Standards for PDRT model files & directories

Files

The fundamental storage unit for a PDR model to be used in the PDR Toolbox is a FITS file. The axes of the FITS file are hydrogen nucleus volume density *n* (AXIS1) and radiation field strength F_{uv} (AXIS2). The pixel values are predicted ratio of two spectral lines, e.g [O I] 63 μm/[CII] 158 μm. Calculation is typically done in 0.125 steps in the log, that is, the axes are logarithmic with CDELT*n* = 0.125. All files shall conform to the FITS 4.0 Standard as much as possible. Units will be in CGS: *n* shall be cm^{-3} and of F_{uv} shall be erg s^{-1} cm^{-2}. The Toolbox will convert F_{uv} to G_0 Habing, χ Draine, etc units if user requests. Data are stored in IEEE floating point;therefore use of BSCALE and BZERO is not recommended. Table 1 lists the recommended keywords for PDR model files. It is expected that model authors will provide as many of these as are relevant to code, but some may be peculiar to a given code (e.g., MASS). See the FITS Standard for more details on general keywords.

File names should be consistent across models internally within a production and externally between productions. The proposed file name format is *numerator_denominator.fits,* where the ratio data in the file are *numerator/denominator,* e.g., OI63_CII158.fits for [O I] 63 μm/[C II] 158 μm, OI145+CII158_FIR.fits for ([O I] 145 μm+[C II] 158 μm)/FIR or CO76_CO43.fits for CO(J=7-6)/CO(J=4-3). The identifier
We need to decide how to deal with varying metallicity. Currently, we also encode this into the file name, e.g., siii35feii26z1, siii35feii26z3, but only when there are multiple metallicity models available. A better choice is that different metallicities be in subdirectories and similar treatment could hold for constant extinction and constant pressure models (see below). Another alternative is to have different planes in the same hypercube be different metallicities. The actual lookup of what file contains what lines and metallicities is driven by an external table which could be modified to work for any of these schemes. We don't want to have to read in a FITS file to know what metallicities are present. The same holds if we choose to make models that vary something else like A_V.

Storage on Disk and Access

The models will be distributed as part of the PDRT python installation. In my test code they are in a *models* subdirectory within the Python module. We further break these apart by origin and version, with a symbolic link *latest* pointing to the latest version, e.g.

```
models/
    wolfire_etal/
                version1.1
                    constant_extinction
                        z=1
                        z=3
                        ...
                    constant_pressure
                        ...
                version1.0
                latest -> version1.1
    kosma-tau/
                version2019a
                version2016
                latest -> version2019a
```

How versions are numbered is up to the software authors, but they should try to follow an internally consistent convention.

Table 1: Recommended FITS Keywords for PDRT Models

Generic FITS Keywords		**Model Specific Keywords**	
KEYWORD	**Explanation or Proposed Value**	**KEYWORD**	**Explanation or Proposed Value**
SIMPLE	T	VERSION	Version of models or modeling software
BITPIX	-32 or -64	DVDOP	Turbulent Doppler Velocity (km/s)
NAXIS	2 or 3, if 3 then NAXIS3 shall be 1	ABUNDC	Carbon Abundance (C/H)
NAXISn	Dimensions of each axis	ABUNDO	Oxygen Abundance (O/H)
CDELTn	Coordinate scale for each axis	ABUNDSI	Silicon Abundance (Si/H)
CRPIXn	Reference pixel of each axis	ABUNDS	Sulfur Abundance (S/H)
CRVALn	Value at reference pixel for each axis	ABUNDFE	Iron Abundance (Fe/H)
		ABUNDMG	Magnesium Abundance (Mg/H)
CUNITn	cm-3 for n, erg s-1 cm-2 for F_{uv}	ABUNDPAH	PAH Abundance (PAH/H)
CTYPEn	log(n) for AXIS1; log(F_{uv}) for AXIS2	ABUNDDST	Dust Abundance wrt local ISM
TITLE	e.g. '[O I] 63 micron/[C II] 158 micron'	ABUNDZ	Dust and Metals wrt local ISM. Z=1 means solar.
BUNIT	‘ ‘ empty string, ratios are unitless	ABUND13C	Carbon 13 Abundance (13C/H)
ORIGIN	institution responsible for creating	ABUNDF	Fluorine Abundance (F/H)
AUTHOR	who compiled the data in the header	ABUNDN	Nitrogen Abundance (N/H)
REFERENC	Bibliographic DOI or ADS identifier	ABUNDHE	Helium Abundance (He/H)
DATAMIN	Minimum of the data	AV	Visual optical depth (mag)
DATAMAX	Maximum of the data	MASS	Clump Mass (solar mass)
DATE	ISO-8601 format *YYYY-MM-DDThh:mm:ss* **UTC**	TAUUVV	Ratio of tau_UV/tau_V
HISTORY	Processing history (multi-line)	TAUFUVV	Ratio of tau_FUV/tau_V
COMMENT	Additional comments (multi-line)	HEAT	Photoelectric Heating model, e.g. “BTF’

			for Bakes & Tielens Flat PAHs