Wavelength calibration sources for the near infrared arm of X-shooter

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ABSTRACT

We have studied the properties of wavelength calibration sources for the near-IR (NIR: 1000-2500 nm) arm of X-shooter. In a novel approach we are combining laboratory measurements from a Fourier Transform Spectrometer (FTS) and literature data with corresponding simulated data derived from a physical model of X-shooter. The sources studied are pen ray lamps filled with the noble gases Ne, Ar, Kr, and Xe and Th-Ar hollow cathode lamps. As a product we provide a quantitative order by order analysis of the expected properties of the calibration lamps during X-shooter operations. The analysis accounts for blending of lines and makes realistic assumptions about the dynamic range available in a typical wavelength calibration exposure. Based on our study we recommend the use of Ne, Kr, and Ar as the best three lamp combination for X-shooter calibration. A detailed comparison between the predicted and actual performance of the calibration system has been started as part of the X-shooter testing and validation phase and first results are very promising. To our knowledge this is the first time that such a detailed and quantitative analysis of a calibration system has been done prior to the operation of the instrument. The combination of laboratory measurements and instrument modeling provides a powerful tool for future instrument development.

Keywords: calibration, wavelength, near infrared, spectroscopy, FTS, X-shooter

1. INTRODUCTION

X-shooter is a single target spectrograph for the Cassegrain focus of one of the VLT UTs covering in a single exposure the spectral range from the UV to the K band (320–2500 nm). It is designed to maximize the sensitivity in this spectral range by splitting the incoming light into three arms (UVB, VIS and NIR) with optimized optics, coatings, dispersive elements and detectors. X-shooter will be a unique instrument on 8 m class telescopes in that it is capable of recording - over such a large wavelength range - the spectrum of an astronomical target in a single exposure. It operates at intermediate resolutions (R=4000–14000, depending on wavelength and slit width) sufficient to address quantitatively a vast number of astrophysical applications while working in a background-limited S/N regime in the regions of the spectrum free from strong atmospheric emission and absorption lines. The instrument is currently undergoing subsystem assembly and commissioning is scheduled for fall 2008. The following table lists the main characteristics of X-shooter:

Table 1: Basic properties of X-shooter

Spectral Format	Prism cross-dispersed echelle (order separation ≥ 12")
Wavelength range	300-2500 nm, split in 3 arms by dichroics
Slit configuration	long slit (~12"); widths: 1" (standard), 0.6" (high resolution), 5" (flux calibration); IFU 1.8" x 4" input area
Detectors	2k x 4k CCDs (UV and Visual-Red arms), 2k x 2k (1k x 2k used) Hawaii LPE MCT (IR)
Auxiliary functions	Calibration Unit; acquisition and guide unit with 1' x 1' field and filter set; ADC for the UV and Visual arms.

2. WAVELENGTH CALIBRATION DURING X-SHOOTER OPERATIONS

X-shooter is equipped with a dedicated calibration unit providing light for flat fielding and wavelength calibration across the entire operating range of the instrument. The unit consists of two arms: one employs a diffuser plate illuminated by faint sources - D_2 lamp used for Flat Field in the UVB arm and the Th-Ar HCL for wavelength calibration of the UVB and VIS); the other uses a 6 inch integrating sphere fed by bright sources (3 Quartz Tungsten Halogen (QTH) for UVB, VIS, and NIR Flat Field and up to 4 pen ray lamps (Ne, Ar, Kr, Xe) for NIR wavelength calibration.

The light of up to four pen ray lamps is superimposed in the integrating sphere and a combined spectrum is fed to the spectrograph. The four pen ray lamps will be operated as a single source that is all lamps, although using separate power supply units (PSUs), will be burning simultaneously and for the same length of time. Hence, the intrinsically different intensity levels of the lamps need to be balanced by the positioning of the lamps inside the integrating sphere and by shielding cylinders mounted around the lamps. In this report we have studied the properties of pen ray lamps with a noble fill gas, Ne, Ar, Kr or Xe in order to provide a basis for the selection of the best lamp combination. So far one set of pen ray spectra has been taken during the X-shooter test phase. Preliminary results are presented in section 7.3. Based on this the actual set-up and performance of the calibration sub-system will be optimized.

3. WAVELENGTH CALIBRATION SOURCES FOR X-SHOOTER

To fully realize the scientific potential of X-shooter excellent wavelength calibration across all three arms is essential. For UVB and VIS, Th-Ar hollow cathode lamps (HCLs) have been chosen as calibration sources following the successful operations of such lamps in e.g. FEROS, FLAMES, HARPS and UVES. At the spectral resolution of X-shooter though blending of lines becomes an issue[1] and the optimum choice of sources will be determined during the X-shooter test phase. For the NIR arm less experience was available and we decided to conduct a dedicated program to select the best combination of calibration sources for this wavelength region which traditionally has relied on atmospheric features for wavelength calibration. Recently, ESO has gained significant experience with NIR wavelength standards in a collaboration with the US National Institute of Standards and Technology (NIST) as part of the CRIRES project[2,3].

Currently, there is no comprehensive database of emission line spectra of commercially available light sources. Based on experience a combination of gas discharge lamps (Ne, Ar, Kr, Xe pen ray lamps) were envisaged. In addition we looked into the possibility of utilizing a Th-Ar HCL also for the NIR arm.

3.1 Pen ray lamps

These lamps are called “Pencil” lamps because of their size and shape. They are made of double bore quartz tubing with two electrodes at one end sealed into a handle. These lamps produce narrow, intense lines from the excitation of various rare gases and metal vapors. They are commercial products widely used for wavelength calibration of spectroscopic instruments such as monochromators, spectrographs, and spectral radiometers e.g. in industrial and chemical analysis applications.

3.2 Th-Ar Hollow cathode lamps

Modern commercial hollow cathode lamps are sealed-off glass tubes that contain a metal cathode, a metal anode and a fill gas at a defined pressure. The lamp is operated by applying a voltage of a few hundred volts across cathode and anode. As a result, a discharge is formed in the low pressure (few hundred Pa) fill gas and positive ions of the plasma are accelerated towards the cathode where they release matter through sputtering. As a result a HCL emits a rich spectrum of narrow emission lines from both the gas and metal atoms and ions in the plasma; for a detailed technical review of HCL and their operations see Kerber at al.[2]. The Th spectrum was studied more than 20 years ago in the range from 278 nm to about 1000 nm at high resolution by Palmer & Engleman[4]. Its emission lines are very narrow and the spectrum is rich over a wide wavelength range. In nature Th has only one isotope, ^{232}Th, which has zero nuclear spin. Thus the use of Th for calibration lines avoids complex and asymmetric line profiles attributable to isotopic or hyperfine structure. Th-Ar HCLs are widely used for wavelength calibration of high resolution spectrographs in the Visual, including many examples at ESO such as FEROS, FLAMES, HARPS, and UVES.

Two valuable studies of the Th-Ar spectrum in the near IR have recently been published, but neither is directly applicable to the operation of X-shooter:

- Hinkle et al.[5] produced an atlas of the Th-Ar spectrum covering selected regions in the range 1000 nm to 2500 nm. Their list of about 500 lines contains significant gaps in wavelength coverage.
- A fundamental analysis of the Th-Ar spectrum was provided by Engleman, Hinkle & Wallace[6]. Their list contains more than 5000 lines. Their high current source is very different from low current commercially available lamps and is not well suited for operation at an astronomical facility. Although the spectrum from the high current lamp is significantly different from commercial Th-Ar lamps, the line list is highly valuable for identification of the lines in low current spectra.

The near-IR spectrum of low current Th-Ar HCLs has been studied extensively at high spectral resolution by a collaboration of ESO and the US Institute of Standards and Technology (NIST) producing NIR wavelength standards for ESO's CRIRES[3]. X-shooter directly benefits from this experience.

4. GOALS OF THE PROJECT

In order to provide a solid basis for the selection of the best combinations of calibration lamps in the NIR we set out to address the following topics:

- measure the spectra of commercially available pen ray lamps filled with Ne, Ar, Kr, Xe,
- determine line density and intensity ratios of lines for each lamp,
- determine the relative intensities of the four lamps,
- select a suitable combination of one to four pen ray lamps,
- compare such a composite gas spectrum to the spectrum of a Th-Ar hollow cathode lamp,
- quantify the number of unblended lines,
- study issues related to the operation of the calibration lamps, such as stability, lifetime, optimal operating current etc.

5. EXPERIMENTAL SETUP

ESO operates a commercial Fourier Transform Spectrometer (FTS) (Thermo 5700) in its laboratory. The spectrometer is equipped with an external port that allows one to feed the light from external light sources to the FTS for analysis. ESO's Integration and Cryo-vacuum Department in Instrumentation Division has built a permanent set-up for the external feed which replicates part of the optical train of the FTS. We used a CaF_2 beamsplitter and a thermo-electrically cooled InGaAs detctor to observe the wavenumber range 10000 – 4000 (1000 – 2500 nm). At a resolution of 1 cm^{-1} that is equivalent to X-shooter (R~10000 at 1000 nm). More details of the set-up and a picture are given in Kerber et al.[7].

Originally, we had planned to emulate the X-shooter calibration unit as closely as possible using all four pen ray lamps inside an integrating sphere. The PSUs for lamp operations on X-shooter provide AC only. The resulting modulated output of the lamps is not suitable for analysis by the FTS. Hence we had to operate the pen ray lamps one at a time using a special PSU that is switchable between AC and DC. Although built for the purpose by the lamp manufacturer, the DC provided by this PSU is not very stable and the resulting interferogram of the FTS shows increased noise due to the residual modulation of the input signal. When using individual lamps inside the integrating sphere the signal from any of the lamps was significantly too low for the FTS to work. Hence we decided to mount the lamps individually in a way that they directly illuminate the FTS feed. The lamps were oriented parallel to the optical path and with their tip facing the FTS feed. Alignment and focusing of the lamps without the integrating sphere is rather critical but the He-Ne laser of the FTS itself gives a very good indication of the optimum position of the lamps.

6. MEASUREMENTS

6.1 Pen Ray lamps

The wavelength range and resolution of the FTS were chosen to match the X-shooter NIR arm. Each lamp was carefully aligned with the optical path in order to see and maximize the signal on the FTS interferogram. The lamps were operated with an AC/DC switchable power supply. For each pen ray lamp we took several spectra varying both the operating current and exposure time. Sample spectra of the lamps are displayed in Fig. 1.

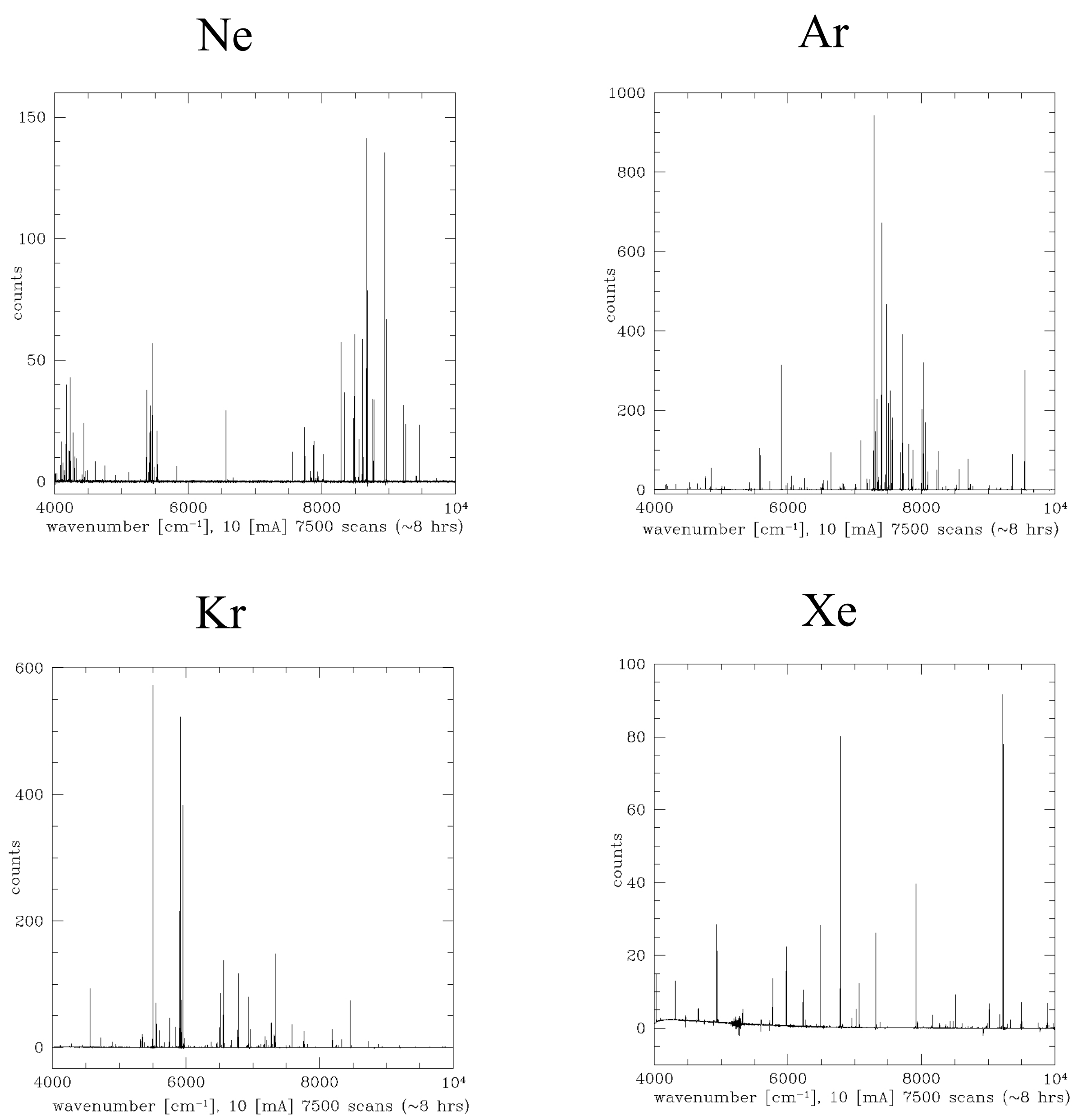

Figure 1: FTS spectra of the Ne, Ar, Kr, Xe pen ray lamps at X-shooter spectral resolution

6.2 Th-Ar Lamp

The settings of the FTS were the same as used for the pen ray lamps. Again, we took several spectra of this lamp, varying both current and exposure time. Long exposure times are essential in order to reach a reasonable S/N. A sample spectrum taken at 10 mA is depicted in Fig. 2.

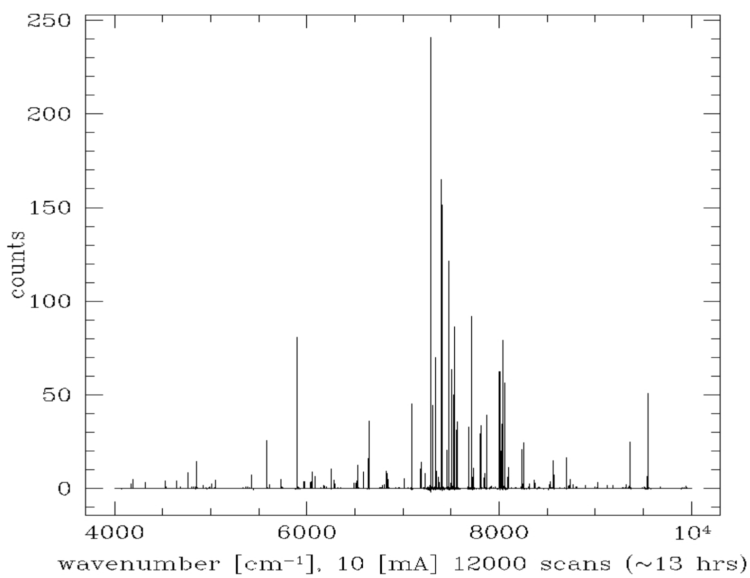

Figure 2: Near-IR spectrum of a Th-Ar hollow cathode lamp taken with ESO's FTS

7. PHYSICAL MODELING AND SIMULATED DATA

7.1 Physical Model

Traditionally the wavelength calibration of spectrographs relies upon an empirical approach. An exposure of a source, usually an emission lamp, with clear, laboratory-calibrated features, is obtained. The location of features on this wavelength calibration exposure are then matched to the catalogued wavelengths of the source, and a low order polynomial is fitted to the data points to provide an empirical relation between positions on the detector and wavelengths. A meaningful polynomial fit will require a sufficient density of useful lines distributed over the wavelength range of interest. Since such an empirical polynomial fit has zero predictive value outside the range defined by data points, a lack of calibration lines at the limits of the wavelength ranges and detector boundaries is particularly critical. We replace this empirical method of wavelength calibration by using our physical understanding of the instrument[8]. In order to avoid computationally expensive, but for the present purpose unnecessary level of detail, those surfaces which do not affect the relative geometry on the detector (e.g. plain folding or pick off mirrors) are neglected. However, the ray tracing at all relevant surfaces is performed by the appropriate 3D matrix transformation[9]. Since the principle goal for the model is to provide wavelength calibration, the orientation, offsets and other properties of dispersive components can be optimised via comparison to calibration data from the instrument. The physical model approach as used for X-shooter wavelength calibration is described in greater detail by Bristow et al.[10].

7.2 Simulated Date 2D Echellograms

The present study requires not only computation of where a photon of a given wavelength arrives on the detector, but also the spectrograph throughput (which we combine with the spectral line intensity) at that wavelength. This is achieved via empirical functions (i.e. they cannot be optimised in the way the physical model parameters can) that describe the quantum efficiency of the detectors and the throughput of the dichroics at each wavelength.

In addition we require a description of the entrance slit. The entrance slit model is rectangular, having a profile in the dispersion direction that is a 1.0" box function convolved with a 0.02" Gaussian and a profile in the cross dispersion direction that is a 12.0" box function convolved with a 0.2" Gaussian.

We use a Monte-Carlo approach to simulate the counts expected on the detector array during an exposure. In this way 2D simulated data containing many photons are produced by multiple calls of the physical model code. We begin with a line list for an emission lamp that specifies wavelengths and relative intensities of spectral features. We scale the intensities appropriately for the signal to noise that we want to achieve. Then, for each feature, the slit model is used to distribute the appropriate number of virtual photons in the entrance slit plane in Monte-Carlo fashion. Next the virtual QE (above), dichroic and blaze functions are used to compute the probability of a photon at this wavelength reaching the detector. At high flux levels (>1000 virtual photons) the fraction of virtual photons arriving on the detector is simply the calculated throughput multiplied by the flux, at low flux levels each photon is treated individually using a pseudo-random number generator.

Using the model in this way we have been able to generate, 2D simulated data for known sources that are being used as test cases for the development of the X-shooter data reduction software. Example of such simulated 2D data and further details of the method are described in Bristow et al.[11].

7.3 Extracted 1D spectra and comparison with X-shooter laboratory measurements

In the current project, we take the 2D simulated data for each lamp and extract a 1D spectrum along the loci traced on the detector array by photons arriving at the centre of the entrance slit, in all orders. To improve statistics we include the counts from pixels within 20 pixels in the cross-dispersion direction.

As a result we have, for each lamp and each order, a 1D extracted spectrum. There is considerable overlap between the orders with features in the centre of the spectrum for one order appearing at the edge of an adjacent order but with a much reduced signal due to the blaze function. Figure 3 shows the blaze function and in Fig. 4 we show a sample 1D spectrum (order #20); the simulation has been done for all 16 orders of X-shooter NIR.

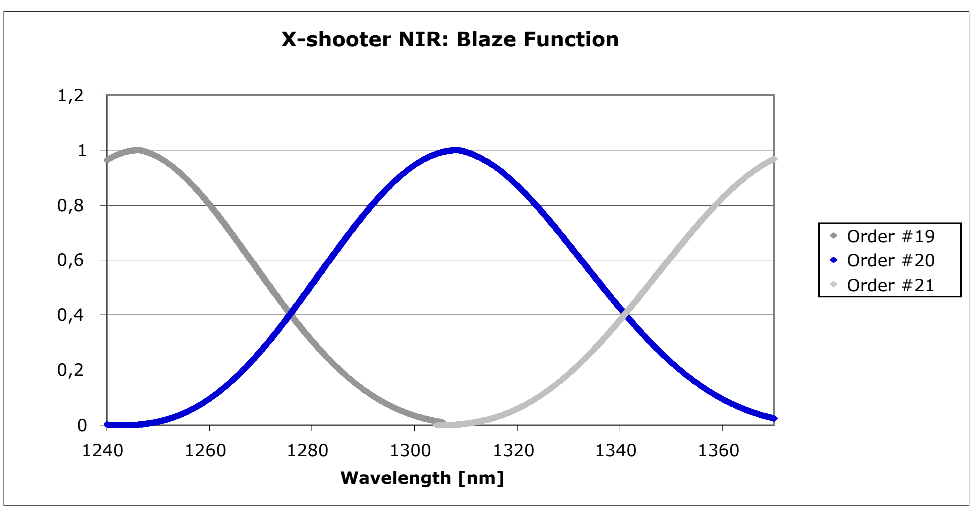

Figure 3: Blaze function of X-shooter NIR: order #20 and adjacent orders.

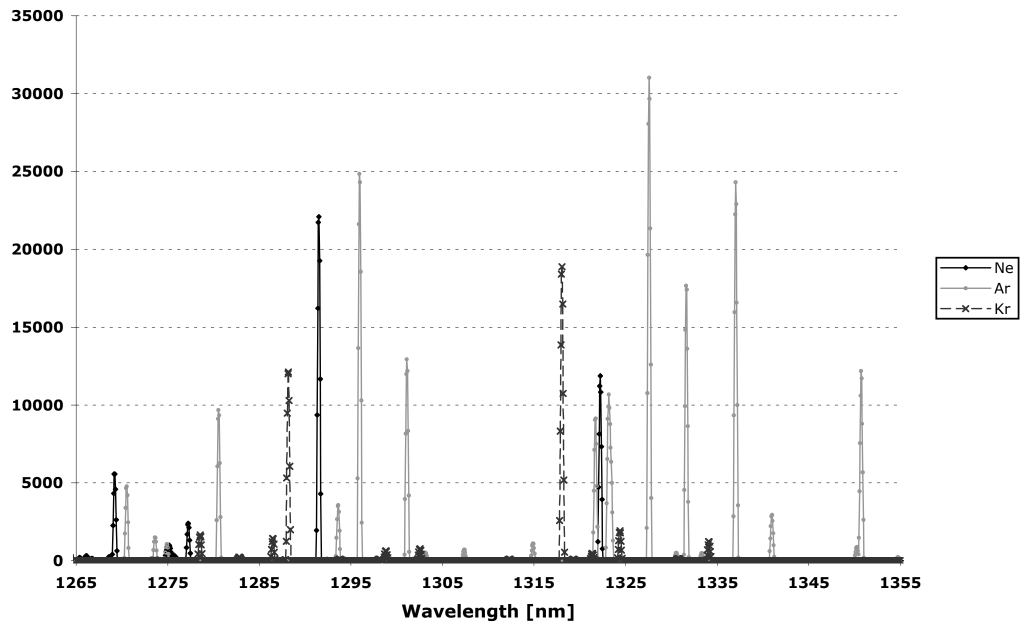

Figure 4: Simulated 1D spectrum of X-shooter NIR order #20. The lines from the different lamps are denoted by different shades of grey and symbols. The flux level of the lamps has been normalized such that the strongest line in all of the lamps yields 100000 counts. Xe has been omitted since it only provides one strong line in this order.

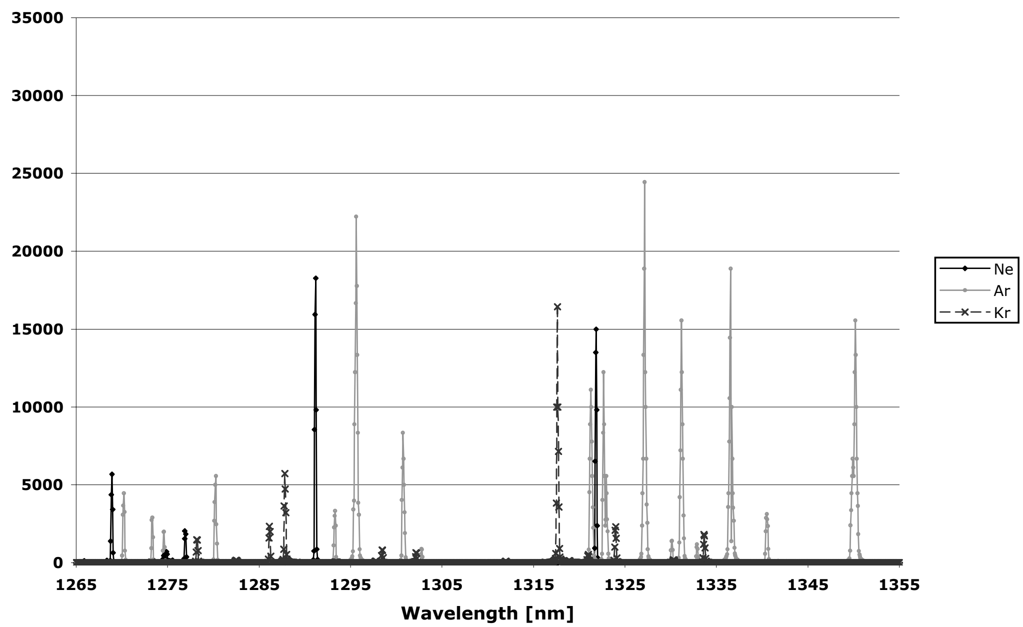

Figure 5: Order #20 as observed with X-shooter. The plot is an overlay of individual exposures taken of each pen ray lamp. The intensity of the strongest lines are somewhat uncertain since they saturated in this test and a correction had to be applied. Still the overall agreement between observation and simulation (Fig. 4) is very satisfactory.

One set of pen ray exposures has so far been taken with the X-shooter NIR arm during integration and testing. Individual spectra of Ne, Ar, Kr and Xe have been recorded and 1-D spectra extracted. They have been scaled individually since the intensity of the lamps needs to be brought to the same level in X-shooter. The results are similar to the ones expected from the simulations (Table 5). Since the strong lines are saturated in the X-shooter data some correction to their flux had to be applied resulting in some uncertainty in the actual intensity. Still the overall agreement between observation (Fig. 5) and simulation (Fig. 4) is very satisfactory. A more precise comparison can be done concentrating on lines that remained with the linearity of the detector (Figs 6 & 7). The spectra are also very similar to the literature line lists used as input for the simulations.

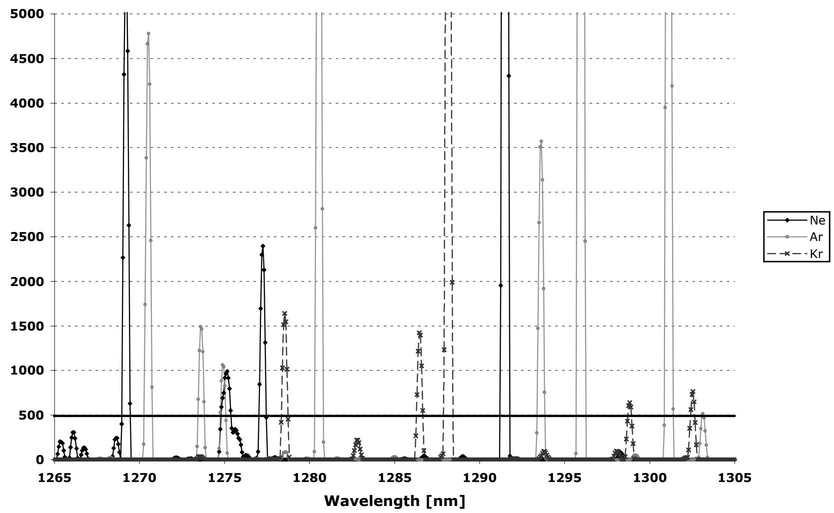

Figure 6: Part of order #20 simulated spectrum

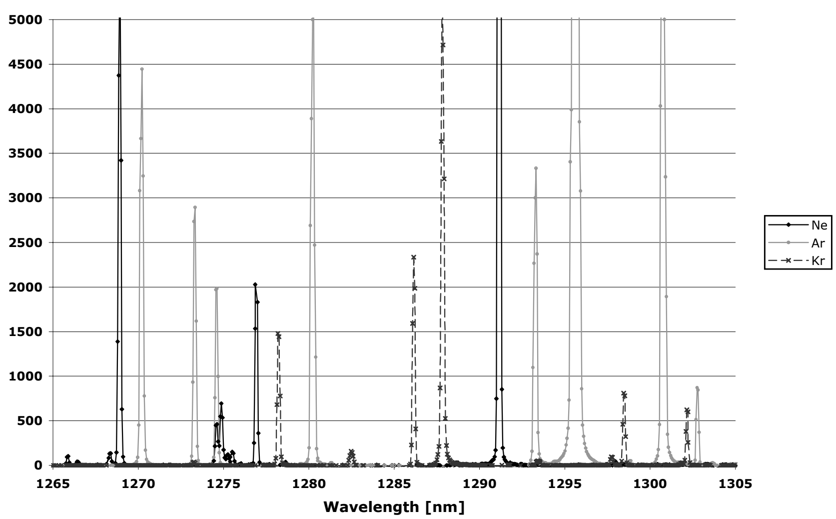

Figure 7: Part of order #20 as observed with X-shooter.

We find that the spectral resolution of X-shooter NIR is actually higher than the design specification and hence more unblended lines will be available. A single scaling factor for each lamp is sufficient to reach agreement of intensities while individual line ratios vary depending on the individual lamp. In summary the validity of the approach is fully confirmed and quantitative predictions based on instrument modeling can be done for calibration systems. We will continue the analysis throughout the X-shooter AIT phase and optimize its calibration system in the process.

8. ANALYSIS AND RESULTS

8.1 Line Identifications

For the identification of the lines we have used compilations available in the literature and some data provided by our colleagues at NIST prior to publication. In the wavelength range of the X-shooter NIR arm 4000–10000 cm^{-1} (1000–2500 nm) we have identified in the observed FTS spectra a total of about 700 lines distributed between the sources as shown in Table 2:

Table 2: Summary of the number of lines observed on the FTS spectra

Source	Number of lines observed with the ESO FTS	Number of lines available in the literature	Reference	Dynamic Range in Literature
Ne	80	350	Sansonetti et al. [12]	$1.5 \cdot 10^4$
Ar	155	360	Whaling et al.[13]	10^5
Kr	130	380	Sansonetti & Greene[14]	$4 \cdot 10^4$
Xe	65	120	Saloman[15]	$5 \cdot 10^3$
Th-Ar	350	> 2400	Kerber et al.[3]	10^4

A combination of Ne, Ar, Kr and Xe will provide a number of lines (~ 350) comparable to the Th-Ar lamp while providing a more even distribution of lines coverage for a given dynamic range. The Th-Ar spectrum includes a large number of faint Th lines (Fig. 2) most of which have not been recovered with our FTS measurements.

8.2 Order by order analysis

We have studied the number of lines for each lamp and each order of X-shooter individually. The following assumptions have been made in the analysis:

- In agreement with the envisaged scheme of operations (Section 2) we have assumed that all lamps have been brought to the same intensity level by appropriate measures. That is the strongest line in each lamp has been normalized to a value of 100000. Whether the same level can actually be achieved and by what means is the subject of the X-shooter integration and test phase.
- The dynamic range achieved in practice for a typical wavelength calibration exposure is limited by the linearity/saturation behaviour of the detector and usually is around 1000. Usually, saturation of the strongest line is avoided by using a short detector integration time (DIT). Then the faintest lines having a S/N suitable for use in wavelength calibration will have an intensity of a few 100 on the above scale. A total wavelength calibration exposure will therefore combine a small number of integrations times (NDIT) and we adopted an intensity of 500 as the lower limit for lines suitable for wavelength calibration purposes.
- A line suitable for wavelength calibration has an intensity in the range 500 - 100000
- A minimum of 10 lines is required for wavelength calibration in any order
- A goal of 30 lines is set for wavelength calibration in any order

In the following tables we summarize the result of this analysis for each lamp and order. We used a grey scale code to visualise the results (Tables 3 & 4).

Table 3: Requirement and goals for number of calibration lines provided

# of lines per lamp	# of lines - complete calibration system
0 – 3	< 10
4 – 6	10 – 19
7 – 9	20 – 29
≥ 10	≥ 30

In Table 4 the number of lines available from each lamp is given. The total includes blended lines, while the net gives the number of unblended lines accounting also for blending across lamps. This net number is the best current estimate of the lines usable for wavelength calibration. While the simulation is detailed and provides quantitative results the actual numbers observed by X-shooter may differ depending on the actual performance of the lamps and instrument. First results from X-shooter testing are promising (Figs 4-7) but a full quantitative comparison and validation of the process as well as optimization of the calibration sub-system is one main objective of the laboratory testing and commissioning phases.

Table 4: Summary of the number of lines provided by each pen ray lamp for a given order

Order # (λ [nm])	Ne	Ar	Kr	Xe	Total	Net
11 (2250-2500)	17	2	4	9	32	27
12 (2060-2270)	7	3	3	6	19	19
13 (1910-2110)	3	2	2	2	9	9
14 (1770-1960)	18	2	10	2	32	24
15 (1650-1825)	5	3	16	5	29	22
16 (1545-1710)	0	8	14	6	28	22
17 (1455-1610)	5	7	12	6	30	24
18 (1375-1520)	1	7	11	6	25	20
19 (1300-1440)	1	16	15	3	35	27
20 (1235-1370)	5	21	10	1	37	30
21 (1180-1305)	15	14	6	2	37	30
22 (1125-1245)	9	10	6	1	26	26
23 (1075-1190)	12	6	4	4	26	24
24 (1040-1140)	6	5	2	8	21	19
25 (1015-1095)	5	4	2	5	16	16
26 (995-1055)	0	0	0	0	0	0

8.3 Summary of various lamp solutions:

No combination of any two lamps provides a spectrum that satisfies the calibration needs of X-shooter. A combination of Ne, Ar and Kr is the best solution using three calibration lamps. Since Xe provides the fewest lines and is the faintest source the combination of Ne, Ar and Kr yields a spectrum almost as good as the full four lamp solution.

8.4 Relative Intensities

The FTS is not an ideal tool for measuring overall intensities of lines. For the current purpose we only need intensities of the lamps relative to each other and we derived these from the integral of the line fluxes in the region of interest. There is a factor of more than an order of magnitude in intensity between the faintest and the most intense source. Similar intensity ratios have been derived from observations with X-shooter (Table 5). In X-shooter the fluxes need to be brought to the same level in the integrations sphere since all calibration sources will be operated simultaneously (Sect. 2). One way to achieve this is to use different operating currents since each lamp has its own PSU.

Table 5: Relative overall intensities of the lamps based on the integrated line flux

Lamp	Relative Integral Intensity FTS (Ne =1)	Relative Integral Intensity X-shooter (Ne =1)
Ne	1.0	1.0
Ar	3.3	5.4
Kr	1.9	4.2
Xe	0.3	0.4
Th-Ar at 10 mA	1.05	-

8.5 Operating Current

We observed all sources at various currents in order to quantify its effect on the spectral output. There is a pronounced difference in the behaviour of the pen ray lamps and the HCLs. This is caused by the fact that pen ray lamps are pure gas discharges while in the HCL the gas discharge drives sputtering of the methods which then causes emission from metal lines. Higher currents lead to higher sputtering rates and hence to an increase in the intensities of the Th lines. A more detailed explanation is given in Kerber et al.[2]. For all pen ray lamps some increase in output is observed for higher currents. In the case of Kr this amounts to a factor of 2 in intensity for a change of current from 5 to 20 mA. For the other three lamps the effect is considerably smaller. We find that the operating current is a parameter that can be easily tuned to vary the relative intensity of the lamps but the effect is limited and most of the attenuation required to bring the individual lamps to the same intensity will have to be achieved by other means.

9. RESULTS

The following results have been derived from our measurements:

- The spectra of pen ray lamps filled with Ne, Ar, Kr, and Xe have been measured at a spectral resolution equivalent to X-shooter NIR. All lamps show sharp, narrow lines in emission. Continuum emission is minimal with the exception of Xe.
- The number of lines and their intensities available from each lamp have been measured and recorded in electronic form. Analysis shows that almost all lines are from neutral atoms and that line intensities are similar to the ones reported in the literature.
- The relative intensities of the lamps have been derived as an integral of the line fluxes measured with the FTS. Ne, Ar and Kr are within a factor of three in intensity while Xe is another 3 times fainter than the next faintest source. Similar intensity ratios have been derived from observations with X-shooter.

- A combination of Ne, Ar and Kr offers the best three lamp solution meeting the requirement of 10 lines per order for all but orders 13 and 26. It also approaches the goal of 30 lines per order for many orders and provide a suitable spectrum for X-shooter calibration.
- The addition of Xe (four lamp solution) will only bring a small overall improvement in the number of lines and coverage. For some orders the improvement would be significant. Since Xe is the faintest source its addition depends on practical considerations such as feasibility of attenuation and added complexity.
- The combined spectrum of Ne, Ar and Kr provides a number of lines suitable for X-shooter wavelength calibration while providing a more even distribution across the spectral range than a Th-Ar lamp. In addition Th has a large number of faint lines many of which are blended at X-shooter resolution.
- Operating current is a straightforward but not very effective means to control the relative intensity of the lamps. Clearly, most of the attenuation needed to achieve equal intensity has to be done by hardware measures.
- The quantitative prediction on the number of lines has been validated through first laboratory tests with X-shooter. Since the spectral resolution of X-shooter is higher than in the design specifications some more unblended lines will be available. A full quantitative analysis will be done in the near future.

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