Spextool User's Manual: iSHELL*

Michael Cushing, William Vacca, John Rayner

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*Version 5.0.3

Contents

1 Significant Changes to Manual & Software

- v5.0.3
  - **Software**: Spextool can now reduce data obtained with NIHTS on the DCT.
  - **Software**: Spextool can now reduce the Lp4 mode of iSHELL.
  - **Manual**: A clearer description of how to set the various extraction parameters (e.g. Ap Radius, PSF Radius) has been added.
  - **Manual**: Added a description of optimal extraction in order to give the user a clearer sense of what the PSF Radius parameter is.
  - **Manual**: Added a note at the end of the `xtellcor` section about the reported uncertainties not including any uncertainty in the absolute flux calibration.
- v5.0.2
  - **Software**: Improved order location to account for the slight movement of iSHELL orders during grating changes.

2 Introduction

Spextool (SPectral EXtraction TOOL) is an Interactive Data Language (IDL)-based data reduction package originally written by Michael Cushing, William Vacca, and John Rayner to reduce data obtained with SpeX on the NASA Infrared Telescope Facility (IRTF). In 2017, it was extensively modified so that it can also reduce data obtained with the new facility high-resolution infrared spectrograph iSHELL. A detailed description of the procedures incorporated into Spextool can be found in Cushing, Vacca, & Rayner (2004, PASP, 116, 362). A description of the telluric correction procedures are described vin Vacca, Cushing, & Rayner (2003, PASP, 115, 389). Note that while some of the procedures have been improved since these papers were published, the general descriptions of the steps and overall philosophy remain the same. This manual is a compilation and amplification of the ASCII help files written by William Vacca in 2000–2001 that were included in Spextool versions earlier than v4.0.

2.1 References

We require users to reference the papers listed below if they use any of the following:

- **SpeX:** Rayner et al. (2003, PASP, 115, 362)
- **iSHELL:** Rayner et al. (2016, SPIE, Vol. 9908, 990884)
- **NIHTS:** Gustafsson et al. (in prep)
- **Spextool:** Cushing, Vacca, & Rayner (2004, PASP, 116, 362)
- **Telluric Correction:** Vacca, Cushing, & Rayner (2003, PASP, 115, 389)

Note: *Although the telluric correction algorithms are contained within the Spextool package, we still ask users to reference both the Spextool and telluric correction papers.*

2.2 Overview of iSHELL

iSHELL is a 1.06–5.3 μm cross-dispersed high-resolution echelle spectrograph in which a resolving power of $R \equiv \lambda/\Delta\lambda$ =75,000 is matched to a slit width of 0.″375 (wider slits are also available). Different wavelength ranges are selected by choosing from the six cross-dispersing (XD) gratings and selecting an XD tilt position. There are 20 standard modes with fixed grating/XD tilt positions covering the 1.1–5.3 μm wavelength range. Object acquisition and guiding is done with an infrared slit-viewing camera. The position angle of the slit on the sky can be changed with an internal instrument rotator. A calibration system consisting of a quartz-tungsten lamp (for the JHK bands), an IR (blackbody) lamp (for the $LL'M$ bands), and a ThAr arc lamp, is used for flat

fielding and wavelength calibration purposes. However, accurate wavelength calibration at thermal wavelengths ($\lambda > 3.0\mu$m; the L2, L3, Lp1, Lp2, Lp3, Lp4, M1, and M2 modes) requires the use of telluric emission features due to a paucity of ThAr emission lines at these wavelengths.

Representative flat field frames for a near-infrared (J3) and thermal mode (Lp2) are shown in Figure 1. For both SpeX and iSHELL, wavelengths increase to the right and angular position on the sky increases to the top. A more detailed look at how the orders fall on the array for all of the orders can be found in the iSHELL manual.

Table 1: iSHELL Modes Reducible with Spextool

Mode	**Orders**	**Wavelength Range (μm)**	**Method**	**Slit Length (arcseconds)**
J0	457-503	1.062–1.165	ThAr lamp	5
J1	432–477	1.115–1.228	ThAr lamp	5
J2	406–442	1.197–1.303	ThAr lamp	5
J3	387–417	1.265–1.364	ThAr lamp	5
H1	311–355	1.473–1.683	ThAr lamp	5
H2	299–388	1.544–1.748	ThAr lamp	5
H3	285–319	1.633–1.832	ThAr lamp	5
K1	233–270	1.918–2.228	ThAr lamp	5
K2	218–248	2.084–2.382	ThAr lamp	5
Kgas	211–238	2.170–2.468	ThAr lamp	5
K3	203–229	2.253–2.549	ThAr lamp	5
L1	172–188	2.749–3.025	ThAr lamp	15
L2	160–175	2.951–3.246	Sky features	15
L3	150–162	3.185–3.460	Sky features	15
Lp1	142–158	3.265–3.657	Sky features	15
Lp2	132–144	3.580–3.934	Sky features	15
Lp3	126–135	3.817–4.122	Sky features	15
Lp4	125–135	3.83–4.14	Sky features	25
M1	99–114	4.52–5.24[a]	Sky features	15
M2	98–114	4.51–5.23[a]	Sky features	15

[a]Wavelength coverage is not continuous.

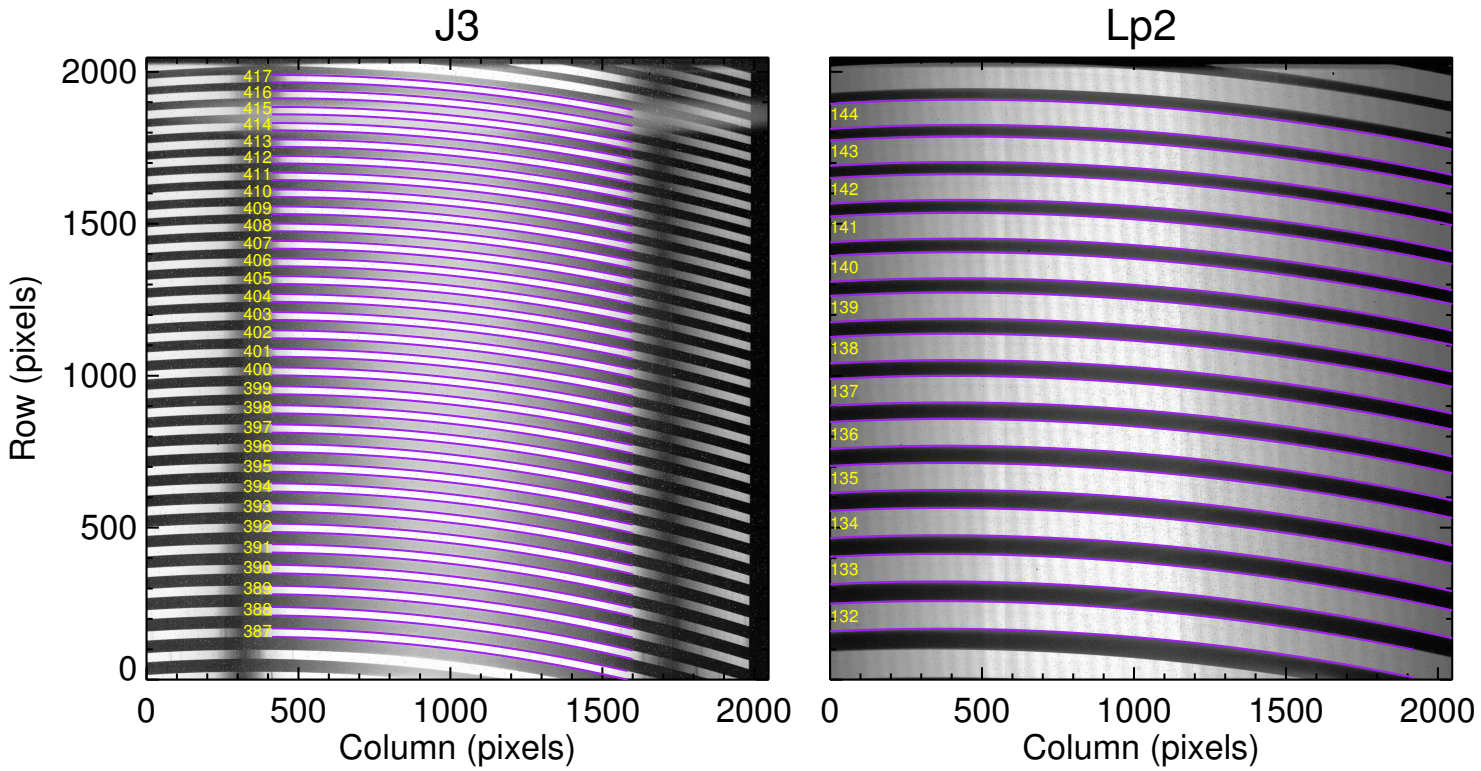

Figure 1: *Raw flat field frames for the J3 (left) and Lp2 (right) modes. The edges of the orders are shown in purple and the order numbers are labelled.*

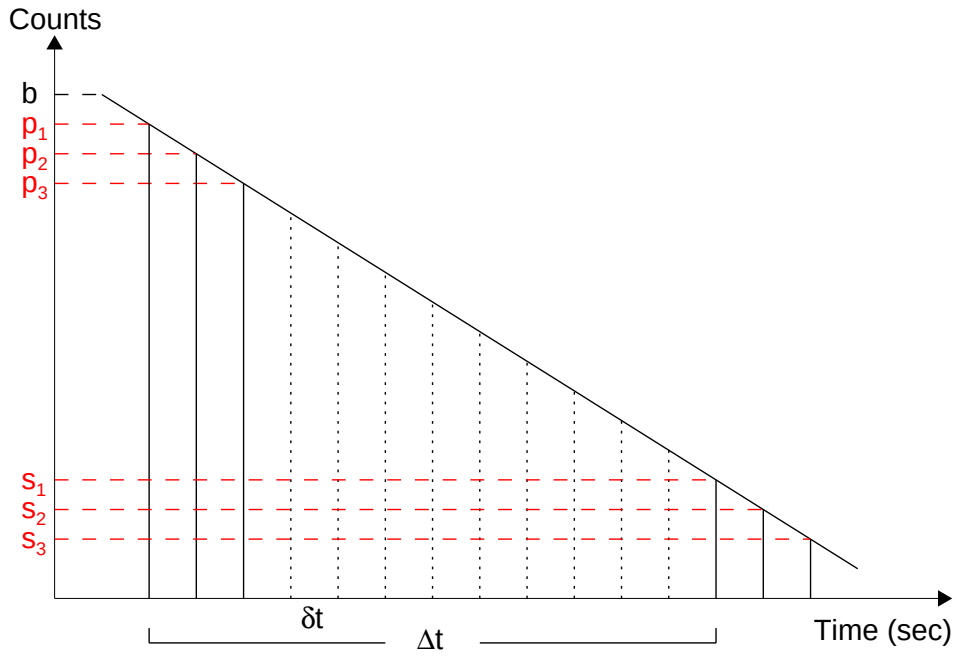

Figure 2: *Schematic of how a pixel on the upgraded SpeX and iSHELL arrays are read out.* Δt *is the exposure time,* δt *is the time between non-destructive reads,* b *is the bias level,* p_i *is the* i^{th} *pedestal read and* s_i *is the* i^{th} *signal read.*

Data obtained with iSHELL are written to disk as multi-extension FITS files (MEF) that contains three extensions. In order to understand what these data values actually represent, it is instructive to inspect Figure 2 which shows a schematic of the signal recorded by a single given pixel as a function of time on a perfectly linear detection with the number of non-destructive reads (n_r) set to 3. After the array is reset to the bias level b, the array is read continuously every δt seconds. The sum of the first n_r reads provides and estimate of the *pedestal* level while the sum of the last n_r reads provides an estimate of the signal level. The value of the (j, k)th pixel in the zeroth extension of the FITS files is given by:

$$S_{jk} = \sum_{i=1}^{n_r} p_{jk,i} - \sum_{i=1}^{n_r} s_{jk,i} \tag{1}$$

The pixel values in the first extension are given by $\sum_{i=1}^{n_r} p_{jk,i}$ while the pixel values in the second extension are given by $\sum_{i=1}^{n_r} s_{jk,i}$.

We note that in principle, each non-destructive read must be corrected for nonlinearity since each read occurs at a different location on the linearity curve. However, the linearity correction routines currently only work on the difference between the pedestal and signal reads S. However, we do use the sum of the pedestal and signal reads to identify pixels that have counts beyond the linearity curve maximum.

3 Installation and Overview

3.1 Backwards Compatibility

Version 5 of Spextool is backwards compatible with all spextool spectral FITS files generated by Spextool beginning with version 2. However, the calibration files generated by previous versions of Spextool are not compatible with version 5 and therefore if the user wishes to re-reduce data with version 5 they will need to create new calibration files.

3.2 Software Installation

1. Spextool requires IDL 7.0 or later. We furthermore assume that the user has successfully installed IDL and can use it before he or she has installed Spextool.

   Note: *Simply starting up IDL is not necessarily an indication that IDL is installed properly. A good test is to attempt to launch the GUI* `xloadct`*. If IDL crashes, then IDL has not been properly installed.*

2. If the user is upgrading from a previous version of Spextool, please delete the previous version of Spextool (or move it out of your IDL path). Download the gzipped tar file from the IRTF website `http://irtfweb.ifa.hawaii.edu/research/dr_resources/` and unpack it. For example, on a Unix-based system you would type `tar zxvf Spextool.tar.gz` on the command line. This will create a directory called Spextool, which is hereafter referred to as the `packagedirectory`, and a number of sub-directories.

3. The user must now add the package directory and ***all*** of its subdirectories to their IDL path. This can be accomplished in various ways.

   - If the user already has a single IDL directory that is searched recursively for IDL libraries, then simply place the Spextool package in this directory. If the user stores other IDL libraries in the same directory but must load them into the IDL path on a case-by-case basis (due to various dependencies), then Spextool may be loaded at any point in the IDL path because it has no path-sensitive dependencies.
   - If this is the first time the user is installing an IDL package, we recommend creating a single directory, .e.g. `userdir/IDL/`, into which the Spextool and other IDL packages can be placed (where for example `userdir` might be `Users/mcushing/Software/`). Then the user must include this directory in their IDL path. This can be done in a number of ways, including adding the path to your `.idl_startup` file, or adding it to your IDL_PATH environment variable.

For example, on a Unix-based machine using the C shell where the environment variable IDL_PATH has already been defined, edit the `.cshrc` file to include the line:

```
setenv IDL_PATH +userdir/IDL:$IDL_PATH
```

If the IDL_PATH environment variable has not been used previously in the .cshrc file, add the following to the file.

```
setenv IDL_PATH +userdir/IDL/:'<IDL_DEFAULT>'
```

In both cases, the + sign tells the system to recursively search the subdirectories in the Spextool package.

4. Spextool requires two additional IDL libraries in order to operate properly:

   - **The Astronomy User's Library**: The main page is locate at the following URL: `http://idlastro.gsfc.nasa.gov/homepage.html`. The user must install both the main library **and** the coyote routines required by the Astronomy User's Library (see below).
   - **The Markwardt IDL Library:** The main page is located at the following URL: `http://www.physics.wisc.edu/~craigm/idl/idl.html`.

   If the user has these libraries already installed on their system, then no further action is required and they can move on to the next step. For the convenience of users who will only ever use IDL to run Spextool, we have included copies of these libraries in `Spextool/other/`. Simply uncompress these libraries in their current location and they will be found if the user has properly installed Spextool. Otherwise, the user should download these packages and install them as described in step #3. The two astronomy libraries (some form of `astron` and the `coyote_astron.tar.gz`) can be downloaded from this URL: `http://idlastro.gsfc.nasa.gov/ftp/`. The Last Modified date on the two libraries should be near earlier than 2018-Jan-18 and 2016-Nov-16, respectively. The Markwardt library (some form of `cmtotal`) can be downloaded from this URL: `http://www.physics.wisc.edu/~craigm/idl/listing.html`. The Last Modified date on the library should be no earlier than 03 Jan 2017.

5. *An incorrect path is one of the most common causes of problems encountered in attempting to run Spextool for the first time.* The user can start IDL and type `mc_testspextoolpath` at the IDL prompt to test whether he/she has set the paths correctly.

6. On a Unix-based system, pop-up menu lists can be made to respond to mouse scroll wheel input by modifying a set of resources associated with the X11 windows environment. Add

the following to your `.Xdefaults` file:

```
*XmList.baseTranslations:  #augment <Btn5Down>:ListNextPage()\n
<Btn4Down>:ListPrevPage() \n

*XmScrollBar.baseTranslations:  #augment <Btn4Down>:
IncrementUpOrLeft(0) IncrementUpOrLeft(1)\n
<Btn5Down>:  IncrementDownOrRight(0) IncrementDownOrRight(1) \n
```

and either restart your X enviroment or incorporate the changes by typing

```
> xrdb -merge $HOME/.Xdefaults
```

in a terminal. Carriage returns should only be placed after the "\n" characters. You can now use the scroll wheel on your mouse to move within popup text windows. Moving the wheel in any text window (e.g., help windows) or file selection window will now perform "page up/page down". Moving the wheel while over a text scroll bar will move one line at a time.

3.3 Test Data

If the user wants to practice using Spextool with real data, they can download data for a near-infrared mode (K3) and/or a thermal mode (Lp3) from the from the iSHELL website (http://irtfweb.ifa.hawaii.edu/~ishell/). The K3 data is of Gl 406 (M6 V) and the Lp3 data is of HD 196610 (M6 III); the A0 V standards are HD 97585 (B=5.374, V=5.404, v_r=+14 km s^{-1}) and HD 196724 (B=4.80, V=4.82, v_r=−17.10 km s^{-1}), respectively. The specific files included are given in Table 2. The data should be placed in the raw directory (see §4.1). Throughout this manual, we will refer to these data when giving examples of how to reduce data.

Table 2: iSHELL K3 and Lp3 Test Data

		Gl 406		HD 196610	
Data Type	**User Prefix**	**Files**	**Exp. time (sec)**	**Files**	**Exp. time (sec)**
flat field	flat	6–10	15	84–88	3.25
arc	arc	11–12	15	80–83	4.60
dark	dark	25–29	200	...	...
object	spc	1– 5	200	61–70	1.40
A0 V Standard	spc	13–17	200	51–60	120

3.4 Overview of Reduction Steps

The Spextool package consists of multiple Graphical User Interfaces (GUIs) that allow the user to extract and calibrate their data. A list of the GUIs and their primary purpose(s) is given below; the name of each step is what the user types at the IDL command line in order to launch the appropriate GUI. All GUIs that plot data are resizable and the user can view this manual at any time by clicking the **Help** button in each GUI.

1. xspextool
    - create normalized flat field images and wavelength calibration files
    - apply non linearity correction to raw data and flat field correction
    - pair subract A and B images or subtract a master dark or sky frame from an A image
    - identify extraction apertures positions
    - trace spectra
    - background subtraction and (optimally) extract spectra
2. xcombspec
    - combine raw multi-order spectra
3. xtellcor (and xtellcor_basic and xtellcor_finish)
    - perform telluric correction and flux calibration on combined multi-order spectra
4. xcombspec (optional)
    - combine telluric-corrected (and possibly multi-order) spectra if multiple obj/std sets were obtained.
5. xmergeorders (optional)
    - merge telluric-corrected (and possibly multi-order) spectra into a single continuous spectrum
6. xcleanspec (optional)
    - clean multi-order spectra or a continuous spectrum by removing/fixing bad pixels and/or smoothing
7. spex2text (optional)
    - convert a Spextool FITS file to an ASCII file

3.5 Reading and Writing Files

Like most instruments, iSHELL write files to disk using an index-based file naming convention. The `xspextool` and `xcombspec` GUIs take advantage of this format by only requiring the user to enter the number of the filename, e.g. `5` for a file called `icm.2016B065.161118.spc.00005.a.fits`[1] or `spectra00005.fits`. There are, however, times when it is more useful to simply provide the fullname of the file. To switch between the two methods of input, the user can switch the File Read Mode from **Index** to **Filename** in the GUIs. If the **Index** mode is selected, the user must provide the prefix of the filename, e.g. `icm.2016B065.161118.spc.` or `spectra` for the files mentioned above, in the **Input Prefix** field. In the `xspextool` GUI, the user can also select the prefix from the pulldown menu. When multiple files are requested, the user can use any combination of the hyphen and comma to describe the files, i.e. `1-3,6,7,10-12` is the equivalent of `1,2,3,6,7,10,11,12`.

Finally, the user will often be required to provide an output file name. In this case, the user ***should not*** provide the `.fits` suffix as it will automatically be applied to the root filenames by Spextool.

3.6 Combination Statistics

At two points in the process of reducing iSHELL data (combining images or spectra), the user will be required to select a statistic with which to combine data. Below, we give a description of each statistic and its associated uncertainty estimate. For the robust statistics, a pixel value I_i is identified as an outlier if

$$\frac{|I_i - \text{med}(\boldsymbol{I})|}{\text{MAD}} > \text{thresh}, \tag{2}$$

where med($\boldsymbol{I}$) is the median of the intensity values, MAD is the median absolute deviation given by $1.482 \times \text{med}(|\boldsymbol{I} - \text{med}(\boldsymbol{I})|$, and thresh is the user set threshold value. The MAD is a robust estimate of the standard deviation and the constant 1.482 is defined such that if the random variable I_i follows a normal distributon, then MAD=σ if the sample size is large. The default statistic is the Robust Weighted Mean with a clipping threshold of 8 (sigma).

- **Robust Weighted Mean:** A sigma clipping algorithm is used to identify outliers. The value at each pixel is then the weighted average of the good pixels and the uncertainty is given by the propagated variance.

[1] As of mid-April 2016, the naming convention for IRTF facility instruments is: `INSTID.PROGRAMID.UTCDATE.PREFIX.IMGNO.BEAM.fits` where `INSTID` is a 3 letter string that describes the instrument and computer that wrote the file (e.g., icm=iSHELL cartman), `PROGRAMID` is a 8 digit code that describes the program (e.g., 2016B075), `UTCDATE` is the 6 digit number giving the UTC date, `PREFIX` is a user defined string, `IMGNO` is a five digit number that gives the file number, and `BEAM` is either 'a' or 'b'.

- **Robust Mean (RMS):** A sigma clipping algorithm is used to identify outliers. The value at each wavelength is the mean of the good pixels and the uncertainty is given by rms deviation of the good pixels.
- **Robust Mean (Std Error):** A sigma clipping algorithm is used to identify outliers. The value at each wavelength is the mean of the good pixels and the uncertainty is given by the standard error on the good pixels ($s/\sqrt{n}$).
- **Weighted Mean:** A weighted mean and uncertainty of all the pixels are given at each wavelength.
- **Mean (RMS):** The value at each pixel is given by the mean and the uncertainty is given by the RMS deviation of the pixels.
- **Mean (Std Error):** The value at each wavelength is the mean of the pixels and the uncertainty is given by the standard error on the pixels ($s/\sqrt{n}$).
- **Median (MAD):** The value at each pixel is given by the median and the uncertainty is given by the median absolute deviation.
- **Median (Std Error):** The value at each pixel is given by the median and the uncertainty is given by the standard error around the median (($\mathrm{MAD}/\sqrt{n}$).) of the pixels.
- **Sum:** The value at each pixel is given by the sum.

Note: *The uncertainty spectrum typically looks very different if a (robust) weighted mean is chosen rather than a statistic that uses the RMS as a measure of the uncertainty. The reason is that the RMS measures the scatter between data and thus is sensitive to small changes in said data. This is particularly important when it comes to combining spectra as the spectra suffer from heterochromatic slit losses (see §5.3.4 for a more indepth discussion of this issue). Although the default statistic is a robust weighted mean, the user should be aware of these issues and choose their statistic appropriately.*

3.7 Bit Mask

Spextool includes a bit mask that give useful information for each output pixel. Currently Spextool uses only the first three bits and sets them as described in Table 3.

Table 3: Bit-mask Flag Values

bit	value	color	Description
0	1	red	one or some of the values that went into this pixel were greater than the linearity correction maximum.
1	2	blue	one or some of the values that went into this pixel were

Table 3: Bit-mask Flag Values

bit	value	color	Description
			identified as bad by Spextool and replaced using a model of the spatial profile.
2	4	cyan	one or some of the values that went into this pixel were fixed in the xcleanspec routine.
3	8	yellow	optimal extraction failed on this pixel.

Note that if optimal extraction is used which is the default case, then bad pixels are ignored and thus the first bit is rarely set.

3.8 Spextool FITS Files and Conversion to ASCII

Spextool FITS files contain an array of size [`nwaves`, `4`, `orders`×`naps`] where `nwaves` is the number of wavelengths, `orders` is the number of orders extracted, and `naps` is the number of apertures that were extracted (Note that `naps` is the number of apertures in a *single order* and not the total number of apertures). The ith image (array[*,*,i]) contains the data for a single extraction aperture within an order such that,

$$\begin{aligned} \text{wavelength} &= \text{array[*,0,i]}, \\ \text{flux} &= \text{array[*,1,i]}, \\ \text{uncertainty} &= \text{array[*,2,i]}, \\ \text{flag} &= \text{array[*,3,i]} \ . \end{aligned}$$

The zeroth image (array[*,*,0]) contains the data for the aperture in the order closest to the bottom of the detector that is closest to the bottom of the slit (i.e. also closest to the bottom of the detector). Moving up the detector, the FITS array is filled in with subsequent extraction apertures, array[*,*,1], array[*,*,2], array[*,*,3], etc. If no orders have been deselected in the extraction process, the contents of the ith aperture in order j can be found as follows:

$$\begin{aligned} \text{wavelength} &= \text{array[*, 0, \{j}-\text{min(orders)}\}\times\text{naps + (i-1)]} \\ \text{flux} &= \text{array[*, 1, \{j}-\text{min(orders)}\}\times\text{naps + (i-1)]} \\ \text{uncertainty} &= \text{array[*, 2, \{j}-\text{min(orders)}\}\times\text{naps + (i-1)]} \\ \text{flag} &= \text{array[*, 3, \{j}-\text{min(orders)}\}\times\text{naps + (i-1)]} \end{aligned}$$

For example, the Lp3 mode of iSHELL covers orders 126–135. If two aperture positions were extracted in each order, then the wavelengths for aperture 1 in order 126 are located in array[*,0,0], the fluxes in array[*,1,0], the uncertainties in array[*,2,0], and the flags in array[*,3,0]. The wavelengths for aperture 1 in order 127 are located in array[*,0,2], the fluxes in array[*,1,2], the uncertainties in array[*,2,2], and the flags in array[*,3,2].

Various FITS keywords are either transferred (and possibly renamed) from the original FITS images or generated by Spextool. Table 4 lists the FITS keywords that Spextool adds to output files.

Table 4: Spextool FITS Keywords

Keyword	Example	Program	Description
INSTR	'iSHELL '	xspextool	Instrument
MODE	'Lp3 '	xspextool	Instrument mode
FILENAME	'spectra00001.fits'	xspextool	File name
DATE	'2016-09-25'	xspextool	Observation date in UTC
TIME	'06:23:47.236007'	xspextool	Observation time in UTC
MJD	'57656.2665189351'	xspextool	Modified Julian date OBSDATE+TIME_OBS
NCOADDS	5	xspextool	Number of coadds
ITIME	119.544500000	xspextool	Integration time (sec)
IMGITIME	119.544500000	xspextool	Image integration time, NCOADDSxITIME (sec)
RA	'20:38:31.84'	xspextool	Right Ascension, FK5 J2000
DEC	'+21:11:55.1'	xspextool	Declination, FK5 J2000
PA	180.000000000	xspextool	Position angle E of N (deg)
HA	'-00:19:21.98'	xspextool	Hour angle (hours)
AM	1.00300	xspextool	Airmass
NIMCOMB	10	xspextool	Number of images combined
IMCOMBAB	1	xspextool	Pair subtraction?: 1=yes, 0=no
CREPROG	xspextool	xspextool	Creation program
VERSION	'5.0.2 '	xspextool	Spextool version
AMPCOR	1	xspextool	Amplifier correction (bit flag)
LINCOR	1	xspextool	Linearity correction (bit flag)
FLATED	1	xspextool	Flat fielded (bit flag)
FIXBDPX	1	xspextool	Fix bad pixels (bit flag)
OPTEXT	1	xspextool	Optimal Extraction (bit flag)
AIMAGE	'icm.2016B999.160924. spc.00051.a.fits'	xspextool	A image
LINCRMAX	30000	xspextool	Linearity correction maximum (DN)
SKYORDRK	'icm.2016B999.160924. spc.00052.b.fits'	xspextool	Sky or dark image
FLAT	'flat84-88.fits'	xspextool	Flat field image
WAVECAL	'wavecal51-60.fits'	xspextool	Wavecal file
WAVETYPE	'Vacuum'	xspextool	Wavelength type

Table 4: Spextool FITS Keywords

Keyword	Example	Program	Description
WCTYPE	'2DXD'	xspextool	Wavelength calibration type
RECTMETH	'interpolation'	xspextool	Rectification method
NAPS	1	xspextool	Number of apertures
NORDERS	10	xspextool	Number of orders
ORDERS	'126,127,128,129,130, 131,132,133,134,135'	xspextool	Order numbers
PLTSCALE	0.125000	xspextool	Plate scale (arcsec pixel-1)
SLTH_PIX	80	xspextool	Nominal slit height (pixels)
SLTH_ARC	15	xspextool	Slit height (arcseconds)
SLTW_PIX	3	xspextool	Slit width (pixels)
SLTW_ARC	0.375000	xspextool	Slit width (arcseconds)
RP	70000	xspextool	Nominal resolving power
XROR*	'8,2038 '	xspextool	Extraction range for order 126
APOSO*	'11.3 '	xspextool	Aperture positions (arcseconds) for order 126
PSFRAD	1.00000	xspextool	PSF radius (arcseconds)
APRADII	1.00000	xspextool	Aperture radii (arcseconds)
BGSTART	1.10000	xspextool	Background start radius (arcseconds)
BGWIDTH	2	xspextool	Background width (arcseconds)
BGR	'0-2,13-15'	xspextool	Background regions (arcseconds)
BGORDER	0	xspextool	Background polynomial fit degree
XUNITS	'um '	xspextool	Units of the X axis
YUNITS	'DN / s '	xspextool	Units of the Y axis
XTITLE	'!7k!5 (!7l!5m)'	xspextool	IDL X title
YTITLE	'f (!5DN s!u-1!N)'	xspextool	IDL Y title
DISPO*	1.66570000000E-05	xspextool	Dispersion (um pixel-1) for order 126
SRT_DATE	'2016-09-25'	xcombspec	Start observation date in UTC
AVE_DATE	'2016-09-25'	xcombspec	Average observation date in UTC
END_DATE	'2016-09-25'	xcombspec	End observation date in UTC
SRT_TIME	'06:23:47.236007'	xcombspec	Start observation time in UTC
AVE_TIME	'06:34:17.371632'	xcombspec	Average observation time in UTC
END_TIME	'06:44:47.505828'	xcombspec	End observation time in UTC
SRT_MJD	'57656.2665189351'	xcombspec	Start Modified Julian date
AVE_MJD	'57656.2738121717'	xcombspec	Average Modified Julian date
END_MJD	'57656.2811053917'	xcombspec	End Modified Julian date
TOTITIME	1195.44500000	xcombspec	Total integration time (sec)
SRT_HA	'-00:19:21.98'	xcombspec	Start hour angle (hours)
AVE_HA	'-00:08:50.02'	xcombspec	Average hour angle (hours)
END_HA	'+00:01:41.93'	xcombspec	End hour angle (hours)
SRT_AM	1.00300000000	xcombspec	Start airmass
AVE_AM	1.00130000000	xcombspec	Average airmass
END_AM	1.00000000000	xcombspec	End airmass

Table 4: Spextool FITS Keywords

Keyword	Example	Program	Description
NSPCOMB	10	xcombspec	Number of spectra files combined
NAPCOMB	0	xcombspec	Number of apertures combined
A0VSTD	'HD 196724'	xtellcor	Telluric Correction A0 V Standard
A0VBMAG	4.80000	xtellcor	B-band magnitude
A0VVMAG	4.82000	xtellcor	V-band magnitude
DELTAAM	-0.000400000	xtellcor	Average of (std-obj) airmass
TELMETH	'IP '	xtellcor	Telluric correction method
VEGADV	0.0723358	xtellcor	Vega velocity shift (km s-1)
TELFILE	'HD196610_telspec.fits'	xtellcor	The telluric correction file
DATES	'2016-11-14,2016-11-14'	xtellcor	Dates of observations in UTC
AVE_AMS	'1.1452000,1.2058000'	xtellcor	Average airmasses
SNRCUT	10	xcleanspec	Xcleanspec S/N cut

The user may convert any FITS spectral files generated by Spextool into ASCII files that can be read by other programs in two ways:

- Start IDL in the directory with the FITS files and at the command line run the program spex2text and follow the instructions, e.g.:

  ```
  IDL> spex2text
  ```

  The contents of the FITS file (including the FITS header) will be written to an ASCII file.

- Load the the spectra(um) in `xvspec` and select **Write ASCII File** from the **File** menu. The user should then enter the output file name and hit return.

3.9 Plot Window Navigation

All the GUIs in Spextool that display spectra in some fashion allow the user to navigate in the plot window using a combination of keyboard commands and mouse clicks, manually changing the plot range by typing in the desired plot limits, or using a scroll bar or the left/right arrow keys to change the abscisa range. The keyboard commands are as follows:

- a - sets the **A**bsolute plot range to the current x and y range

  This is very useful if the spectrum has a bad pixel as this x and y range is what will be used when the user types 'w' rather than the true min/max of the spectrum.

- c - **C**lear any current keyboard command

- i - to zoom **I**n in whatever zoom mode the cursor is currently in. For example, if the plot window is currently in the 'x' zoom mode, typing 'i' will zoom in

- o - to zoom **O**ut in whatever zoom mode the cursor is currently in
- w - to plot the **W**hole spectrum, i.e. the full range of the spectrum. By default the plot ranges are set to the minima and maxmima of the spectrum. However if the user has set the absolute range by using the 'a' cursor, then these values are used instead.
- x - enters the **X** zoom mode

  Press and release left mouse button at lower x value and then again at upper x value or type 'i' or 'o'
- y - enters the **Y** zoom mode

  Press and release left mouse button at lower y value and then again at upper y value or type 'i' or 'o'
- z - enters the **Z**oom mode

  Press and release the left mouse button in one corner of the zoom box and then move the cursor to the other corner and press and release the left mouse button or press 'i' or 'o'

Please see the following section (§3.10.2) to learn how to practice with these commands.

3.10 Additional GUIs: ximgtool, xvspec, xzoomplot

In addition to the GUIs described above, there are three additional GUIs that the user can interact with, `ximgtool`, `xvspec`, `xzoomplot`. All three GUIs are resizable.

3.10.1 ximgtool

`ximgtool` is a multi-buffer, resizable, array/FITS viewer which in appearance is based on the older ximtool display tool. Although `ximgtool` can be used as a stand-alone routine and has a rich set of features (see the Help menu), Spextool users typically only need to pan around the image and browse through the buffers. To pan around the image the user can use a mouse in the following way:

- Left mouse click - center at pixel and zoom in by a factor of two
- Middle mouse click - center at pixel
- Right mouse click - center at pixel and zoom out by a factor of two

The user can also use keyboard commands to pan around the image. Simply type the following letters in the window to active the command.

- i- zoom **I**n by a factor of two
- o- zoom **O**n by a factor of two
- t- zoom **T**o fit the display window

- left arrow - move the cursor one pixel to the left
- right arrow - move the cursor one pixel to the right
- up arrow - move the cursor one pixel up
- down arrow - move the cursor one pixel down

Finally, the user can browse through the buffers using the keyboard commands:

- f- to move (**F**orward) to the next buffer
- b- to move (**B**ackwards) to the previous buffer

3.10.2 xvspec & xzoomplot

`xvspec` is a general-purpose, resizable, spectrum viewer specifically designed to work with the spectral FITS files produced by Spextool. It can be launched at any time by typing `xvspec` at the IDL command line. The most used features are shown in a menu bar below the top menu. The user can learn about the full list of keyboard commands via the **Help** menu, but the primary way a Spextool user will interact with it is to view the **Flux**, **Uncertainty**, and **S/N** spectra. The atmospheric transmission can also be overplotted by clicking the **Atmosphere** button. By default, `xvspec` will display the bit-mask flags (see §3.7) stored in the Spextool FITS files. These can be toggled on and off using the **Flags** pulldown menu.

`xvspec` can display multi-order spectra in two ways: 1) the spectrum of each order is plotted separately one on top of each other (i.e. "**Ladder**"), and 2) the spectra are plotted on a single plot covering the entire wavelength range (i.e. "**Continuous**"). If the Continuous mode is used, the user has access to the keyboard command described in §3.9. If Ladder mode is used, the user can view the various orders by using either the vertical scroll bar or the up and down arrow keys. In addition, the user can click on a spectrum in the Ladder mode and `xvspec` will launch the `xzoomplot` which allows the user to exam a single spectrum. Three additional useful features in `xvspec` are the ability to plot the hydrogen lines on the spectra (**Plot** $>$ **Plot Hydrogen Lines**), clip the spectrum based on the S/N to make viewing the spectrum easier (**Tools** $>$ **S/N Cut**), and the ability to plot the multi-order spectra using three colors (**3 color** in the menu bar or **Plot** $>$ **3-Color Alternate Color**.

To practice both using `xvspec` and the keyboard commands list described in §3.9, simply launch `xvspec`, i.e.,

```
IDL> xvspec
```

4 Spectral Extraction: xspextool

The `xspextool` GUI allows the user to flat field, extract, and wavelength calibrate spectra from raw data.

4.1 Starting up and Loading the Paths

8. Start IDL and bring up the main Spextool GUI by typing `xspextool` at the IDL prompt, e.g.

   ```
   IDL> xspextool
   ```

   Once the GUI has appeared, please check the title bar to make sure you are running the correction version (v5.0.3) and that the correct instrument is loaded.

9. Click on the **Paths** button in the middle of the Spextool GUI. This will bring up the Paths Panel. Spextool will automatically load the paths last entered by the user. If this is the first time that Spextool is being run, or if the user wants to reduce data in a directory that is different from the last time Spextool was used, the user will have to change the paths.

   Spextool *requires* that the raw data, processed data needed for calibrations (e.g., normalized flats and wavelength calibration files), and completely reduced data be kept in separate directories. Typically these directories will be called `raw` (for raw data), `cal` (for processed **cal**ibration files) and `proc` (for **proc**essed data files). Type or (click) the paths for these three subdirectories in the fields listed in the Paths panel. Spextool will remember these directories, so that next time you start Spextool these fields will be loaded automatically.

4.2 Flat Field, Wavelength Calibration, Dark, and Sky Frames

Note: *Because of flexure and the variable nature of atmospheric absorption, it is recommended that each set of object and standard star images of a given object be reduced with its own set of flats, arcs, and telluric standards.*

4.2.1 Flat Field Frames

The creation of a flat field frame is required to not only remove pixel-to-pixel quantum efficiency variations in the array, but also to identify the locations of the orders on the array.

10. Click the **Cals** button in the middle of the GUI to bring up a panel that allows the user to create both normalized flat fields and wavelength calibration files.

11. To create a flat field, provide the prefix of the raw flat field frames in the File Read Mode panel (K3:`icm.2017A999.170525.flat.`, Lp3:`icm.2016B999.160924.flat.`) and then type the frames numbers of raw flat field frames into the **Raw Flat Images** field in Box #1 (K3:`6-10`, Lp3:`84-88`).

12. Type the name of the flat field file to be written to disk (without the .fits suffix) in the **Flat Output Name** field (K3:`flat6-10`, Lp3:`flat84-88`). and then click **Generate Flat Field**. Spextool will then perform a number of steps including loading the frames into memory, scaling the average flux

level in each order to a common value, median combining the scaled images, displaying the result in `ximgtool`, identifying the edges of the orders, and then normalizing each order by fitting a 2D model to the data and then dividing the model into the data. The resulting normalized flat field frame will be written as a FITS file to the `cal/` directory.

The FITS file is actually a Multi-Extension FITS (MEF) files that can be viewed with ximgtool or any FITS viewer, e.g. DS9. It has four extensions: the zeroth extension contains the FITS header and all of the ancillary information necessary for extraction, the first extension contains the normalized flat field, the second extension contains the variance image, and the third extension contains a bit-mask image that flags pixels identified as bad and pixels that were generated from saturated pixels.

4.2.2 Wavelength Calibration Frames

The wavelength calibration files (so-called "wavecal" files) are not technically required for extraction, but are required if the user wishes to have wavelength calibrated data (duh). Wavelength calibration is accomplished in any of the JHK modes and the $L1$ mode using a ThAr arc lamp. However at longer wavelengths, there are not enough ThAr emission lines available and Spextool uses telluric emission features in the science or sky frames for wavelength calibration. A line list and line atlas for each mode is provided in the `Spextool/instruments/ishell/data/` directory.

The image of the slit is not aligned with the columns of the detector (due to the non-zero γ angle of the echelle grating illumination that is used for best efficiency) which means that emissions lines appear tilted and/or curved greatly complicating the wavelength calibration of iSHELL data. Spextool generates a wavelength solution in two steps. Briefly[2], Spextool first creates a so-called 1DXD wavelength solution (because we determine a 1D wavelength solution for all orders at once) which assigns a wavelength to the mid-point of the slit on a column-by-column basis for each order. Next Spextool traces the positions of the emissions lines on the array to make how the distortion of the slit varies across the array. The final result of the 2DXD wavelength calibration process is an array of (x,y) indices that describe lines of constant wavelength and angle on the sky within each order. These indices can then be used to rectify an order so that lines of constant wavelength and sky angle are aligned with the columns and rows of an array.

13. If the user has not already done so, click the **Cals** button in the middle of the GUI to bring up the panel that allows the user to create both normalized flat field and wavecal files.

14. Select the observing mode from the **Mode** pulldown menu in box #2. If the user is creating a wavecal file for any of the J, H, or K modes or the $L1$ mode, provide the prefix of the arc frames taken by the iSHELL calibration macros in the File Read Mode panel (K3:`icm.2017A999.170525.arc.`) and then type the numbers of the arc frames taken by the iSHELL calibration macros into the **Arc Images** field (K3:`11-12`).

    If the user is creating a wavecal file for the any of other L modes, or any of the Lp or M modes, then the user should select the prefix of science frames that exhibit strong telluric emission features in the File Read Mode panel Lp3:`icm.2016B999.160924.spc.`). Unlike the near-infrared modes in which two arc frames (a "arc on" and "arc off" frame) are used, multiple exposures can be used

[2] A more detailed explanation of the process will be included in the manual in a future release.

for the wavelength calibration at thermal wavelengths. If the user obtained sky frames, then select **A** and type the numbers of the sky frames into **Sky Images** field. If the user was observing in the A-B mode, then selected **A-B** and type the numbers of the science frames into the **Sky Images** field (Lp3:`51-60`). In the latter case, Spextool will create sky emission image according to the equation,

$$\text{sky} = (A + B) - |(A - B)|, \tag{3}$$

which effectively removes the signal from the source.

15. If the user is creating a wavecal file directly after creating a normalized flat field then the name of said flat field will have automatically been placed in the **Full Flat Name** field. Otherwise, the user should type (or click) the full name of the normalized flat field frame in the **Full Flat Name**.

16. Finally, type the output file name of the wavecal file in the **Wavecal Output Name** field (K3:`wavecal11-12`, Lp3:`wavecal51-60`) and click the **Generate Wavelength Calibration** button. Spextool will first construct the 1DXD wavelength solution by extracting an emission spectrum and identifying lines contained in the line list stored on disk. To do so, Spextool must know where to look for the lines and so we store a fully wavelength calibrated spectrum on disk and then cross correlate the disk spectrum of one order against the extracted spectrum of the same order. The results will be shown to the user in the `XCorrelate Spectra` GUI for inspection; the wavelength range over which the cross correlation was performed is shown as two dashed vertical cyan lines. Typical offsets are of order <3 pixels and so if the offset is much larger than this (due typically to a hot pixel), then the user will have to select a different wavelength range over which to perform the cross correlation. To do so, simply type 's' for **S**elect in the plot window, click the left-most mouse button on the left-most extent of the new wavelength range and then click on the right-most extend of the new wavelength range and the program will recompute the offset. Once the user is happy with the offset, click **Accept** at the bottom of the GUI. The `XCorrelate Spectra` GUI is fully resizable and the user has access to all the zoom keyboard commands available in the `xzoomplot` GUI (see §3.9).

Spextool will now finish the process of generating the wavecal file. This includes tracing the emission lines (which will be shown in `ximgtool` in real time), determining their shapes (as encapsulated in the polynomial coefficients derived by fitting their positions), mapping how their shapes (i.e. coefficients) change with position on the array, and then finally deriving rectification indices. The resulting wavecal file will be written to disk as a multi-extension FITS file in the `cal/` directory. The zeroth extension contains the FITS header, the first extension contains an image where each pixel within an order is set to its wavelength, the second extension contains an image where each pixel within an order is set to its angle on the sky, and the remaining extensions contain the rectification indices, wavelengths, and angles on the sky for each order.

During the creation of the wavecal file, Spextool with generate two Quality Assurance (QA) plots in the `cal/` directory. The first QA file, which has the suffix `_1DXDResiduals.pdf`[3], shows the residuals to the 1DXD fit. An example for the K3 test data is shown in Figure 3. As described in the Spextool paper, we derive a 1D solution for all of the orders at once by fitting the wavelengths of the lines as a function of both x and order number o, $\lambda = f(x, o)$. The plot shows the marginalized residuals of this 2D fit as a

[3]IDL can only make postscript files and so Spextool attempts to convert the postscript files to pdf files using ghostscript (gs). If Spextool cannot find ghostscript, the files will remain as postcript files.

function of column number and order number. Points identified as outliers in the fit are identified as squares. Non-random residuals or many bad data points suggest that something went wrong with the fit.

Note: *Currently the residuals are not random in the near-infrared and L1 modes of iSHELL. Please see the §A for a detailed description of this issue.*

The second QA file, which has the suffix `_2DCoeffFit.pdf`, is a multi-page file showing various plots relating to the mapping of the line tilt/curvature as a function of position on the array. An example of the first page for the K3 mode is shown in Figure 4 and shows the positions of all the lines relative to their center (so-called "zero lines" or "zlines" for short). Lines that show an obvious deviation from the cloud of lines may indicate a problem with the wavelength calibration. The second page is shown in Figure 5 and shows the slopes of the zeroed lines ($c_{\rm zline}$) as a function of position on the array and the marginal distributions of these points. The top two panels of Figure 6 show the 2D polynomial model of the data; data points that were identified as bad during the fit are marked using an open square. The lower left panel shows the data points for comparison and the lower right panel is an *attempt* to create a 2D surface via interpolation to compare with the upper right panel. Finally, Figure 7 shows the percent fraction residuals between the data and the model. The marginalized residuals should be close to random. If the mode being reduced has a $15''$ or $25''$ slit (e.g. the test Lp3 data), then there will be four additional pages in the QA plot dealing with the $c2_{\rm zline}$ coefficient.

4.2.3 Dark Frames

The near-infrared modes of iSHELL have a slit length of only $5''$ and so the standard infrared method of moving the object between two positions on the slit to facilitate the subtraction of the bias, dark current, and sky background cannot be employed. Therefore a dark frame (which includes any bias) must be subtracted from each science frame before extraction. Typically a series of dark frames are taken and so the user should combine them into a master dark frame.

17. Click on the **Combine Images** button in the middle of the GUI. This panel is used to combine a variety of images and so the **Scale Orders** and **Column BG Sub** options are not required to create a master dark and thus can be ignored.

18. Select the prefix of the dark frames in the File Read Mode panel (K3:`icm.2017A999.170525.dark.`), select the **A** beam switching mode, type the numbers of the dark frames in the **Images** field (K3:`25-29`), and select the statistic that will be used to combine the frames (see §3.6 for a description of the various statistics).

19. Select **cal/** for the directory in which to write the master dark and then type a file name (without the suffix .fits) in the **Output Name** field (K3:`dark25-29`).

20. Click **Combine Images** and the dark frames will be loaded into memory, combined using the statistic chosen by the user, and written to disk in the `cal/` directory.

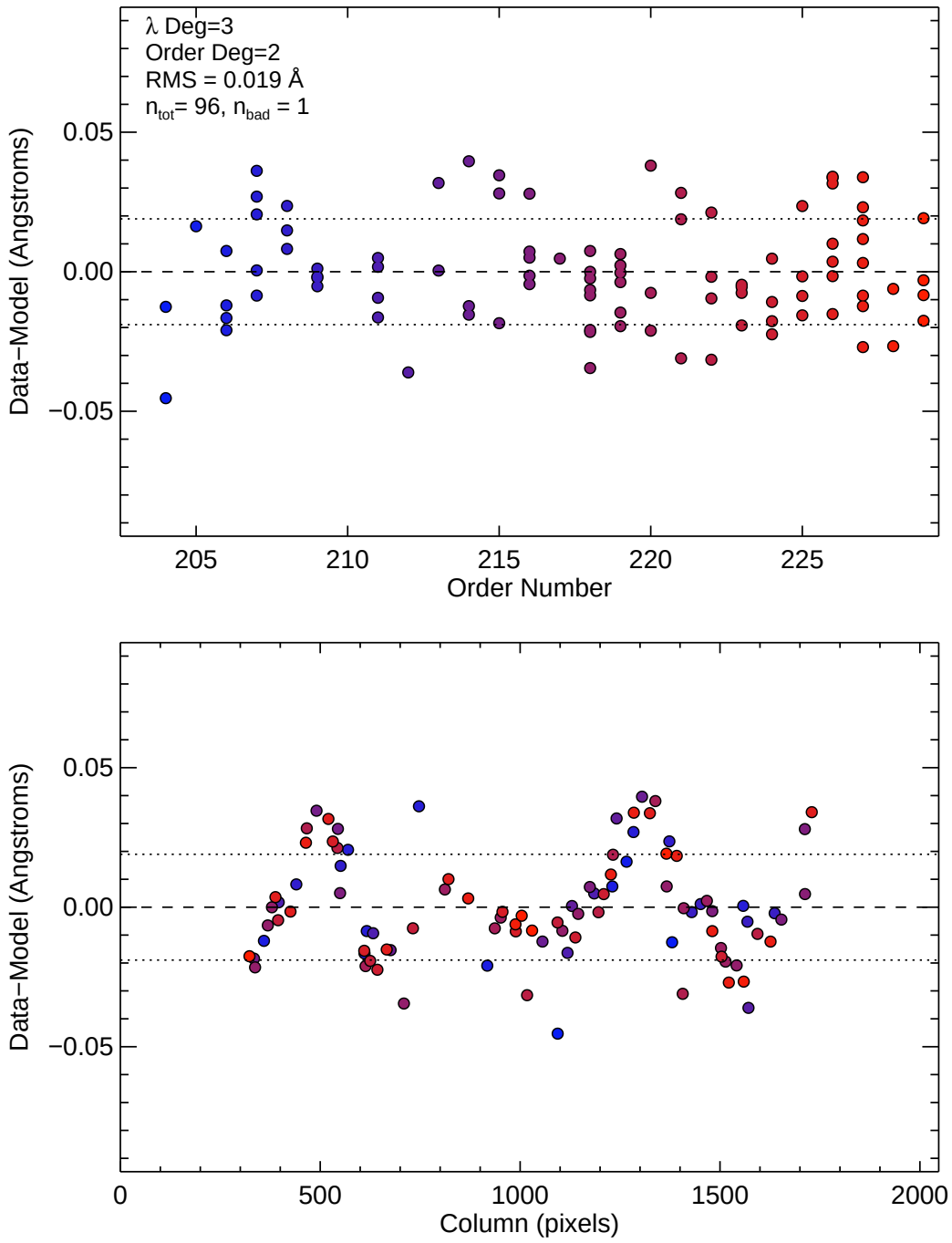

Figure 3: *QA plot for the 1DXD wavelength calibration of the K3 mode. The two panels show the marginalized residuals from the 1DXD wavelength calibration fit* $\lambda = f(x, o)$*, where* x *is the column number of the line and* o *is the order number of the line. Points identified as outliers in the fit are identified using squares, although none are shown in this figure because the one bad point identified in the fit is located outside the plot range.*

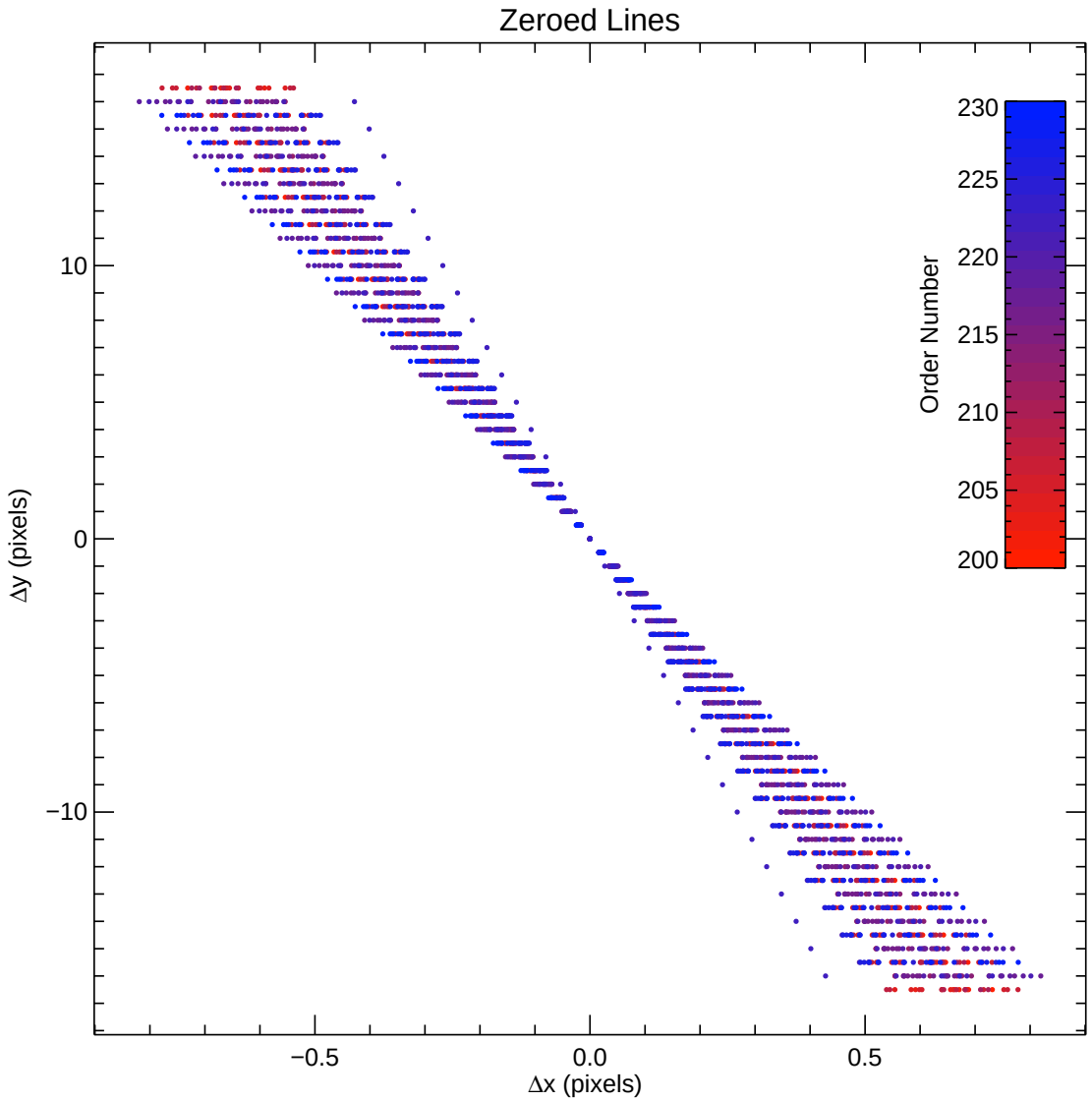

Figure 4: *Page 1 of the* `_2DCoeffFit.pdf` *QA file.*

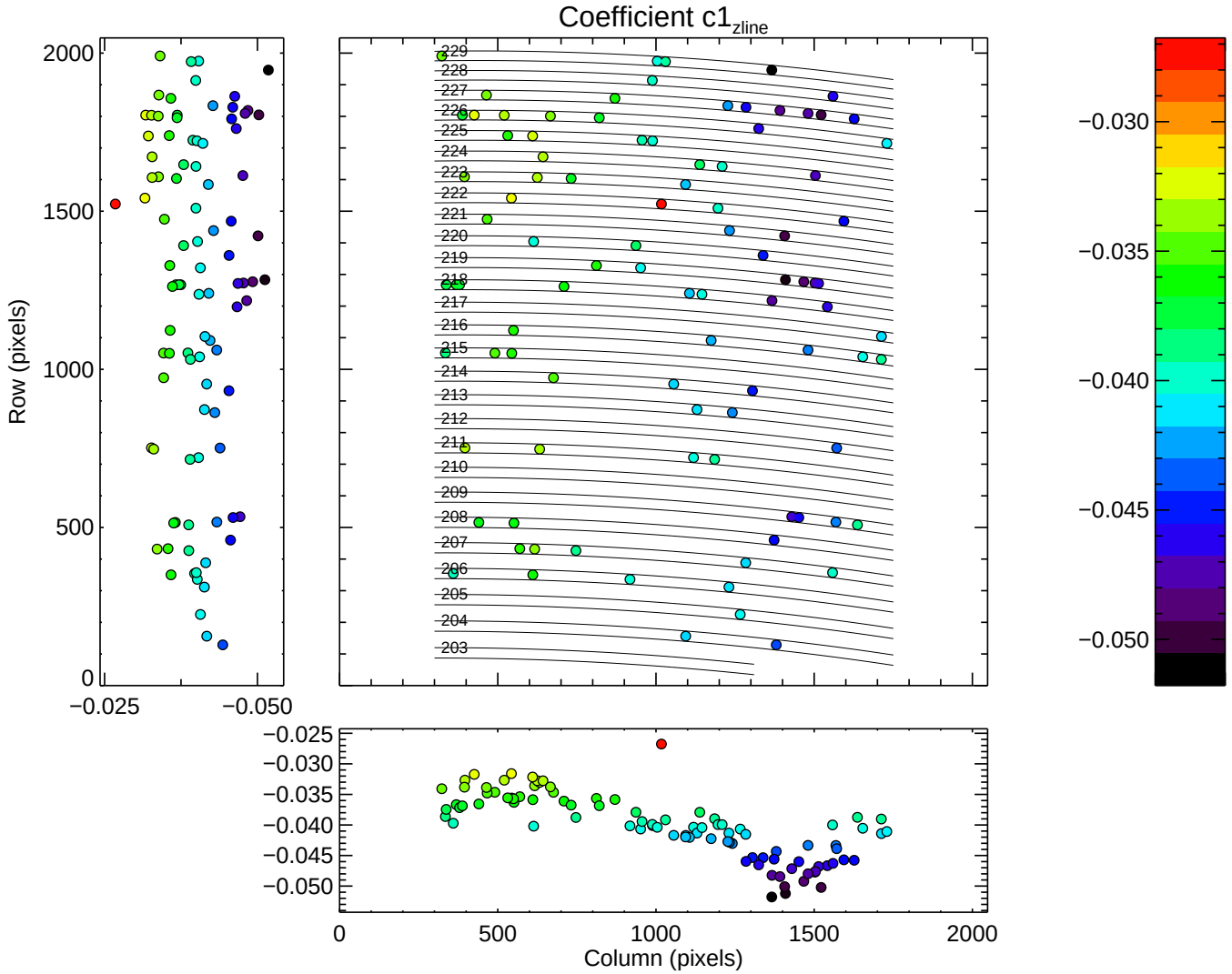

Figure 5: *Page 2 of the* `_2DCoeffFit.pdf` *QA file.*

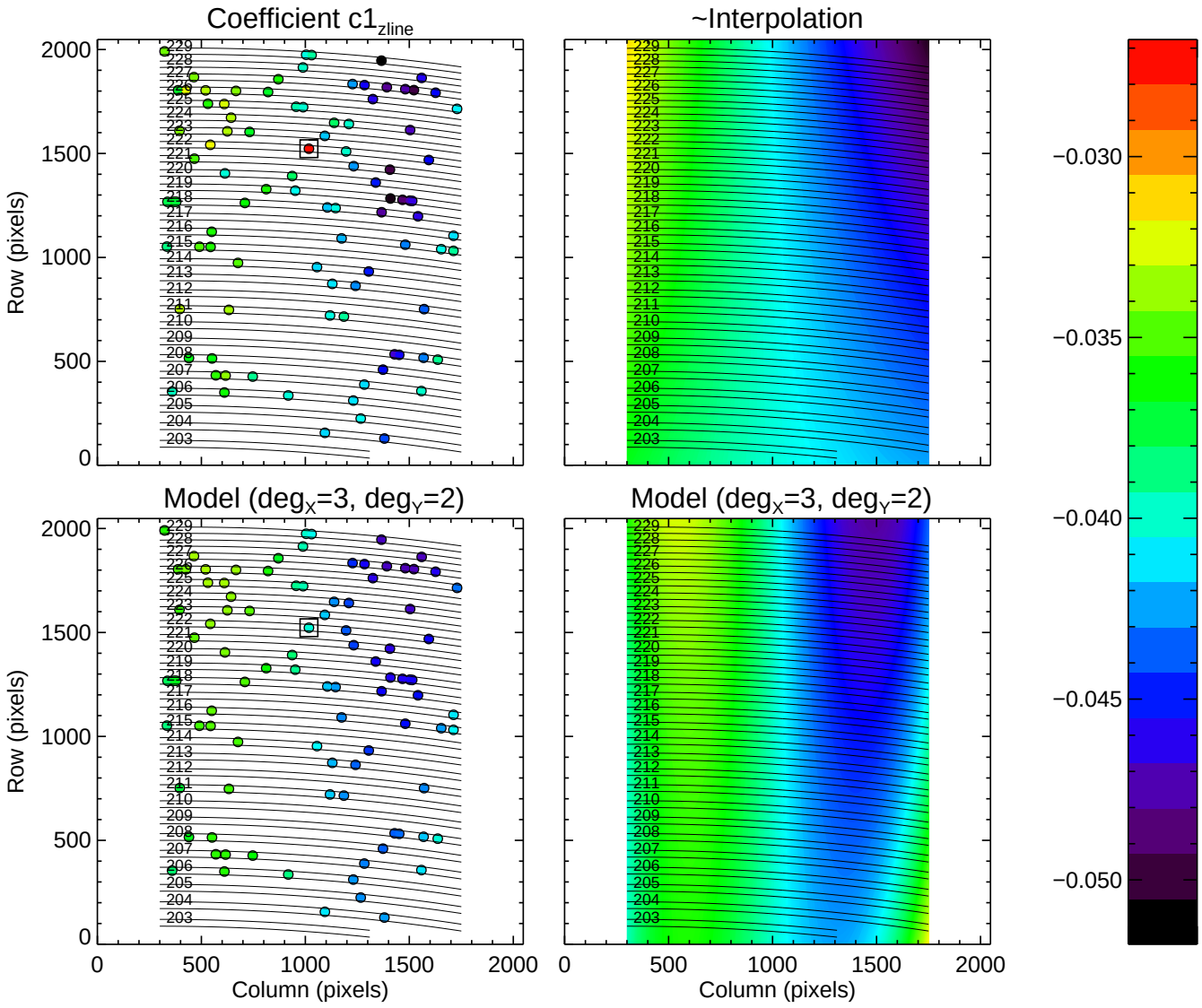

Figure 6: *Page 3 of the* `_2DCoeffFit.pdf` *QA file*

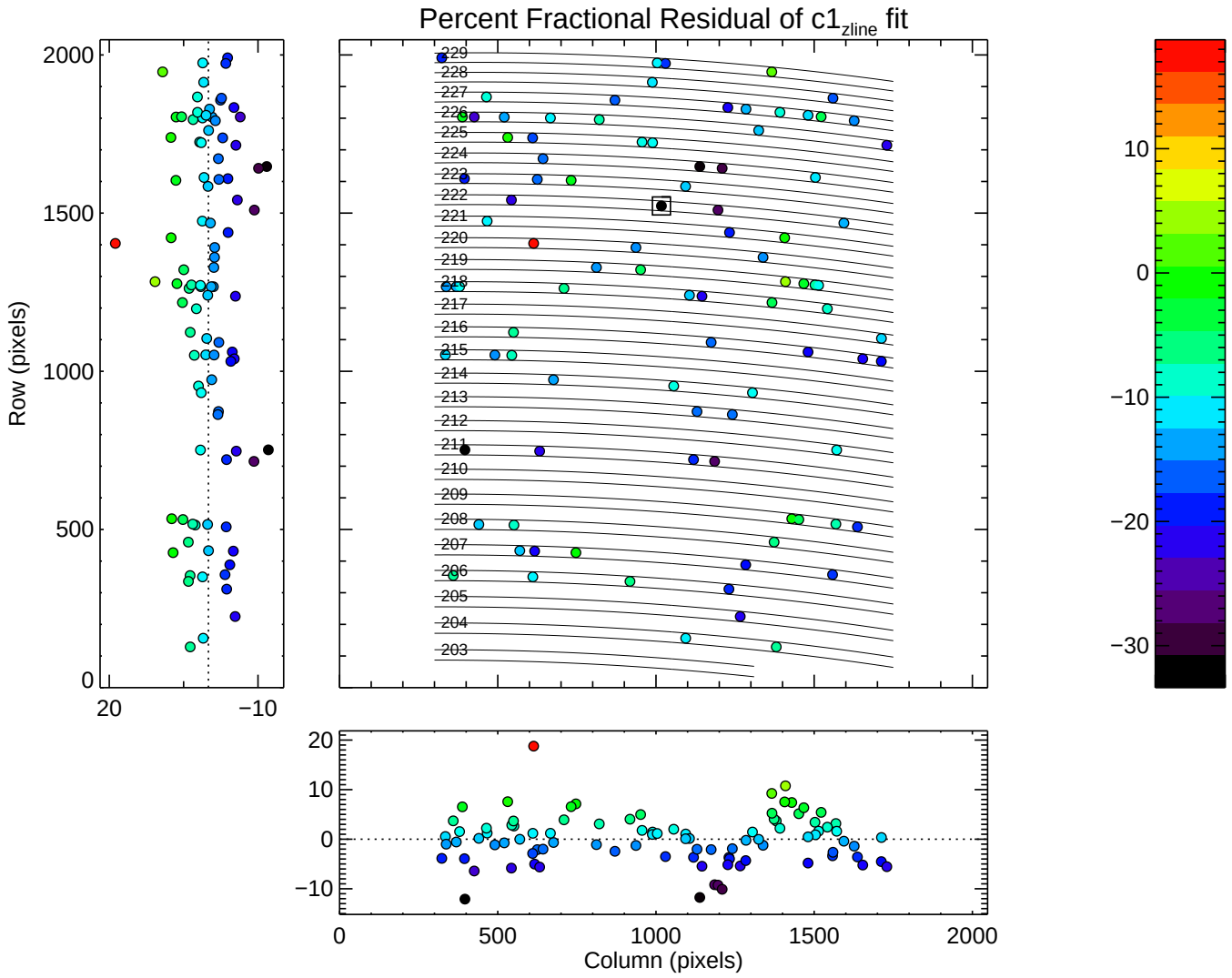

Figure 7: *Page 4 of the* `_2DCoeffFit.pdf` *QA file*

4.2.4 Sky Frames

If the user acquired data by nodding to sky between object frames, then they may want to create a master sky frame that can be subtracted from each of the object frames.

21. Click on the **Combine Images** button in the middle of the GUI. This panel is used to combine a variety of images and so **Column BG Sub** button is not required to create a master sky frame and thus can be ignored.

22. Select the prefix of the sky frames in the File Read Mode panel, select the **A** beam switching mode and type the numbers of the sky frames in the **Files** field.

23. Once the frames are loaded into memory, there are several ways they can be processed before being combined. If the user wishes to scale the average flux level in each order to a common value before combining, click the **Scale Orders** button and then either type (or click) the name of the associated normalized flat field exposure created in §4.2.1 in the **Full Flat Name** field.

24. Select the statistic that will be used to combine the frames (see §3.6 for a description of the various statistics), select **cal/** for the directory in which to write the master sky, and then type a file name (without the suffix .fits) in the **Output Name** field.

25. Click **Combine Images** and the sky frames will be loaded into memory, combined using the statistic chosen by the user, processed as requested, and written to disk in the `cal/` directory.

4.3 Extraction of Bright Sources

Targets observed with iSHELL can have a range of brightnesses. For the purposes of this manual, we consider "bright" targets to be those where the object is easily visible in a single image or pair-subtraction in all of the orders the user wishes to extract. We recommend that first-time users extract a bright source (typically, but not always, the standard star) first in order to get a feel for the extraction process. A description of how to extract "faint" objects is given in §4.4. As users become more comfortable with Spextool, they will no doubt develop a sense of which sources are "bright" and which sources are "faint".

4.3.1 Loading the Data

26. Prepare for extraction of your spectra by clicking either the **Point Source** or **Extended Source** button in the middle of the GUI. This will bring up a set of boxes for the chosen source type.

27. The user should select the File Read Mode in the upper left hand panel of the GUI; the default mode of **Index** is by far the most common mode. If **Index** is selected, the user should also select the prefix of the filenames that will be reduced (K3:`icm.2017A999.170525.spc.`, Lp3:`icm.2016B999.160924.spc.`).

28. In the Reduction Mode panel (upper right hand panel of the GUI), the user should select the **Reduction mode**. If the user wishes to extract raw data choose **A**. If the data were acquired in the standard

infrared method of moving the object between two positions on the slit (the "pair" method), or if the B frames are sky frames for an extended source, choose **A-B** (the appropriate method for the Lp3 test data). If you are subtracting a master sky or master dark frame, choose **A-Sky/Dark** (the appropriate method for the K3 data)

29. Now fill in the fields below the Reduction Mode buttons. If the Reduction mode is **A** or **A-Dark/Sky** type in the number of the object frame in the **Images** field (K3:`1`) while if the Reduction Mode is **A-B** type in the numbers of the first two object frames in the **Images** field (Lp3:`51,52`).. Give the full name of the normalized flat field in the **Full Flat Name** field (K3:`flat6-10.fits`, Lp3:`flat84-88.fits`)and give the full name of the Wavecal file in the **Full Wavecal Name** field (K3:`wavecal11-12.fits`, Lp3:`wavecal51-60.fits`).

    ***Note:**. The directory button next to the **Images** field which contains the choices, `raw/`, `cal/`, and `proc/` defaults to `raw/`. However, in principle the user can extract from images in either the `cal/` or `proc/` directory, e.g, see §4.4.*

    Click the **Load Image** button. Spextool will apply linearity corrections to the image(s), pair subtract the two images or subtract a master dark or sky if required, and divide the result by the normalized flat field. Spextool will then rectify the orders using the rectification indices stored in the wavecal file and stack them on top of each other in a sythetic image. The flux, uncertainty, and S/N images will be displayed in `ximgtool`. The user can scroll through the buffers by typing 'f' for **F**orward and 'b' for **B**ackwards in the `ximgtool` window and the order number, wavelength, and sky angle along the slit for each pixel are displayed in the lower right hand corner of the display. Pixels in either the A or B frame that have values above the maximum value that can be corrected by the linearity correction ∼30,000 DN are colored red in `ximgtool`.

4.3.2 Point Source Extraction

Identify Apertures (Box #1)

30. Click the **Make Spatial Profiles** button and Spextool will construct an "average" spatial profile in the various orders by effectively calculating the average value along the wavelength direction at each spatial point. An atmospheric transmission curve is used to weight wavelengths with higher transmission more heavily. The spatial profiles are displayed in a separate GUI (`Spatial Profiles`) which can be resized as required. If there are more orders than can be plotted on screen, the user can view the other orders using the scroll bar, the **up** and **down** arrow keys, or the **View Orders** menu at the top of the GUI.

31. Aperture positions can now be identified in ways:

    - **Auto**: If the stellar peaks are clearly discernible in each order, select the **Auto** button and then the number of apertures to be found. For spectra obtained in pair, or A-B mode, there will be two apertures, corresponding to the object in the A frame and its negative counterpart in the B frame. Spextool will identify the positions of the peaks in each order and plot them as solid

cyan lines in the `Plot Profiles` window. The user should confirm that the aperture(s) in each order were properly identified.

- **Guess:** Sometimes the automatic aperture identification routine fails and thus the user must give the routine guess positions. In this case, the user should click **Guess** and then the number of apertures to be identified. Click the **Find Aperture Positions** button and the window focus will shift to the `Plot Profiles` GUI and the user can identify guess positions (for all orders) by clicking with the left-most mouse button. A dashed cyan line will appear in each order to denote the selected guess position. Once the guess positions are identified, Spextool will attempt to identify the aperture positions and will plot the results as solid cyan lines.

  If one or more of the apertures is still not identified properly, the user can either attempt to identify new guess positions or modify the guess positions within a given order by typing 'm' (for **M**odify) and then dragging the dotted cyan line left or right by clicking and holding the left-most mouse button while moving the cursor. When the user releases the mouse button, Spextool will attempt to refit all of the aperture positions.

Choose Orders

32. If the user is extracting data with only a single order, they may skip to the next section. Normally the observer will want to extract all spectral orders. However, if an order contains so little flux that the aperture position cannot be identified or the spectrum cannot be traced, the user should unselect that order in the `Spatial Profiles` window by typing 's' for **S**elect over the order and the profile plot will turn grey; typing 's' again will re-select the order for extraction. If the user wants to only extract a few orders, it is faster to unselect all orders at once, and then select the few orders to extract. This can be accomplished using the **Select Orders** menu or by typing 'n' for **N**one. To select all orders at once, use the **Select Orders** menu or type 'a' for **A**ll.

Trace Objects (Box #2)

33. Because of atmospheric dispersion, the spatial position of a point source does not fall along a line of constant angle on the sky. The user should therefore click the **Trace Objects** button and Spextool will fit a Gaussian to the spatial profile at every column, using the aperture positions determined above as the initial guess. The centers of the Gaussians are then fit with a polynomial to derive the trace position as a function of column. The resulting trace will be displayed in the `ximgtool` window.

    Note: *The extraction of the spectra are based on the positions determined from the trace and not the aperture positions determined in the previous step.*

Define Extraction Parameters (Box #3)

The extraction parameters can now be defined in the **Define Extraction Parameters** box. By default, Spextool carries out a so-called "optimal" extraction for point sources but since the user is more likely familiar with simple aperture photometry, we first describe how the user can perform a non-optimal extraction. We recommend the user read the follow step even if they plan to use the optimal extraction mode because it describes parameters that the user will be required to provide during the optimal extraction. Figure 8 shows a graphical representation of the extraction parameters described below.

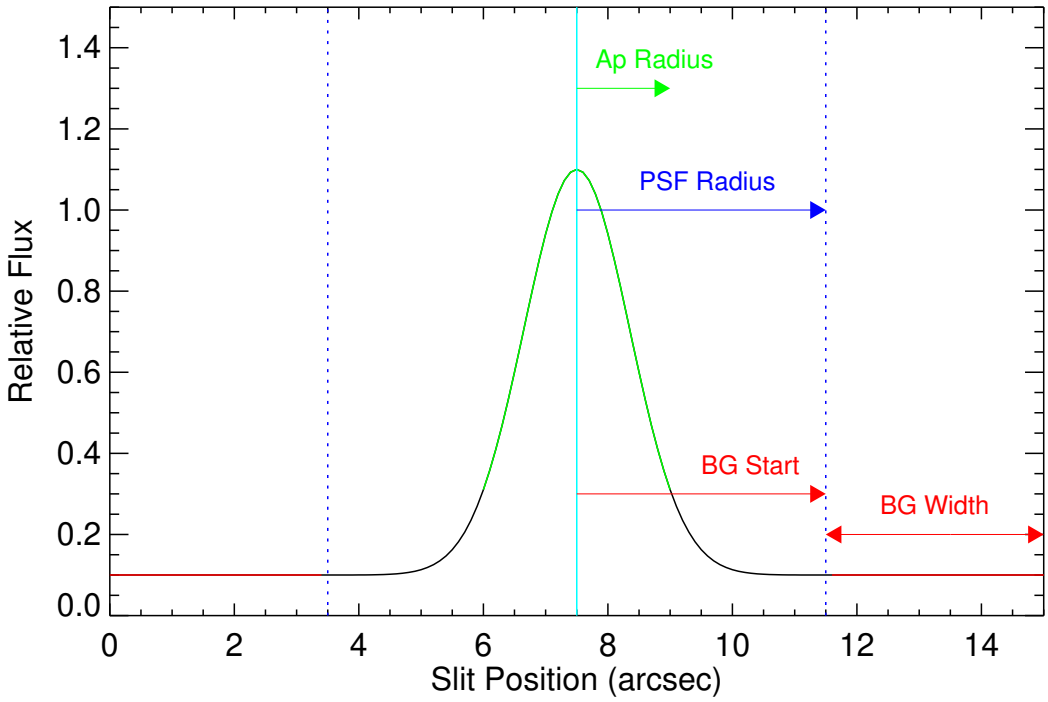

Figure 8: Extraction parameters for a point source.

34. To perform a simple sum (non-optimal) extraction, the user should first un-select the **Optimal** button. The user must then provide values for four parameters: **Ap Radius**, **BG Start**, **BG Width**, and **Fit Deg**. The first three are the one-dimensional equivalents of the standard two-dimensional aperture photometry parameters, i.e. the **Ap Radius** is the size of the aperture that Spextool uses to compute the source count rate at each column by summing the pixels in the aperture, the **BG Start** value is the inner radius of the background annulus, and **BG Width** is the width of the background annulus (see Figure 8). The final parameter, **Fit Deg**, specifies the degree of the polynomial used to fit the background across the object aperture - degree = 0 is a constant while degree = 1 is a linear fit with slope and offset.

    The user should determine the values of these parameters by using the `Plot Profiles` window and the **Show Apertures** button which will display the apertures (in green) in the `Spatial Profile` and `ximgtool` windows and the background region (in red) in the `Spatial Profiles` window. The user also has the option to perform a sum extraction without background subtraction by un-selecting the **BG Sub On** button.

35. To perform an optimal extraction, the user should first select the **Optimal** button. Rather than summing the values of the pixels in the aperture to determine the count rate, optimal extraction[4] uses each pixel in the aperture as an estimate of the count rate and combines these estimates in an optimal way which delivers the maximum possible S/N. To see how this is done, consider the spatial profile

[4]for a detailed description please see Horne (1986, PASP, 98, 609).

of a star (e.g. Figure 8) at a wavelength λ and let $C_{\lambda,i}$ and $V_{\lambda,i}$ be the count rate and variance of the count rate in the ith pixel of the profile (you can think of λ as a particular column on the detector and i as the row number as you move up the slit in a given order). Further assume that we have perfect knowledge of the spatial distribution of starlight P_λ such that $P_{\lambda,i}$ gives the probability of detecting a photon at pixel i. The quantities $C_{\lambda,i}/P_{\lambda,i}$ and $V_{\lambda,i}/P_{\lambda,i}^2$ then become estimates of the source count rate and variance of the source count rate at λ. These estimates can be combined optimally using a weighted mean as,

$$C_\lambda = \frac{\sum_i W_{\lambda,i} C_{\lambda,i}/P_{\lambda,i}}{\sum_i W_{\lambda,i}}, \quad \mathrm{var}[C_\lambda] = \frac{1}{\sum_i W_{\lambda,i}} \tag{4}$$

where the weights are given by the inverse variance values of each estimate $C_{\lambda,i}/P_{\lambda,i}$ or,

$$W_{\lambda,i} = \frac{P_{\lambda,i}^2}{V_{\lambda,i}}. \tag{5}$$

The profile $P_{\lambda,i}$ is generated from the data by Spextool but the profile must be properly normalized in order for the optimal extraction to work. The **PSF Radius** parameter gives the angle at which the profile is effectively zero thus allowing Spextool to normalize the profile at each wavelength. The user should determine the values of this parameter by using the `Plot Profiles` window and the **Show Apertures** button which will display the **PSF Radius** with a blue vertical dashed line. Note that the **Ap Radius** can be as large as the **PSF Radius**.

Extract and Write Spectra to Disk

36. In the File Read Mode panel, type in the desired prefix for the output files (the default is `spectra`) if Spextool is in **Index** mode, or the full output file name if Spextool is in **Filename** mode.

    Note: *The .fits extension will automatically be added to filenames by Spextool. That is, if Spextool is in the* ***Filename*** *read mode and if the final desired filename is* `Jupiter.fits`*, then the user should enter* `Jupiter` *in the* ***Output File Name*** *field.*

37. Click **Extract Spectra** and Spextool will extract the spectra and write them to the `proc/` directory as FITS files (K3:`spectra00001.fits`, Lp3:`spectra00051.fits`, `spectra00052.fits`) the format of which is described in §3.8. The spectrum or spectra will be displayed in the `xvspec` GUI for inspection. If two spectra are written to disk because the **A-B** reduction mode was chosen, the user can switch between the A and B buffers by either using the **Buffer** pulldown menu or clicking the **A** and **B** buttons. `xvspec` is described in more detail in §3.10.2.

    Note: *Spextool handles bad pixels differently depending on which extraction mode is chosen. If optimal extraction is chosen, then bad pixels are simply ignored. If sum extraction is being performed, Spextool replaces bad pixels using a model, wavelength-dependent spatial profile. Any output spectral pixel that is generated using an array pixel that has been replaced is flagged in the bit mask (see §3.7).*

Reducing the Rest of the Data

38. The user may now extract *all* of the remaining point source data with the same extraction parameters by entered the remaining frames into the **Images** field (K3:`1-5,13-17`, Lp3:`53-60,61-70`) and clicking **Do All Steps**.

    Note: *In the case where dark or sky frames are being subtracted, it may be necessary extract the object and standard star spectra separately because their exposure times differ. In this case, the user will need to set up the extraction again by going through all the steps before using* ***Do All Steps****.*

4.3.3 Extended Source Extraction

Identify Apertures (Box #1)

11. The user can identify the aperture positions in one two ways:

    - Cursor Mode: The user should type the number of aperture positions to be identified in the **Number of Apertures** field and then click **Identify Aperture Positions**. The mouse focus will shift to `Spatial Profiles` window and the user can identify aperture positions (for all orders) by clicking with the left-most mouse button. A cyan line will appear in each order to denote the selected aperture.
    - Keyboard Mode: The user should select **Keyboard** and simply enter the aperture positions in arcseconds, separated by commas, and then click **Store Aperture Positions**. Cyan lines will appear in each order to denote the aperture positions.

    Once all of the aperture positions have been identified, the user can (in principle) modify the aperture positions on an order-by-order basis by typing 'm' (for **M**odify) in the `Spatial Profiles` window and then dragging an aperture left or right.

Choose Orders

12. If the user is extracting data with only a single order, they may skip to the next section. Normally the observer will want to extract all spectral orders. However, if an order contains so little flux that the aperture position cannot be identified or the spectrum cannot be traced, the user should unselect that order in the `Spatial Profiles` window by typing 's' for **S**elect over the order and the profile plot will turn grey; typing 's' again will re-select the order for extraction. If the user wants to only extract a few orders, it is faster to unselect all orders at once, and then select the few orders to extract. This can be accomplished using the **Select Orders** menu or by typing 'n' for **N**one. To select all orders at once, use the **Select Orders** menu or type 'a' for **A**ll.

Trace Objects (Box #2)

13. Since the aperture positions are fixed when extracting extended sources, there is no reason to trace the object's position across an order. However, for historical reasons a trace based on the aperture positions must still be generated so the user must click **Create Trace** in the Trace Objects box (box #2). The aperture positions will appear in the `ximgtool` window as cyan lines.

Define Extraction Parameters (Box #3)

14. The extraction parameters can now be defined in the Define Extraction Parameters box. The aperture radii (in arcseconds) of each aperture must be entered in the **Ap Radius** field (e.g., 1.5,1.5 for 2 apertures). The positions (in arcseconds), of the background windows must also be specified in the **BG Reg** field. An example might be 0-2, 13-15. Finally, the user can select the degree of the polynomial that is used to fit the background in the **BG Fit Degree** field.

    Note: *that differential atmospheric refraction will cause a fixed position on the extended source to have slightly different angular positions on the sky. The user should keep this in mind and make sure the extraction aperture widths are large enough to account for the variation in position of the spectrum with order. The user can mitigate the order-by-order variation by moving the apertures as described in step 11 of §4.3.3.*

15. Now click on the **Show Apertures** button. Spextool will show the apertures used for both the background (in red) and the object (in green) in the `Spatial Profiles` window and the apertures (in green) in `ximgtool`.

Extract and Write Spectra to Disk

16. In the File Read Mode panel, type in the desired prefix for the output files (the default is `spectra`) if Spextool is in **Index** mode, or the full output file name if Spextool is in **Filename** mode.

17. Click **Extract Spectra** and Spextool will extract the spectra and write them to the **proc** directory as FITS files. The spectra will be displayed in the `xvspec` GUI for inspection. The user can switch between apertures using the **Aperture** pulldown menu.

Reducing the Rest of the Data

18. The user may now extract *all* of the remaining extended source data with the same extraction parameters by entered the remaining frames into the **Images** field and clicking **Do All Steps**.

4.4 Extraction of Faint Sources

If this is the first time a user is extracting a spectrum with Spextool, we recommend that they return to §4.3 to learn how to extract bright sources if they have not already done so. Extracting the spectra of faint point sources can be difficult because Spextool may have problems accurately identifying the aperture positions and/or tracing the objects across the array. Several methods to deal with such a situation are described below. While each method can be used, we recommend the third option described in §4.4.3.

4.4.1 Method #1: Use Aperture Positions

19. If the user is extracting a point source and Spextool can identify the aperture positions, in either **Auto** or **Guess** mode, but cannot accurately trace the object across the array, then one option is to simply force Spextool to extract the spectrum at these apertures positions. To do so, the user should click the **Use Ap Positions** in the Trace Objects box (box #2) before clicking **Trace Objects**.

    Note: *Differential atmospheric refraction will cause the peak of a point source to be located at slightly different positions along the slit. While using the aperture positions to define the trace will mitigate the change of position between orders, it will not mitigate the change in position within an order.*

4.4.2 Method #2: Fix Aperture Positions

20. If the user is extracting a point source and Spextool cannot identify the aperture positions using either the **Auto** or **Guess** mode, then the user can simply fix the positions of the apertures by clicking **Fix** in the Identify Apertures box (box #1), the number of apertures to be identified, and then **Find Apertures Positions**. The window focus will shift to the `Spatial Profiles` windows and the user can identify aperture positions (for all orders) by clicking with the left-most mouse button. A cyan line will appear in each order to denote the selected aperture.

    Once all of the aperture positions have been identified, the user can modify the aperture positions on an order-by-order basis by typing 'm' (for **M**odify) in the `Spatial Profiles` window and then dragging the aperture left or right.

4.4.3 Method #3: Combine Images

21. The user can combine all of the images of a fainter source together in order to create a higher S/N image from which Spextool can extract the spectra. Move to the Combine Images panel by clicking on the **Combine Images** button in the middle of the main GUI.

22. The user should select the File Read Mode in the upper left hand panel of the GUI and select the prefix of the filenames if **Index** is selected.

23. If the data were acquired by moving the object between two positions on the slit (the pair method), choose **A-B** for the **Beam Switching Mode**; if not, choose **A**. Then type or click the image into the **Image** field.

24. The user can modify the images if they choose before they are combined in two ways:

    - **Scale Orders**: On an order by order basis, the flux values in each order will be scaled to the median of all pixels in that order in all of the images. Typically this would be used for combining sky frames.
    - **Column BG Sub:** The median background level will be subtracted off each column in each order. This effectively is a zeroth order sky subtraction.

In either case, Spextool requires the normalized flat field created in §4.2 so enter the full name of the normalized flat field in the **Full Flat Name** field.

Note: *The images will not actually be flat-fielded. Rather, Spextool requires information stored in the flat field header to locate the orders.*

25. Choose the statistic that will be used to combine the images. §3.6 gives a summary of each statistic.

26. Finally, select the directory into which the file should be written (we recommend **proc/**) and give the full name of the output file in the **Output Name** field and click on the **Combine Images** button. Spextool will then combine the images, write the result to disk as a multi-extension FITS file, and display the results in `ximgtool`. The zeroth extension will contain the FITS header, the first extension will contain the combined image, the second extension will contain the variance image, and the third extension will contain the bit-mask flag array.

27. The combined image may now be extracted as described in the previous sections. After selecting whether to perform a point or extended source extraction, the File Read Mode should be set to **Filename** and the **Reduction Mode** set to **A**. The user can then select the directory where the combined image was written (e.g. **cal/** or **proc/**), enter the full name of the combined image into the **Images** field, fill in the remaining fields and then click **Load Image**.

Note #1: *To perform optimal extraction or fix bad pixels, Spextool creates a wavelength dependent model spatial profile. However, sometimes the data have such low S/N that this spatial profiles fail to adequately model the shape of the PSF. In this case, the user can select* ***Average Profile*** *button and Spextool will use the higher S/N, wavelength-independent profiles shown in the* `Plot Profiles` *GUI.*

Note: *If the data were obtained in the A-B mode, Spextool will write both the positive and negative aperture to a single file. The user can switch between apertures in the* `xvspec` *GUI using the* ***Apertures*** *pulldown menu. These beams can be combined in* `xcombspec` *(see next section).*

5 Combining Spectra: xcombspec

The `xcombspec` GUI allows the user to combine multi-order spectra generated by `xspextool` or `xtellcor`.

5.1 Additional Keyboard Commands

- s - **S**elect a wavelength range.

5.2 Starting up and Loading the Data

1. Typing `xcombspec` at the IDL prompt will launch the `xcombspec` GUI.
2. In Box #1, the user can either click on the **Path** button and select the path containing the spectra to be combined or they can simply type the path into the field. If the user started IDL and launched the `xcombspec` in the directory with the spectra to be combined, then the field can be left blank.
3. There are three ways in which `xcombspec` can be used to combine spectra:
   - **Normal spectra**: Spectra extracted in the standard way, i.e. any way except as described in §4.4.3.
   - **Combine-Images spectra**: Spectra extracted from a combined image as described in §4.4.3.
   - **Telluric-corrected spectra**: If the user observed a target over a large range in airmass, then object/standard sets that were extracted, combined, and telluric corrected separately can be combined to increase the S/N of the final spectra before being merged with `xmergeorders`.

   The user should next select the File Read Mode. If the user is combining standard spectra, select **Index**, type the prefix into the field (the default is `spectra`) and then type the file numbers into the **Files** field (K3:`1-5`, Lp3:`61-70` for the object or K3:`13-17`, Lp3:`51-60` for the standard). If the user is combining combined-images spectra or telluric-corrected spectra, selected **Filename** and then click on the **Files** button and highlighting the file names from the list that is displayed.
4. Click on the **Load Spectra** button to load the spectra. The individual spectra will then be displayed in the plot window. If the data files contain multiple orders, all of the orders will be displayed at once (hereafter we will assume this is the case since it is the most common case). The user has several ways of viewing the data. To view different orders, the user can use the scroll bar, the up and down arrow keys, or the **Order** pull-down menu. If the data have more than one aperture, the user can view the different apertures using the **Aperture** pull-down menu. The user also has the choice of displaying the fluxes, uncertainties, or S/N ratios using the **Type** pull-down menu. On loading the spectra `xcombspec` will combine the spectra using the statistic shown at the top of the plot window. The combined spectra can be view by selecting **Combined** from the **Plot** pull-down menu.

   Note: It is critical that the user actually look at all of the orders to ensure that the extraction process was successful. The easiest way to do this is to use the up and down arrow keys while

the cursor is in the plot window. If some spectra look bad, it may be necessary to re-extract them or simply exclude them from the combination process.

5.3 Modifying the Spectra: Scale, Prune, Correct Shape

While the combined spectra could now be written to disk, there are typically several modifications to the spectra that should be performed before doing so. As a result of variable slit losses, the average flux levels of each spectrum are different, and thus the spectra sometimes appear to fan out. This can be corrected by scaling the spectra to a common flux level as described in §5.3.1. A second order correction to the flux levels is often required because we see a heterochromatic (i.e. wavelength dependent) component to these slit losses that affects the overall shape of the spectra. This correction is described in §5.3.4. The scale and shape corrections are particularly important if the user is going to use the dispersion of flux values at a given wavelength as a measure of the uncertainty in the flux density at that wavelength (see §3.6 for a more in depth discussion of this issue).

A final modification that is seldom needed is to prune sections of spectra or an entire spectrum. This may be necessary if some of the spectra have a similar defect, e.g. a cluster of bad pixels affecting the 'A' beam spectra, such that the robust sigma clipping cannot remove the bad pixels or if a single spectrum shows clear deviations from the rest. These modifications are described in §5.3.3.

5.3.1 Scaling the Spectra

5. The purpose of combining spectra is to increase the S/N of the source spectrum by averaging out the fluctuations due to noise. However as noted previously, as a result of guiding errors, variable sky transmission, etc., rarely will it be the case that all of the individual spectra in a given order have the same flux level. If the final uncertainty on a flux density value in the combined spectrum is computed using some form of the standard deviation of the flux density values, then combining spectra with different flux levels can defeat the purpose of the combining process, by increasing, rather than decreasing, the noise.

   `Xcombspec` determines a *single* scale factor that is applied to all orders of a given spectrum[5]. That is, the factor determined for spectrum 2 in order 5 is also applied to the corresponding spectrum 2 in order 3. Therefore, we suggest that the scale factors should generally be determined from the middle orders, unless the user has a particular reason for choosing another order (for example, if no flux is detected in some of orders). We also recommend choosing an order with a high overall S/N value. In Box #2, the user should choose the order with which the scaling should be determined from the **Order** pulldown menu, click **Scale Spectra** and the `xscalespec` GUI will appear.

6. By default, the spectra will be scaled to the median of the set of spectra using the wavelength range denoted by the dotted cyan lines. If the user would like to change the wavelength range, type 's' (for **S**elect) and click with the left most mouse button to specify the short wavelength limit of the selected range. Click again with the left most button to specify the long wavelength limit. The user can also choose to scale the spectra to one of the spectra instead of the median spectrum. To do

[5]The reason for this choice is discussed in more detail in §9.

so, select **Spectrum** from the **Scale to:** pull down menu in the upper left of the plot window and then the number of the desired reference spectrum should be chosen from the ther pull down menu. `Xcombspec` will then determine the scale factors to be applied to each spectrum, and will scale them appropriately. If **None** is chosen at any point in this process, the original unscaled spectra will be re-plotted. We recommend using the **Median** for the scaling.

7. Once the user is satisfied with the scaling, s/he should click on the **Accept** button. At this point, the scale factors determined for each spectrum will be applied to all the spectra in all the orders. If the results are not acceptable, the scaling can be re-determined by choosing a new scaling order, a new reference spectrum, a different wavelength range, or the spectra can be re-loaded and the process repeated from the beginning.

8. Ideally, by scaling all spectra in every order to a common value all the spectra should now lie perfectly on top of one another. However, we have found that this is not the case. After scaling, often the spectra in orders farthest from that used to determine the scale factor exhibit a large dispersion about the mean. This implies that the spectral slope is varying from one spectrum to another over the various orders. One can see this change in spectral slope even across a single order if the spectra are examined closely. We believe this slope change is the result of guiding errors, atmospheric dispersion, and time-variable, wavelength-dependent changes in seeing. Based on our tests, we do not believe it is due to any procedures carried out by Spextool during the data reduction. The user can correct for this dispersion in §5.3.4.

5.3.2 Shifting the Spectra

9. Due to reasons we do not yet fully understand, the spectra in the wider slits may be shifted relative to each other by a constant (in units of pixels). We therefore recommend the user click on the **Shift Spectra** button in Box #2 and 1) inspect the spectra for this shift and 2) correct for it if necessary. The easiest place to see the shift is near the telluric CO_2 absorption features near $\sim$2.05 μm. If the spectra appear shifted relative to each other, the user type 's' (for **S**elect) and click with the left most mouse button to specify the short wavelength limit of the selected range. Click again with the left most button to specify the long wavelength limit. The GUI will perform a cross correlation against the telluric absorption spectrum in order to determine the shift (in pixels) relative to the telluric absorption band and then adjust the spectra accordingly.

5.3.3 Pruning the Spectra

10. The user can both remove spectra from an order and/or mask out parts of a spectrum before they are combined, although this step can typically be skipped. To do so, the user should select **Prune** from the **Modify Spectra** pull down menu and then select an order from the **Order:** pull down menu and the `maskspec` GUI will appear.

11. At any time the user can control which spectra are displayed by **Plot** from the pull down menu and then selecting which orders to display. At any time, the user can select **All** and all of the spectra will be displayed or **None** and none of the spectra will be displayed.

12. If the user would like to remove an entire spectrum, he/she should select **Remove** from the pull down menu and select which spectra to remove. The **All** button is grayed out because at least one spectrum must be present. However, the user can click the **None** button at any time and all the spectra with be displayed.

13. If the user would like to mask parts of a spectrum, he/she should select **Mask** from the pull down menu and then select which spectra will be masked. The user can choose the wavelength range to mask by typing 's' (for **S**elect) and then left-clicking the mouse button on the left and right wavelength limits. To **U**ndone **all** of the masks, type 'u'.

    ***Note**: Once the user modifies which spectra are to be masked, they can no longer undo any previously generated masks.*

14. When the user is satisfied with the selection of spectra to remove and the regions to be masked, he/she should click the **Accept** button at the bottom of the GUI.

5.3.4 Correcting the Shape of the Spectra

15. The user may choose to reduce the dispersion in the spectra about the mean (and therefore increase the S/N of the final combined spectrum) by correcting for these slope variations. This can be done by clicking on the **Correct Spectral Shape** in box #2. In each spectrum **xcombspec** will then remove the low order variations, relative to the reference spectrum, from each spectrum, order by order. After this has been done, all the spectra in a given order should lie on top of one another, which will then increase the S/N in the resulting combined spectrum.

    ***Note:** The results of the Correction should be inspected carefully. While we have set the parameters of the procedure such that it should work in most cases, it can sometimes generate obviously spurious results. This is particularly true if the input spectra have very low S/N. If the user is uncertain about the results, do not perform the shape correction.*

    The **Correct Spectral Shape** step cannot be undone. If the user wishes to undo this correction, s/he will have to re-load the spectra and start the combining procedure from the beginning.

5.4 Write the File to Disk

16. Give the root of the output file name in the **File Name** field in Box #3 (K3:`cspectra1-5`, Lp3:`cspectra61-70` for the object or K3:`cspectra13-17`, Lp3:`cspectra51-60` for the standard) and click on the **Write File** button. The spectra will be written to disk in the directory given in the **Path** field in Box #1. The combined spectra will be displayed in the `xvspec` GUI. The FITS headers of the input spectra are combined and as a result and the keywords listed in Table 4 are added to the output file.

6 Telluric Correction and Flux Calibration: xtellcor

`Xtellcor` is the telluric correction program originally written by Bill Vacca and Mike Cushing for use with SpeX. Users can find a description of the code in the paper by Vacca, Cushing, & Rayner (2003, PASP, 115, 389) and we would ask all users to reference this paper if they use `xtellcor`. `Xtellcor` uses observations of an A0 V standard and a high resolution model of Vega to remove both telluric absorption and the instrument throughput. In brief,

$$f_{\rm obj}^{\rm intr}(\lambda) = f_{\rm obj}^{\rm obs}(\lambda) \left[\frac{f_{\rm vega}^{\rm mod}(\lambda)}{f_{\rm A0\,V}^{\rm obs}(\lambda)} \right] \tag{6}$$

where $f_{\rm obj}^{\rm intr}(\lambda)$ is the instrinsic spectrum of the source, $f_{\rm obj}^{\rm obs}(\lambda)$ is the observed spectrum of the source, $f_{\rm vega}^{\rm mod}(\lambda)$ is a model spectrum of Vega modified to match the radial velocity, reddening, resolving power, and H I equivalent widths of the A0 V standard star, and $f_{\rm A0\,V}^{\rm obs}(\lambda)$ is the observed spectrum of the A0 V standard star. Most of the steps in the `xtellcor` GUI are aimed at properly modifiying the Vega model.

Three additional programs associated with `xtellcor` are `xtellcor_finish`, `xtellcor_basic`, and `xtellcor_general`. `Xtellcor_finish` allows the user to apply previously generated telluric correction spectra to data, `xtellcor_basic` allows the user to divide by a standard star (and optionally multiple by a Planck function) which can be useful for solar system observations or for quick telluric corrections, and `xtellcor_general` is a general version of the code for use with other instruments. The first two routines are described in more detail in Sections 6.3 and 6.4 while the latter routine is described in its own user manual which can be found in the directory `Spextool/manuals/` of the Spextool package.

Note: *`Xtellcor` is used with a variety of instruments and so there will be buttons and fields that may not be necessary for your particular instrument configuration. These buttons and fields will be greyed out as needed to avoid confusion.*

Note for iSHELL users: *One of the critical steps in the telluric correction process is matching the equivalent widths of the hydrogen lines in the Vega model to those in the observed A0 V star. However, the current procedure to match the equivalent widths requires that the lines are completely contained within an order. Given the high spectral resolution of iSHELL, the wavelength grasps of iSHELL orders are small and thus hydrogen lines often span multiple orders. As a result, xtellcor for iSHELL makes no attempt to adjust the equivalent widths and so there may be residuals in the data due to the mismatch in the equivalent widths.*

6.1 Additional Keyboard Commands

The following keyboard commands are used in various subroutines described below.

- s - to **S**elect a wavelength region in the `xfindshift` GUIs

6.2 xtellcor

6.2.1 Starting up and Loading the Data

1. Typing `xtellcor` at the IDL prompt will launch the `xtellcor` GUI, which is divided into five sections corresponding to the steps to be carried out in performing the telluric correction.
2. Enter the name of the A0 V standard star in the **A0 V Standard** field (`HD 196610`) and the fullpath of the standard star file in the **Std Spectra** field (K3:`proc/cspectra13-17.fits`, Lp3:`proc/cspectra51-60.fits`).

   Note: *The standard star file must contain only a single aperture. If the standard star was extracted from combined images (e.g., §4.4.3), then the two apertures must first be combined using* ***xcombspec****.*

3. Enter the B- and V-band magnitudes (easily obtained from SIMBAD) in the **Std Mag (B,V)** fields (K3:`5.374` and `5.404`, Lp3:`4.80` and `4.82`). If the magnitudes are unknown, the user can enter the same magnitude (any number) for B and V. However in this case, the pseudo flux calibration will not be correct.
4. Enter the fullpath of the object spectra in the **Obj Spectra** field (K3:`proc/cspectra1-5.fits`, Lp3:`proc/cspectra61-70.fits`).
5. Click the **Load Spectra** button to load the spectra into memory. Note that the airmass values for both spectra and the airmass difference will appear at the top of the `xtellcor` panel. The panel is colored coded such that it is green if the absolute value of the airmass difference is less than 0.1 and red if it is greater than 0.1. Typically airmass differences greater than $\sim$0.1 result in spectra that are poorly corrected at wavelengths with strong telluric absorption. Finally, depending on which instrument and mode were used to obtain the data, certain buttons and fields will be greyed out.

6.2.2 Constructing Convolution Kernel

The next step involves generating a kernel that will be convolved with the Vega model spectrum in order to simulate the observed spectrum of the A0V standard star at the resolution of the data. The division of the observed stellar spectrum $f^{\rm obs}_{\rm A0\,V}(\lambda)$ by the convolved and scaled Vega spectrum $f^{\rm mod}_{\rm vega}(\lambda)$ will then yield the telluric correction spectrum that will be applied to the object spectrum. There are two methods with which to generate the convolution kernel:

- **Deconvolution Method:** The observed A0 V star spectrum is used to generate the kernel be preforming a deconvolution between the data and model using an H line free from telluric absorption, e.g. the Pa δ line at 1.0052128 μm. During this process, the velocity shift between the data and model is computed and the resulting kernel automatically accounts for any rotation of the A0 V star.
- **IP Method:** If no H line free from telluric absorption can be found (e.g. the LXD mode of SpeX), or if the line spans more than one order (i.e. iSHELL), then the deconvolution method cannot be used. Instead we use a pre-computed instrument profile as the convolution kernel. However, the rotation of the A0 V star is not accounted for in this process.

6. The deconvolution method is not available for ISHELL data so simply click the **Construct Kernel** button in Box #2 and the appropriate kernel for the slit width will be loaded into memory.

6.2.3 Constructing the Telluric Spectrum

7. The user should enter the radial velocity of the A0 V standard (km s^{-1}) in the **Std Vrad** field (K3:$v_{\rm rad}$=14 km s^{-1}, Lp3:$v_{\rm rad}$=-17.10 km s^{-1}) and then select the units of the output spectrum.

8. Click **Construct Telluric Spectra** and `xtellor` will shift the Vega model to the velocity of the A0 V standard (by combining the $v_{\rm rad}$ entered by the user and the motion of the Earth towards the star at the time of the observation which is computed from information contained within the FITS header), convolve the shifted model with the kernel, and then divide the results $f^{\rm mod}_{\rm vega}(\lambda)$ into the observed stellar spectrum $f^{\rm obs}_{\rm A0\,V}(\lambda)$ to yield the telluric correction spectra.

6.2.4 Determining Residual Wavelength Shifts

Note: *This step is effectively a cosmetic adjustment to the data and thus can be skipped if the user so desires.*

We often find there are slight wavelength shifts between the telluric correction spectra and the spectra of the object to be corrected. Division of the two spectra can sometimes result in spurious artifacts which occur primarily at wavelengths with sharp and deep telluric absorption features. These artifacts appear as either noise spikes or, if the shifts are large enough, s-shaped profiles (the result of dividing two slightly shifted telluric absorption lines). These artifacts can partially be mitigated using the procedure described below if the S/N of the data at these wavelengths is high enough; if the telluric absorption features are deep (i.e. near zero transmission) resulting in a very low S/N, then the user may be better off simply removing the noisy wavelengths in `xcleanspec` (see §7).

9. Click on the **Find Shifts** button and the `xmc_findshifts` GUI will appear. The upper window will also show the raw telluric-corrected spectra. The bottom panel shows either the shifted spectra or the shift values for each order, depending on the plot type selected (using the buttons in between the two panels). When the GUI first appears, both panels will appear identical. If the object file has more than one aperture, the user can select between apertures using the **Ap** pulldown menu at the top of the GUI.

   Note:*If the spectra do not appear to show artifacts, then it is probably not necessary to continue and the user can simply click* ***Cancel*** *at the top of the GUI.*

10. The wavelength shift between the telluric correction spectra and the spectra of the object to be corrected probably arises from the sub-pixel flexure of the instrument as the telescope moves between the object and standard. Therefore in principle a single pixel shift can be applied to all of the spectra. The user can determine this shift using two methods:

Single Order

11. Identify an order that exhibits strong artifacts and **S**elect it by typing 's' anywhere in the wavelength range of the order or by selecting the order number from the **Select Order** pull-down menu at the top of the GUI. The spectrum will be automatically centered in the plot window and the other orders will disappear. Select a wavelength range that contains artifacts by typing 's' for **S**elect at which point the red cursor crosshair will turn into a cyan vertical line. Press and release the left-most mouse button on the left and right side of the wavelength range. **xmc_findshifts** will shift the telluric correction spectra by 0.02 pixels from -1.5 to $+1.5$ pixels (and will update the lower panel as it does so) and search for the shift that minimizes the RMS over the user-selected wavelength range. The result will be given in **Shift (pixels)** field at the top of the GUI.

12. If the user is unsatisfied with the shift determined, They can select a new wavelength or add or subtract 0.02 pixels from the shift value using the $+$ and $-$ buttons. When the user is satisfied with this order, they can type 'd' for **D**one or click the **Done** button and continue the process of determining the pixel shifts for other orders, or click **Apply to All** and the shift will be applied to all of the orders and apertures in the file.

Multi Order

13. An alternative method to determining the shift is to compute the shifts for multiple orders at once. To do so, simply type the order numbers (e.g., Lp3:`134-131`) in the **Orders** field and `xmc_findshifts` will determine the orders for these orders. To view the values simply click the **Shifts** button in the middle of the GUI.

14. If the user chooses, he/she can apply the shift computed for one order to all orders by selecting the order (in either panel) and then clicking **Apply to All**.

15. When the user is happy with the shift or shift values, simply click **Accept** at the bottom of the GUI.

6.2.5 Write the File to Disk

16. Give the root of the output file name in the **File Name** field in Box #5. The user can also choose to output the telluric correction spectrum as well as the modified Vega model spectrum (shifted in velocity to account for the Earth's motion and the radial velocity of the A0 V star, scaled to the optical mag of the input standard star, convolved with the kernel, and multiplied by the equivalent width scale factor array). Click on the **Write File** button to generate the output files; the files will be written to the directory in which the object spectrum was located. The spectra will be displayed in the `xvspec` GUI. If the user chose to output the telluric correction spectrum or the modified Vega spectrum, they will be written to disk with the file names `root_tellspec.fits` and `root_modvega.fits`. The FITS keywords listed in Table 4 are added to the output file.

    Note: *The uncertainties contained in the FITS file written to disk do not include the uncertainty in the absolute flux calibration that arises because of variable slit losses in standard and/or target. If the user requires precise absolute flux density values, then they may have to absolute flux calibrate the spectra with photometry.*

6.3 xtelcorr_finish

If one observation of an A0V standard is being used to perform telluric corrections for multiple objects, it is not necessary to re-generate the telluric correction curve each time. The user should generate the curve once using `xtellcor`, making sure that the telluric correction spectrum is saved and written out at the end of the process (the default is to do this). For the next object to be corrected, the user should type `xtellcor,/FINISH` at the command line. `Xtellcor_finish` will take the previously generated telluric curve (e.g. root_tellspec.fits) and the target object as input. The user will be able to shift the two spectra, as in §6.2.4 and after the best shift is found, `xtellcor_finish` will divide the two spectra and output the corrected object spectrum.

6.4 xtellcor_basic

`Xtellcor_basic` is a GUI that that performs basic telluric correction and flux calibration by simply dividing the science observation by a standard star. Not attempt is made to remove intrinsic stellar features but the continuum can be restored by multiplying the result by a Planck function of the appropriate temperature. `Xtellcor_basic` can be used to correct observations of solar system objects where the signal is due to reflected sunlight.

6.4.1 Starting up and Loading the Data

1. Type `xtellcor_basic` at the IDL prompt. This will bring up the `xtellcor_basic` GUI, which is divided into four sections corresponding to the steps to be carried out in performing the telluric correction.
2. Enter the fullpath of the standard star file in the **Std Spectra** field.

   Note: *The standard star file must contain only a single aperture. If the standard star was extracted from a set of combined images, then the two apertures must first be combined using* ***xcombspec*** *(select combine apertures in Box #1 of the GUI).*

3. Enter the fullpath of the object spectra in the **Obj Spectra** field.
4. Click the **Load Spectra** button to load the spectra into memory. Note that the airmass values for both spectra and the airmass difference will appear at the top of the Xtellcor panel. The panel is colored coded such that it is green if the absolute value of the airmass difference is less than 0.1 and red if it is greater than 0.1. Typically airmass differences of greater than 0.1 result in spectra that are poorly corrected at wavelengths with strong telluric absorption.

6.4.2 Determining Residual Wavelength Shifts

We often find there are slight wavelength shifts between the standard star used to construct the telluric spectrum and the object to be corrected. These shifts need to be removed in order to avoid introducing spurious

noise and artifacts when dividing the object spectrum by the telluric spectrum.

Note: *This step is optional and can be skipped if the user so desires.*

5. To estimate the wavelength shift for a given spectrum and correct for it, choose an Aperture and an Order from the pull-down menus in Box #2. Click on the **Get Shift** button and the `xfindshift` GUI will appear. The object spectrum (white) and the telluric spectrum (green) are both plotted in the upper window along with the atmospheric transmission at the resolving power of the data (yellow). The result of dividing one by the other is shown in the bottom window.

6. Select a region in the top window containing a reasonably strong atmospheric features in both spectra (and preferably one not containing strong absorption or emission features in the object spectrum). This is done by typing 's' (for **s**elect) and click with the left-most mouse button on either side of the features. Then click on the **Auto Find** button in the upper left of the window. `xfindshift` will shift the telluric spectrum by fractions of a pixel and search for the best value, corresponding to a minimum in the RMS computed from the telluric corrected spectrum in the selected region. Alternatively, if the user desires a specific shift value (perhaps as the result of determining the shift from another order), s/he can enter the value directly in the **Shift** field and hitting return. Similarly, wavelength shifts can be reset to zero by entering zero in the **Shift** field and hitting return. The user can determine the shift obtained from a different wavelength region by typing 's' and selecting a new wavelength region. When the user is satisfied with the shift found by `xfindshift`, s/he should click on the **Accept** button at the bottom of the window.

7. The user should determine shift values for each order/aperture independently by selecting a new order/aperture in Box #2 and repeating the previous step.

6.4.3 Restore the Continuum

If the user wishes, they can restore the continuum shape of the spectrum and approximately absolutely flux calibrate the spectrum by multiplying the ratio of the observed object and standard star spectra by a Planck function, e.g,

$$F_{\rm obj}^{\rm intr}(\lambda) = F_{\rm obj}^{\rm obs}(\lambda) \left(\frac{B(T,\lambda)}{F_{\rm std}^{\rm obs}(\lambda)} \right). \tag{7}$$

This implicitly assumes that the star can be modelled accurately as a Planck function. Since this is almost never the case, residuals due to intrinsic stellar lines and differences between the stellar continuum and a Planck function will be present in the final spectrum.

8. If the user does not wish to restore the continuum, s/he should select **No** and move to step 10.

9. The user should enter the temperature of blackbody and the V-band magnitude of the standard star. The latter quantity is used to approximately absolutely flux calibrate the final spectrum. Finally, select the units desired for the output telluric-corrected spectrum from the **Units** pulldown menu.

6.4.4 Write the File to Disk

10. Give the root of the output file name in the **File Name** field in Box #5 (the .fits suffix will be automatically appended to the root). The user can also choose to output the telluric correction spectrum as well as the modified Vega model spectrum (shifted to the radial velocity, scaled to the optical mag of the input standard star, convolved with the kernel, and multiplied by the equivalent width scale factor array). Click on the **Write File** button to generate the output files. The spectra will be displayed in the `xvspec` GUI.

7 Cleaning, Fixing, and Smoothing Spectra: xcleanspec

The `xcleanspec` GUI allows the user to 1) linearly interpolate over bad/noisy pixels, 2) remove regions of the spectra (e.g. regions with high telluric noise) and 3) smooth the spectra.

7.1 Additional Keyboard Commands

- d - **D**one editing a spectrum
- f - to **F**ix a region of the spectrum
- r - to **R**emove a region of the spectrum
- s - to **S**elect an order or to **S**ave and edit
- u - to **U**ndo an edit

7.2 Starting Up and Loading the Data

1. Type `xcleanspec` at the IDL prompt which will bring up the GUI.
2. In Box #1, click the **Input Spectrum** Button and choose the file that contains the spectrum or spectra. Alternatively, the user can type the full path of the filename in the field.
3. Click the **Load Spectra** button and the data will be displayed in the plot window. If the spectra are multi-order, then the order numbers will be displayed at the top of the plot window. The user can view the **Flux**, **Uncertainty**, and **S/N** spectrum/spectra, as well as overplot the transmission of the **Atmosphere**. In addition, the user can plot the linearity correction flags and fixed flags (see §3.7). If the spectrum/spectra exhibit/s a large range in flux due to spiky pixels, we recommend the user first find a zoom range that nicely shows the entire spectrum and then type 'a' to set the **A**bsolute zoom level. Whenever the user needs to return to the entire spectrum, type 'w' for **W**hole spectrum.
4. If the file has more than one aperture, the user should then select the aperture they wish to clean or smooth in box #2.

7.3 S/N Cut

5. If the user wishes to clip the spectra based on the S/N, they should enter the S/N limit in the **S/N Limit** field and hit return. The pixels with S/N below the limit will be set to NaN and the masked region will be displayed above the plot window in the Remove Mask. Setting the limit to zero is equivalent to performing not cut.

   Note: *The user must determine the appripriate S/N cut, if any, before moving on to interactively clean or remove pixels as described in the next two sections. Once a pixels have been cleaned or removed, the S/N Limit field will be greyed out. To perform another S/N cut, the user must reload the spectra.*

7.4 Cleaning

6. If the multi-order data were loaded, then the user should choose an order to clean by typing 's' for **Select** anywhere in the wavelength range of the order or by selecting the order number from the **Select Order** pull-down menu in box #3. The spectrum will be automatically centered in the plot window and the other orders will turn grey. The **Fix**, **Remove**, **Undo**, and **Save** buttons will also become sensitive in box #3. If the user is cleaning a single spectrum, then the **Select Order** pull-down menu will be insensitive.

7. At this point, the user has two options to clean the spectrum:

   - Removing pixels: To remove pixels from the spectrum by replacing their values with NaNs, type 'r' or click the **Remove** button in box #3. The red cursor cross hair will become a cyan vertical line at which point the user should press and release the left-most mouse button on the left and right side of the wavelength range to be removed. The pixels in the user selected wavelength range will be set to NaN and the masked region will be displayed above the plot window in the Remove Mask. To **U**ndo the edit type 'u' or click the **Undo** button in box #3. To **S**ave the edit, type 's' or click the **Save** button in box #3.
   - Fixing pixels: To **F**ix a region of the spectrum, type 'f' or click the **Fix** button in box #3. The red cursor cross hair will become a cyan vertical line at which point the user should press and release the left-most mouse button on the left and right side of the wavelength range to be fixed. The pixels in the user selected wavelength range are replaced using the edge pixels to define a line. To **U**ndo the edit type 'u' or click the **Undo** button in box #3. To **S**ave the edit, type 's' or click the **Save** button in box #3. The bit-mask flag array will be updated to reflect the fact that pixels were replaced.

8. If the user is cleaning a single spectrum, then they can continue the cleaning process. If the user is cleaning multi-order spectra, then when the user is done editing the order, they can either select another order to clean, or type 'd' (for **Done**) or select **None** from **Select Order** pull-down menu in box #3. In the latter case, the grey-colored orders will return to their normal alternating white/green colors and the user can continue cleaning orders by selecting another order.

7.5 Smoothing

9. At any point in the process, the user can smooth the spectra in one of two ways. However once executed, the user cannot smooth the data again and box #4 will become insensitive. The user has two options to smooth a spectrum.

   - Savitzky-Golay (SG) smoothing, which is described in detail in Numerical Recipes, will smooth the spectrum while preserving the average resolving power. `xcleanspec` will automatically provide an estimate of the best SG window in units of pixels (in box #4) based on the slit width. The best window size is typically 1 to 2 times the slit width, although we have found that for the 0.3 arcsecond slit, 1.5 times the slit width does nothing. The degree of the smoothing function can also be chosen (in Box #4), but must always be less than the window size.

- Gaussian smoothing will smooth the spectrum with a Gaussian kernel with the requested FWHM (in box #4). Note since the resolving power changes as a function of wavelength, only the average resolving power will be modified. The default FWHM is the slit width given in pixels.

Note: *Please check the final spectrum to make sure you are happy with the results. If not, you will have to reload the data and start again.*

7.6 Write the File to Disk

10. When the user is done editing and/or smoothing the spectrum, give the root of the output file name in the **File Name** field (the .fits suffix will be automatically appended to the output name). `xcleanspec` automatically copies the root of the filename to the field in case the users wishes to simply append a string, e.g., 'm', to the file name. Click the **Write File** button in Box #5 and the file will be written to disk in the directory the input file is located. The spectrum will be displayed in the `xvspec` GUI.

8 FAQ

1. *Are the wavelengths returned by Spextool in vacuo or air?*

   All wavelengths generated by Spextool in are in vacuo.

2. *My SpeX calibration files do not have the prefixes "flat" and "arc" or my data are so old that I cannot use the Cal Panel.*

3. *How do I convert the Spextool FITS files to something useful like ASCII?*

   See §3.8

9 Miscellaneous Notes

9.1 xcombspec

As of v3.3, xcombspec applies a single scale factor, determined from the user-selected order, to all the orders. Older versions determined separate scale factors for each order. The switch to a single scale factor per spectrum was made because (1) we found that the use of separate scale factors for each order resulted in mismatches in the flux levels in the order overlap regions in the final combined spectrum; and (2) scale factors could not be determined reliably in those orders with low S/N. The use of a single scale factor determined from a high S/N order obviates problem (2) while simultaneously yielding excellent flux level agreement in the order overlap regions of the combined spectrum.

Nevertheless, the adoption of a single scale factor has revealed another challenge for the combining procedure and software. If there were no systematic/instrumental effects, the use of a single scale factor for a given spectrum across all orders should give the same result as applying separate scale factors for each order. However, as explained above, we have found that, after adopting a single scale factor for each spectrum across all orders, the slopes of spectra recorded by SpeX for a single object within a block of 5 A-B pairs taken one after another can vary by a few percent.

Although it is not yet clear exactly what causes this variation, we believe it results from a combination of physical effects (flexure, guiding errors, atmospheric dispersion, variable transmission, etc.) and it does not appear to be due to any procedures involved in the data reduction. We believe that xcombspec incorporates the appropriate procedure for combining these spectra (yielding the median spectrum with the correct slope). Nevertheless, **we urge users to perform the same steps and use the same statistics for their standard stars as for their objects.**

10 Version History

The most recent version of Spextool is v5.0.3.

v5.0.1: 2017-10-18

- added J0 and Kgas mode.
- Fixed line atlas plotting error (no longer duplicating lines)
- Fixed loss of final significant digit in some line wavelengths
- Added the `WCTYPE` and `RECTMETH` keywords

v5.0: 2017-10-09

- iSHELL data can now be reduced with Spextool.
- Large additions and modifications to the code to allow for the extraction of data where the spatial axis is not aligned with the columns of the detector.
- Major changes to the GUIs to deal with the large number of orders present in iSHELL data.

v4.2: 2015-02-XX

- General bug fixes.
- Major re-write of the manual to improve the description of both bright and faint sources and extended sources.
- Major update in the way user's identify apertures and select orders for extraction.

v4.1: 2015-01-20

- General bug fixes.
- Added a new flag that identifies pixels that cannot be optimally extracted.
- `xvspec` can now write Spextool FITS files and ASCII files to disk.
- `xvspec` can now display both the A and B extractions. The user can switch between buffers by typing 'a' or 'b' or using the pulldown menus.
- `xvspec` can now plot multi-order extractions in a single plot window. This method is now known as "Contiunous" display while the older method is known as "Ladder" display.
- `xvspec` can now plot the atmospheric transmission on the spectra (use Plot pulldown menu).

v4.0: 2015-01-XX

- A full pdf manual supercedes the ASCII help files.
- Spextool now lets the user choose the file prefix in the read mode panel by a pulldown menu instead of having to type them in.
- A median spatial profile can be used for optimal extraction instead of a wavelength dependent one (useful in low S/N cases).
- The cal panel now has a prefix column to allow for different sky frames with different file prefixes.
- Added an ITOT keyword to the output FITS files.
- The default plot ranges are now derived intelligently to avoid bad pixels.
- Major internal re-write to allow incorporating new instruments easier.
- Ximgtool has been completely re-written and boasts more capabilities.
- The appearence of the ximgtool and xvspec widgets are improved.
- Lines and symbols plotted on ximgtool are now permanent when the user zooms or pans around the image.
- More FITS headers keywords have been added to the ouput files and the histories are no labelled and self-consistent.
- Spextool will now check to make sure that there are not multiple file names with the same index number but a different prefix (e.g. spc0001.a.fits and arc0001.a.fits).
- Atmospheric transmission curves at the correct resolving power are now displayed in xcleanspec and xtellcor.
- Output images are now stored as multi-extension FITS files.
- Wavecal files are now full array images that include the wavelength solution and the spatial solution.
- Almost all routines have the prefix 'mc_' in order to avoid conflicts with other libraries.
- Spextool now includes a flag array on its output that allow the user to identify flux density values that have been affected by bad pixels or saturated pixels.
- Quality assurance plots are generated for all wavelength solutions except the prism mode.

v3.4: 2005-11-08

- Fixed image math base in ximgtool
- Fixed an xmergexd error and added both the SXD and LXD HISTORY fields to the final FITS file

- Fixed bug when concatanating headers that do not have the same sized HISTORY fields
- Renamed xfit2text to xspex2text and fits2text to spex2text
- Updated plotting character sizes to scale with the plot window sizes
- Added a rountine to test the seeing for optimal extraction (See step 16).
- Added an IDLWAVE catalog file
- Added ability to specify aperture positions independently in each order
- Postscript plots (ShortXD_IDs.ps, LongXD_IDs.ps) showing the identification of the lines used for wavelength calibration are included in Spextool/data
- Fixed bug in `xtellcor_finish` regarding the YUNITS FITS keyword.
- Spextool is now Windows compatible (thanks to Dan Clemens, BU and Joshua Kim, UA)

v2.1: 2001-Oct-09

- Fixed bugs in xcombspec
- Added xsmoothspec widget to smooth spectra by a Gaussian with FWHM equal to the slit width in pixels
- Added a fits2text program to convert a SpeX FITS file to a text file
- Improved bad pixel replacement
- Added a data set to allow the user to practice using Spextool

v2.0: 2001-Aug-17, Major revisions

- Errors are now propagated through the extraction process. An error vector is now produced and appears as a third dimension in the FITS array or another column in the text array.
- All output names (i.e. arcs, flats, etc) should NOT have the suffix .fits added now. Spextool will add it automatically. When loading images in using full names, the entire name, including the .fits, should be entered.
- Xplotprofiles now shows the raw data and and has cursor tracking.
- Xvspec can show the error spectra and compute the signal-to-noise in each spectrum.
- Xvspec can now smooth the spectra (convolve with a Gaussian of FWHM = npixels) and propagate the error.
- To launch a zoom window (xzspec) in xvspec, click on the order you want to examine. Xzspec is fully resizable. To learn the keyboard commands, type 'h' in the plot window.

- A new widget called xmkcals allows the user to construct the flats and arcs for the entire night.
- The xcombspec widget has been completely redesigned to allow more user input.

v1.5: 2001-Mar-09

- Improved wavelength calibration for the LXD1.9 and LXD2.3. See step 8.
- Improved flat fielding (To be described later).
- Prism mode can now be fully reduced.
- Modified Path input.
- XQTV can now perform image arithmetic (under file menu button).
- xcombspec has been modified to combine apertures if requested. This is useful when point source data is combined before being extracted. In this case, Spextool writes both apertures to the same file.
- Wavelength calibration now requires a user input which gives the pixel offset of an arc spectrum relative to a standard arc spectrum.

v1.4: 2000-Dec-18

- Fixed bug where the spectra returned using the extended source extraction base WERE NOT in DN/s. The values are now returned as DN/s.
- Added Combine base (see below).
- Fixed a bug which made the spectra appear to have some sort of fringing when small apertures, < 1 arcsecond, were used.
- Modified the way the arcs, flats and skys are stored. As a result, arcs, flats and skys made using earlier versions of Spextool have to modified as follows: At an IDL prompt:

  IDL> `i = readfits('filename',hdr)`
  IDL> `writefits, 'filename',rotate(i,7), hdr`

  The flats, arcs, and skys can now be used with version 1.4.

v1.3: 2000-Oct-24

- bug fixes in xcombspec

v1.2: 2000-Oct-20

- added xcombspec

- modified PS extraction
- added description of xvspec

v1.1: 2000-Oct-18

- Bug fixes and added a sky base

v1.0: 2000-Oct-13

- Original release

A iSHELL Wavelength Calibration with the ThAr Lamp

Wavelength calibration in the near-infrared and L1 modes of iSHELL is accomplished using a low-pressure ThAr arc lamp that is moved directly in front of the entrance aperture of iSHELL when required. The fact that the lamp light does not have the same beam as the light from the sky has a number of effects that users of these modes must be aware of in interpreting their data.

A.1 Line Shapes

Figure 9 shows the line traces of emission lines in the L1 and H2 modes; ThAr lines were obtained using the low-pressure lamp while the OH line was obtained on sky. All the data were obtained using a 15″ slit.

Note: *The axes are reversed so that we are plotting column position as a function of row position.*

The top panels show the positions of the lines along with a second order polynomial fit to the data. The lower panels show the residuals between the data and the model. The left and middle columns show the trace for a ThAr emission line (the 15″-long slit was used for the H2 mode instead of the default 5″-long slit) while the right column shows the trace for an OH emission line. The ThAr lines show non-random residuals while the OH emission line shows random residuals. We believe this is a result of the fact that the ThAr arc lamp is placed directly in front of the entrance aperture (because is not bright enough to pass through the integrating sphere and still be detectable in reasonable integration times).

A.2 1DXD Solution

Figure 10 shows the 1DXD QA plot (see 4.2.2) for the H2 mode using ThAr lines (*left panel*) and OH sky lines (*right panel*) to determine the solution. The ThAr residuals are both larger and are non-random while the OH line residuals are smaller and random. While in principle this could mean that there are systematic errors in the ThAr wavelengths, we see similar patterns in other near-infrared modes (e.g. the K3 mode shown in Figure 3) and thus we believe this is also a result of the fact that the ThAr arc lamp is placed directly in front of the entrance aperture instead of passing through an integrating sphere.

A.3 Distortion

As part of the wavelength calibration procedure, we fit the positions of each line on the array with a polynomial model. Modes with a 5″ slit only require a linear model to accurately model their positions. The left panels of Figure 11 show the c1 coefficients (i.e. slopes) for the ThAr and OH lines in the H2 mode.

Note:*We actually fit the x position as a function of the y position of the line. As a result, a line with c1=0 is perfectly aligned with the columns of the detector. We nevertheless call the c1 coefficient the "slope".*

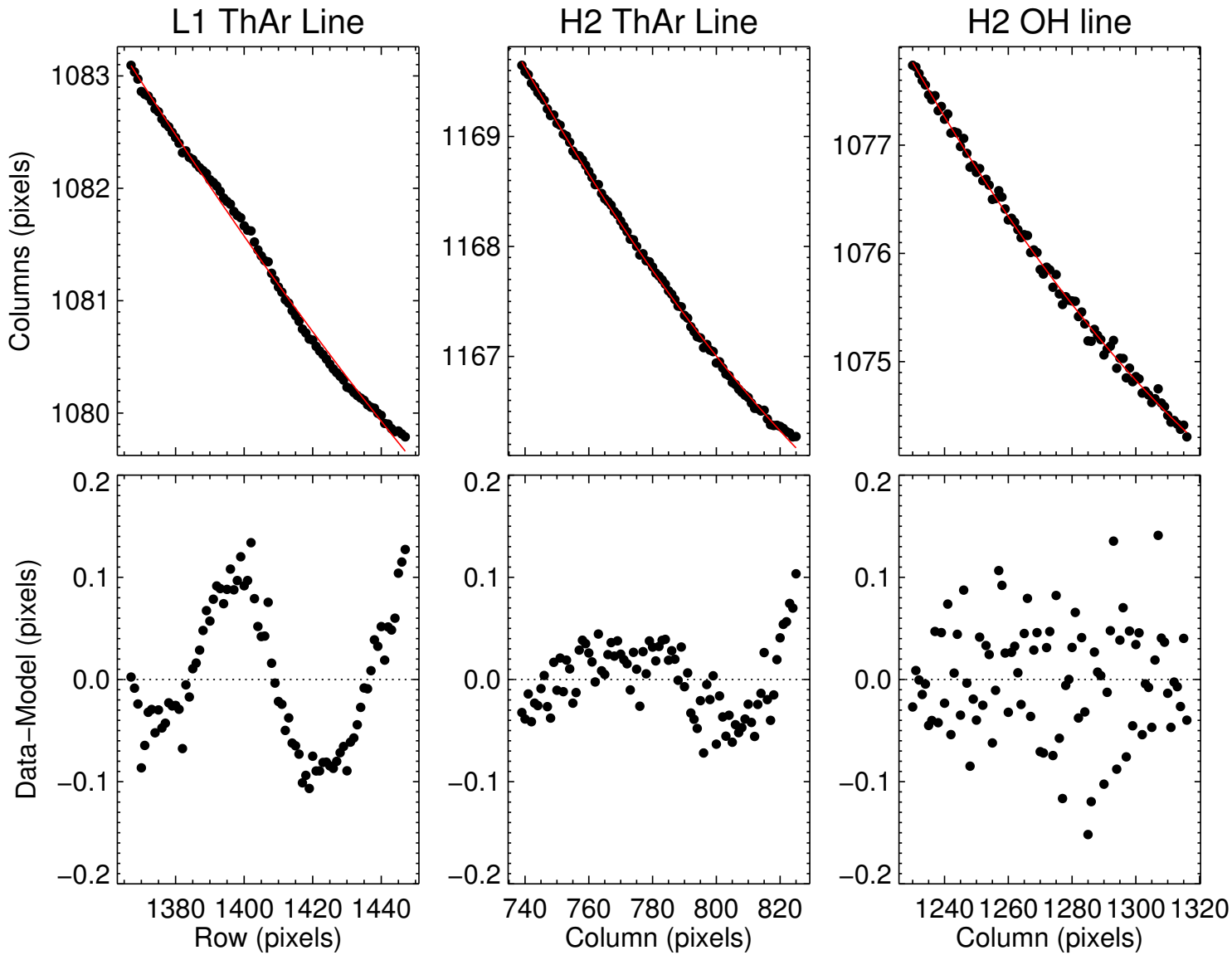

Figure 9: *Line traces of emission lines in the L1 and H2 modes. The top panels show the positions of the lines along with a second order polynomial fit to the data. The lower panels show the residuals between the data and the model.*

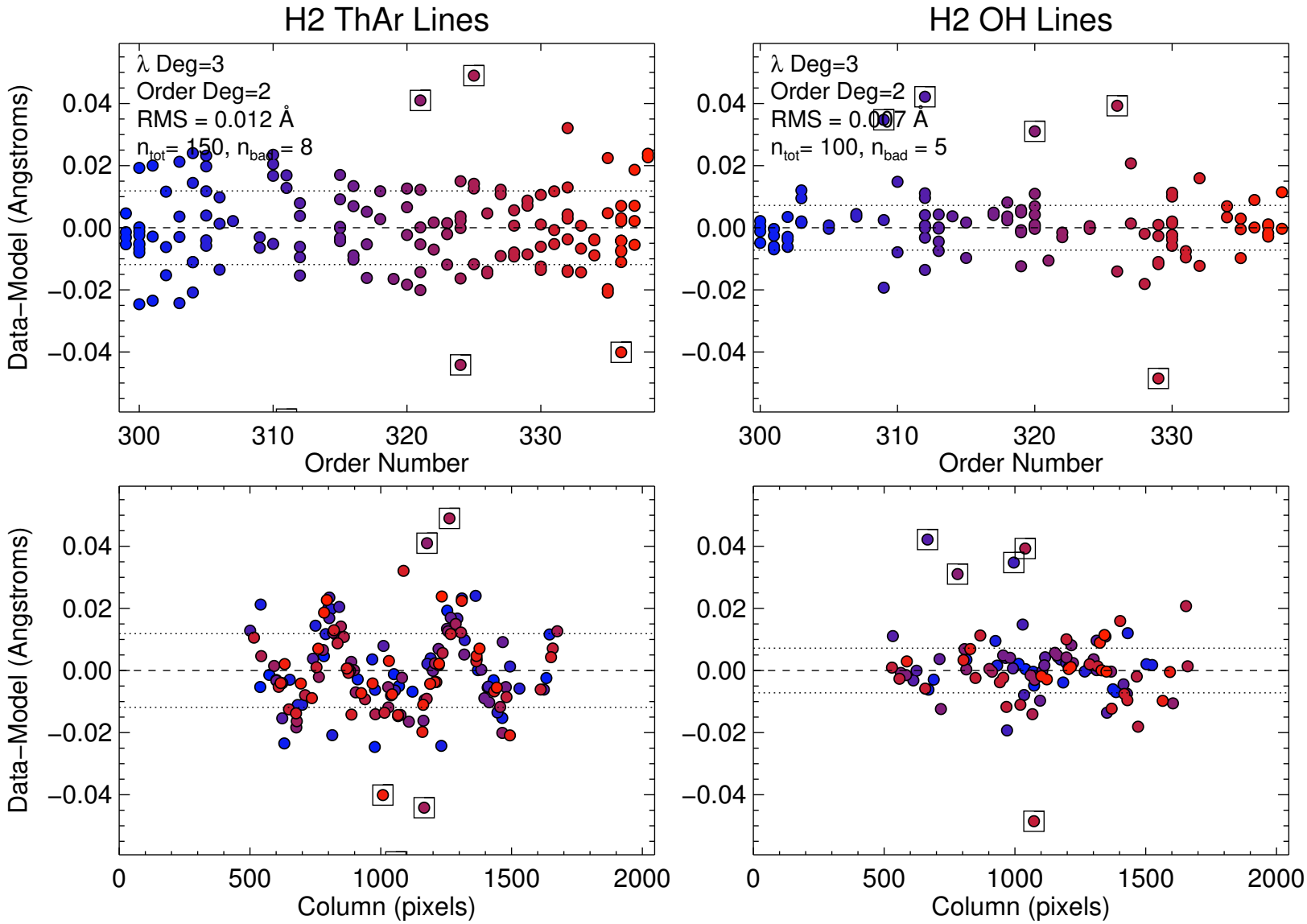

Figure 10: *1DXD QA plots for the H2 mode. The left panel was generated using ThAr lines while the right panel was generated using OH lines.*

The right panels shown an polynomial interpolation of the data points to guide the reader's eye. The ThAr lines show a larger (negative) slope in the upper right hand corner of the array, a result we also believe is due to the ThAr arc lamp is placed directly in front of the entrance aperture instead of passing through an integrating sphere.

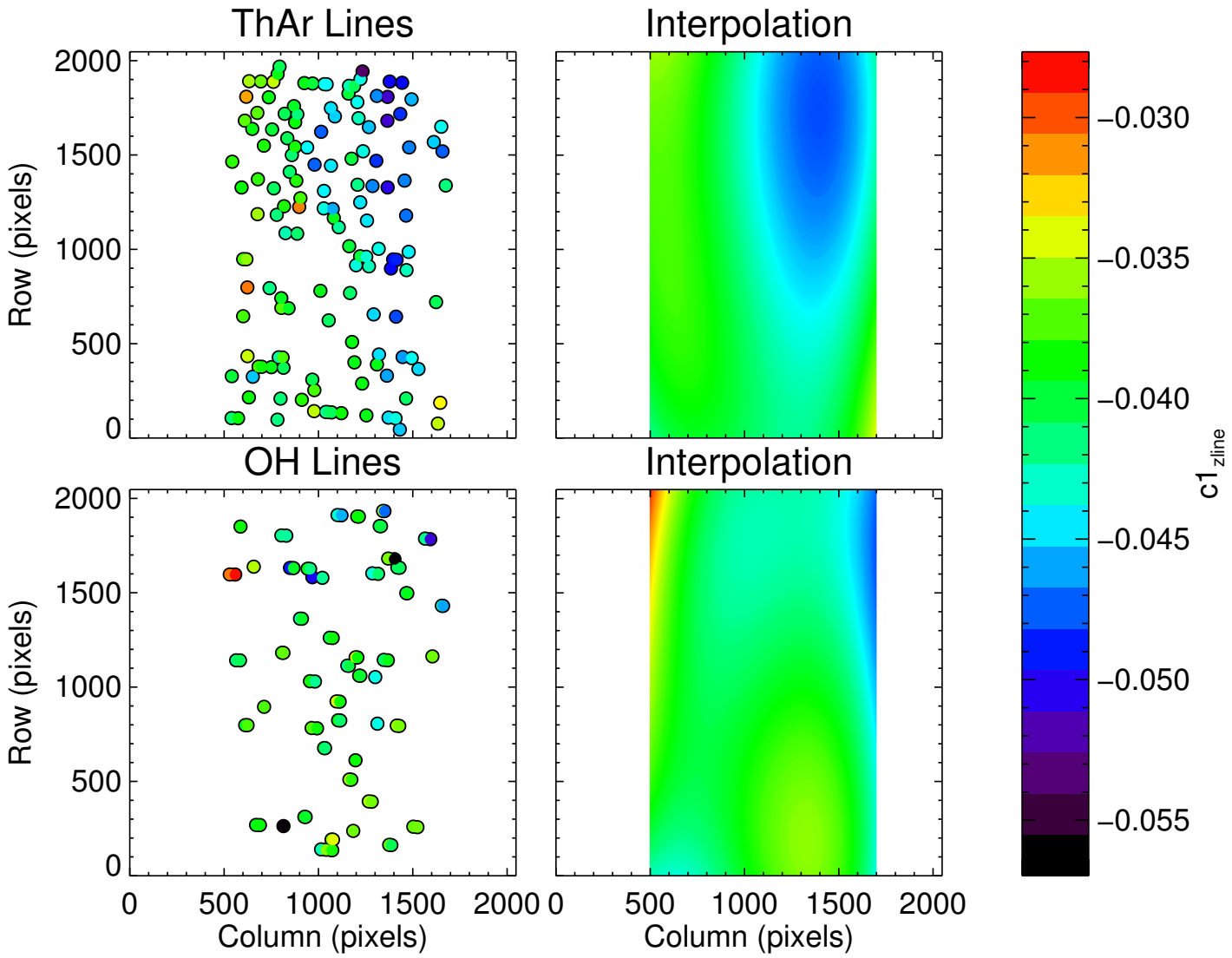

Figure 11: *c1 coefficient values (slopes) of lines in the H2 mode. The top panels are for the ThAr lines while the bottom panels are for the OH lines.*