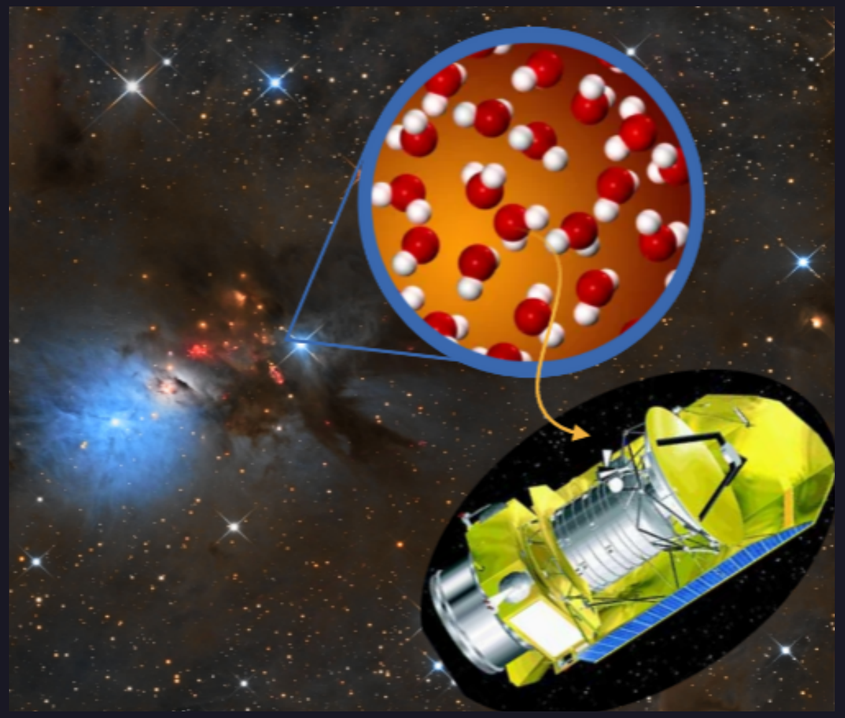



Interstellar Dust Lifecycle.
Figure by M. Perssons; credit NASA/ESO/ESA/ALMA

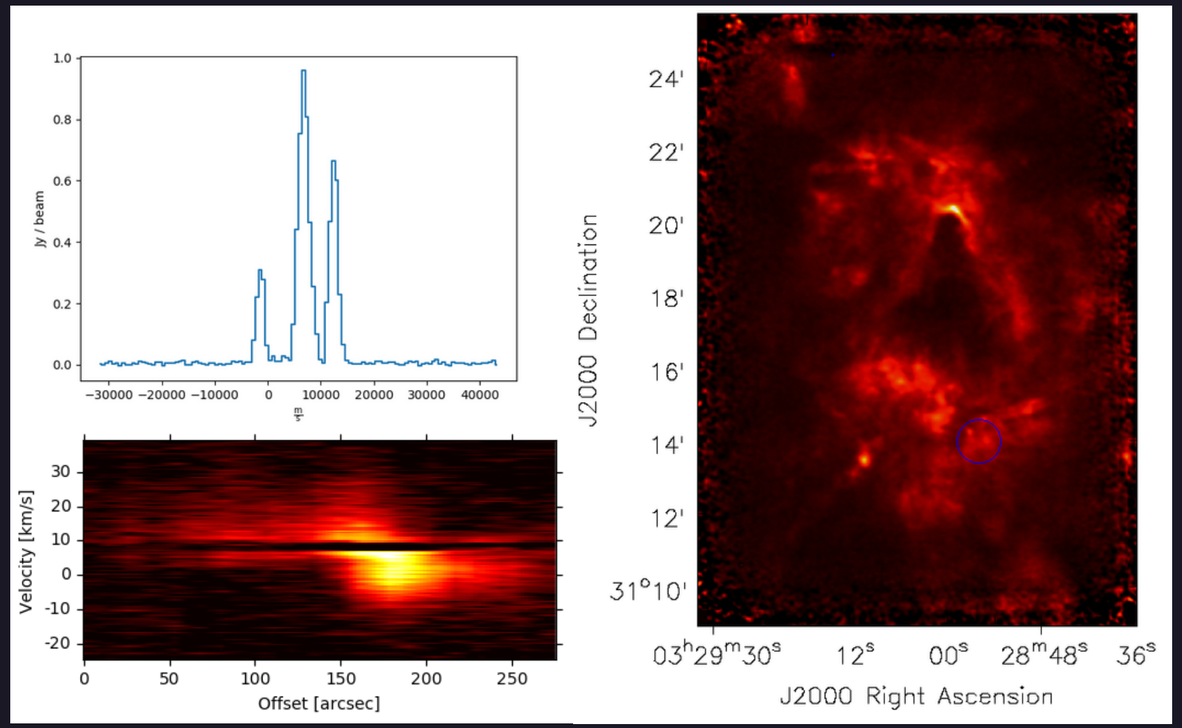
Molecular Cloud NGC1333; Spitzer Space Telescope.
Credit R. Gutenmuth NASA/JPL-Caltch

# WHAT DO I USE PYTHON FOR?

Python Software Packages are used for data processing and analysis, such as: mapping regions, obtain line spectra, make specific diagrams, create contour maps, and much more.

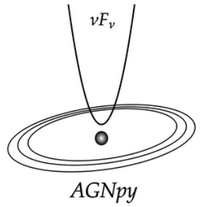


Molecular water emission from Molecular Clouds can be detected with various Space Telescope.




Results obtained using AstroPy packages.

# OPEN SOURCE PYTHON PACKAGES FOR ASTRONOMY





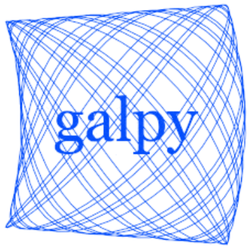


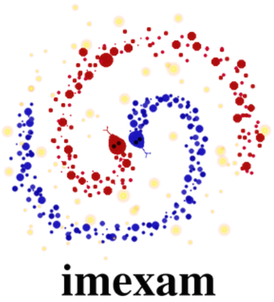












# ASTROPY: A CORE PACKAGE FOR ASTRONOMY IN PYTHON

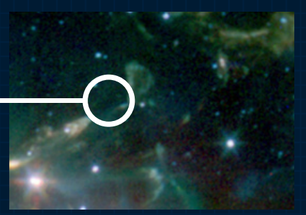
- Single free software that contains key functionality and common tools needed for performing astronomy and astrophysics with python
- Concise and readable code
- Complemented by general Scientific packages (Numpy, SciPy, etc.) and affiliated packages for specific functions (APLPy, GammaPy, PySpec, etc.)

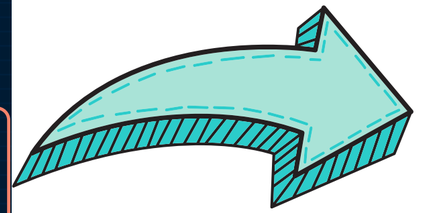
A Fiscally Sponsored Project of NUMFOCUS
OPEN CODE = BETTER SCIENCE

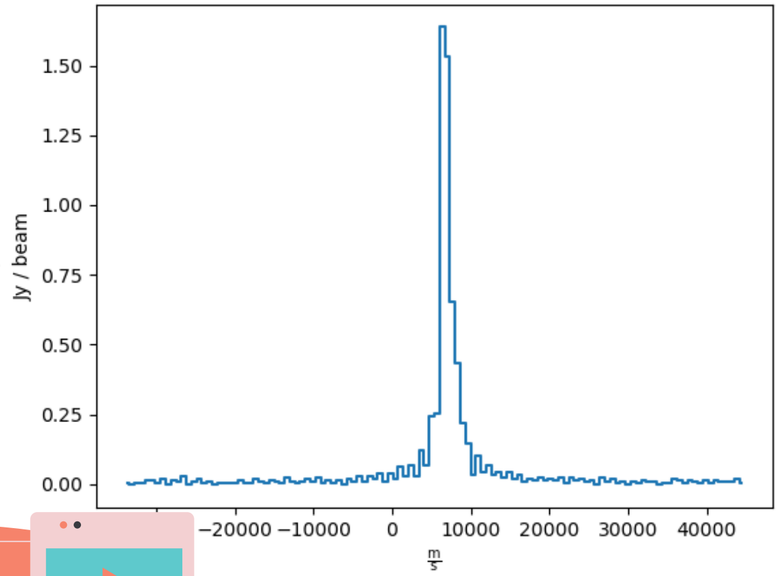
astropy
A Community Python Library for Astronomy

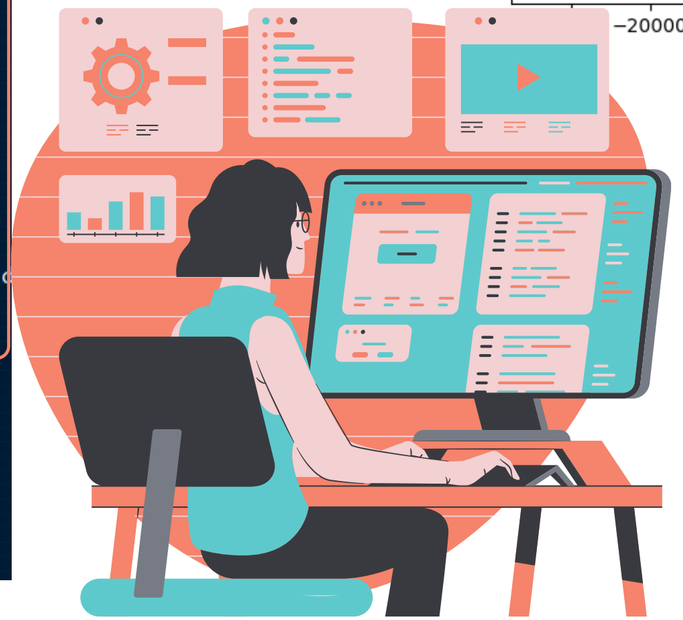
# Example: Using AstroPy to obtain Line Spectra

```python
import numpy as np
import matplotlib.pyplot as plt
from matplotlib.colors import LogNorm
import astropy.units as u
from astropy.io import fits
from astropy.utils import data
from spectral_cube import SpectralCube
from astropy.wcs import WCS

hdulist = fits.open('ngc1333_13co32_jcmt.fits')
r = 0.01111
y = float(input('Enter ra:'))
x = float(input('Enter dec:'))
imgname= input('Enter region name: ')

hdulist[0].data = hdulist[0].data.squeeze()
cube = SpectralCube.read(hdulist)

_, dec, _ = cube.world[0, :, 0]
_, _, ra = cube.world[0, 0, :]

dec_range = [(x-r), (x+r)] * u.deg
ra_range = [(y-r), (y+r)] * u.deg
subcube = cube.subcube(xlo=ra_range[0], xhi=ra_range[1],ylo=dec_range[0], yhi=d

spectrum = subcube.mean(axis=(1, 2))
spectrum.quicklook()
fig = plt.gcf()
plt.show()
plt.draw()

fig.savefig('spec_13co32_'+imgname)
```







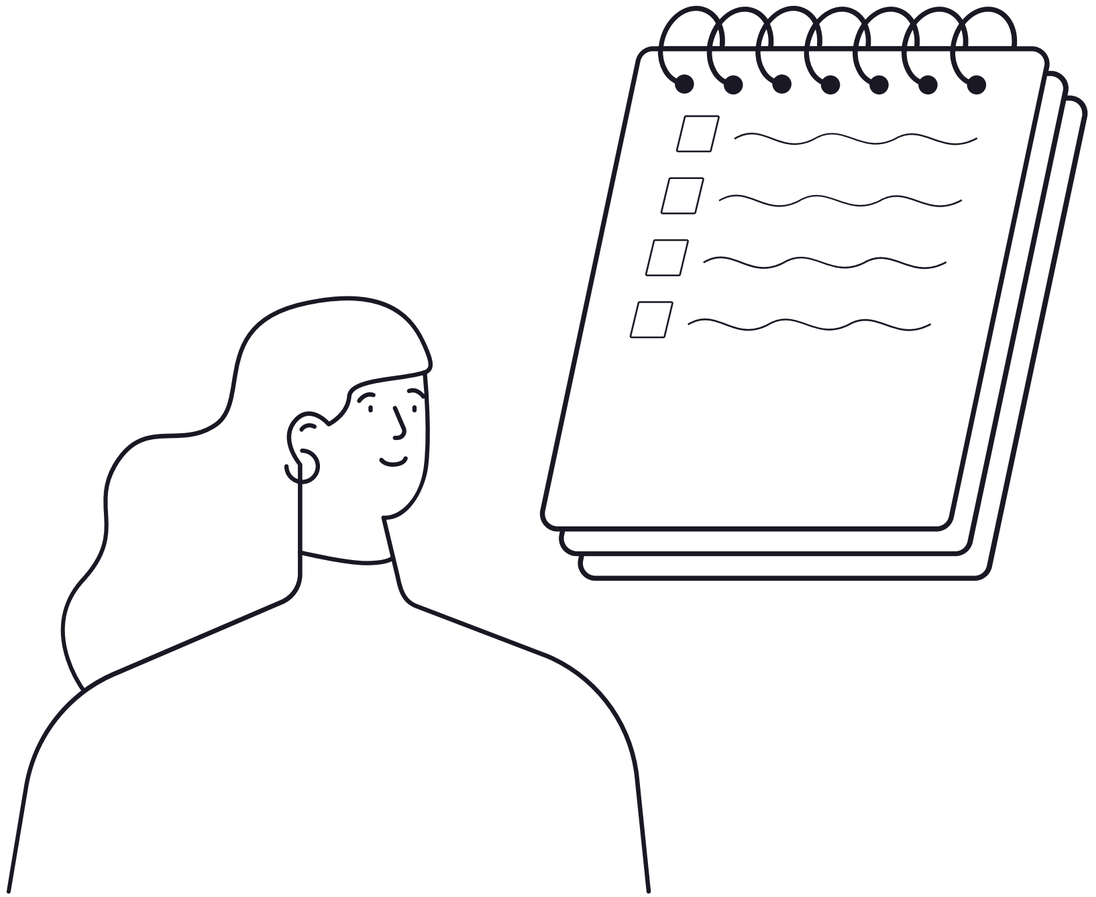
# Why use Python Packages for Astrochemistry?

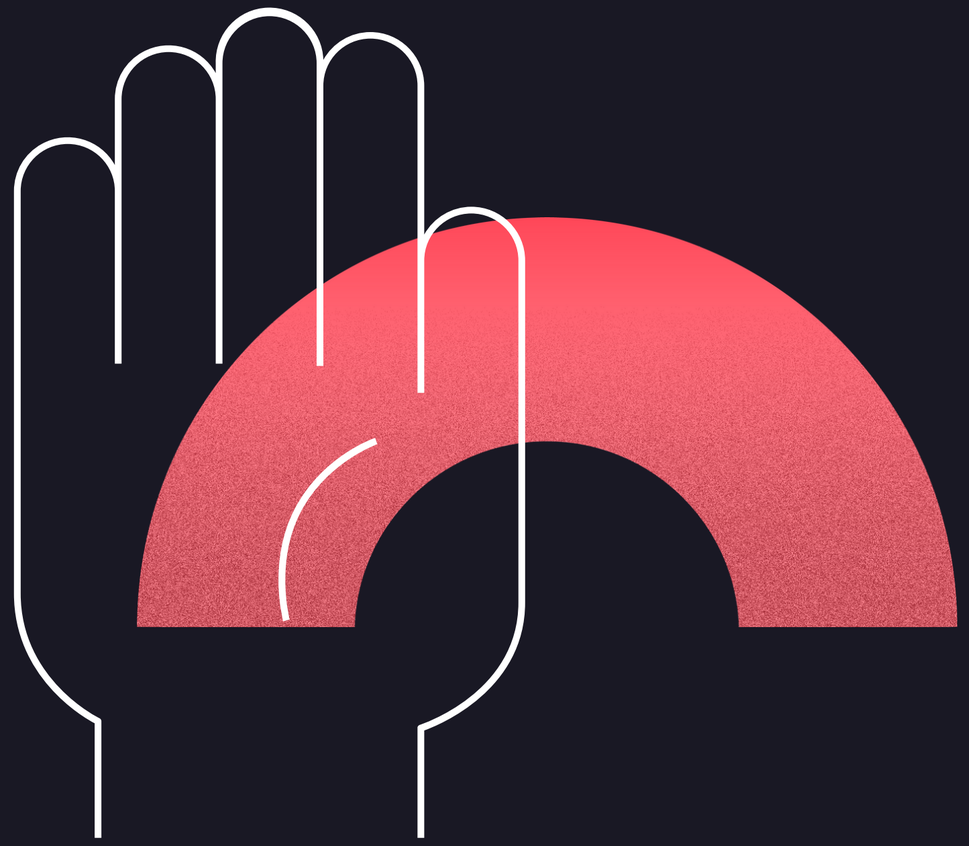
When compared to software programs and apps used for Astrochemical Research, using python packages for data processing and analysis are preferred because they are:

- Beginner friendly: easy to learn, understand, and use
- Compatible with many platforms
- Cost-effective
- Flexible and versatile (It can be easily modified to each scientist's needs)

For my research, AstroPy is the most useful tool for elucidating the chemical parameters from the molecular line emission.

# Summary and Key Takeaways





# QUESTIONS OR COMMENTS?

# Thank you!