Wavelength calibration sources for instruments on extremely large telescopes

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ABSTRACT

Extremely large telescopes (ELTs) and most of their instruments will be optimized for operating in the near infrared (IR) because of the wavelength dependent performance of adaptive optics. Few established sources for wavelength calibration exist in this wavelength domain. This project aims to provide the basic data to select the best calibration sources for instruments at the European ELT (E-ELT) as a function of wavelength range and spectral resolution. We have made use of the existing databases such as the NIST Atomic Spectra Database as well as first principle physics and practical considerations to select about 20 hollow cathode lamps for study. We are investigating their spectral and operational properties through laboratory measurements using a Fourier Transform spectrometer at the European Southern Observatory (ESO). The most interesting sources will then be studied at atomic physics laboratories, such as the US National Institute of Standards and Technology (NIST), in order to produce accurate wavelength standards and calibration reference data directly applicable to operations of E-ELT instruments. The resulting data archive will be used to recommend the best suited sources for the instruments proposed for the E-ELT.

Keywords: calibration, wavelength, spectroscopy, FT spectrometer, hollow cathode lamp, E-ELT

1. INTRODUCTION

The near infrared (IR) region promises to become the most powerful domain of the electromagnetic spectrum for astronomy during the next decades. This evolution of astronomy is partially based on scientific needs and partially driven by technological development.

1.1 Science Drivers

• Study of dust-obscured objects

Because infrared wavelengths are less attenuated by dust than shorter wavelengths, they allow the study of dust obscured objects. Many young objects such as proto-stars and proto-planets are still embedded in the cloud from which they formed and are hidden from view at visible wavelengths.

• Study of Molecules and Dust

The near-IR H_2 emission lines can be used to derive the rotational and vibrational excitation temperatures and the dominant excitation mechanism in gas clouds. In astro-mineralogy it is now possible to make very specific identifications of minerals known from Earth, in particular for crystalline silicates.

• Study of cool objects

Here the IR is often favored simply because faint targets can be observed at the maximum of their spectral energy distribution. Hence all attempts to directly image extra-solar planets focus on the IR where the contrast between planet and host star is more favorable than in the visible and where adaptive optics combined with other techniques can be used to boost the contrast.

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● **Distant Universe**

For an observer on Earth objects at cosmological distances have their emitted light shifted towards longer wavelengths because of the expansion of the Universe. Therefore, near-IR spectroscopy is required in order to observe restframe ultraviolet (UV) astrophysics at high red-shifts.

1.2 Technological Drivers

During the past decade, sophisticated IR instruments, including cryogenic instruments, have become routine at many observatories, partly because of developments in IR detectors. These have made the IR a very important wavelength region for ground-based astronomy.

The next generation of extremely large telescopes (ELTs) will benefit from developments in adaptive optics. Adaptive optics are far more effective in the IR than in the visible. Artificial guide stars can be created by lasers ($\lambda = 589$ nm) that excite the Na atoms in an atmospheric layer about 90 km above the ground. These laser guide stars (LGSs) are then used to correct for the atmospheric turbulence, knowing that a plane wavefront was launched upwards from the telescope. Since the lasers are co-aligned with the telescopes, the LGSs are created close to the science target and one no longer has to rely on the presence of a suitable natural star for wavefront correction. This increases the sky coverage for full adaptive optics correction to virtually 100 %. The information collected by the wavefront sensing corresponds to a detailed sounding of the atmosphere above the telescope and can in the future be used to fully reconstruct the point spread function of an astronomical source. Hence such telescopes assisted by potent adaptive optics systems will approach the diffraction limit in terms of spatial resolution.

As a result of the above considerations, the most powerful combinations of telescopes and instruments within the next 10 years will operate in the near-IR. In order to support the quantitative work needed to address some of the fundamental questions of astrophysics it will be essential to have adequate wavelength calibration sources in this region.

2. SELECTION OF WAVELENGTH CALIBRATION SOURCES

Since the focus of astronomy and laboratory atomic physics has been on UV and visible wavelengths for more than 100 years, a wealth of reliable atomic data exists in this wavelength range. In contrast, existing data for most elements are sparse at near-IR wavelengths and a better knowledge of the spectral properties is clearly needed for both the analysis of astronomical spectra and for selecting possible calibration sources. No comprehensive database of near-IR spectra is available. ESO and NIST are collaborating on a project to provide the necessary basic data to help select the best calibrations sources for E-ELT instruments both as a function of wavelength range and spectral resolution.

2.1 Requirements of E-ELT spectrographs

Instruments at the ELTs will cover a variety of wavelength regions and spectral resolutions. The projected large size of E-ELT instruments will make it possible to deliver excellent calibration by combining optimized sets of calibrations lamps, provided such lamps can be identified in advance.

Recent developments indicate that frequency based systems such as the laser frequency comb may provide wavelength calibration of unprecedented accuracy and stability for future high-resolution spectrographs such as CODEX. At lower resolution, and for instruments with less stringent calibration requirements, classical calibration sources such as hollow cathode lamps (HCLs) are expected to remain the preferred choice for many ELT instruments.

Currently, conceptual designs for six instruments suitable for the E-ELT are being made, with another two designs to start soon. Our project will directly support these studies by providing information on possible calibration sources for a given spectrograph. Figure 1 shows the parameter space of a suite of spectrographs currently under study. The values used in the diagram are very preliminary since both wavelength range and spectral resolution are parameters that will be optimized during the conceptual design based on the proposed science and technical feasibility. Still, it is obvious that the emphasis of E-ELT spectrographs will be in the near-IR covering a large range of spectral resolution.
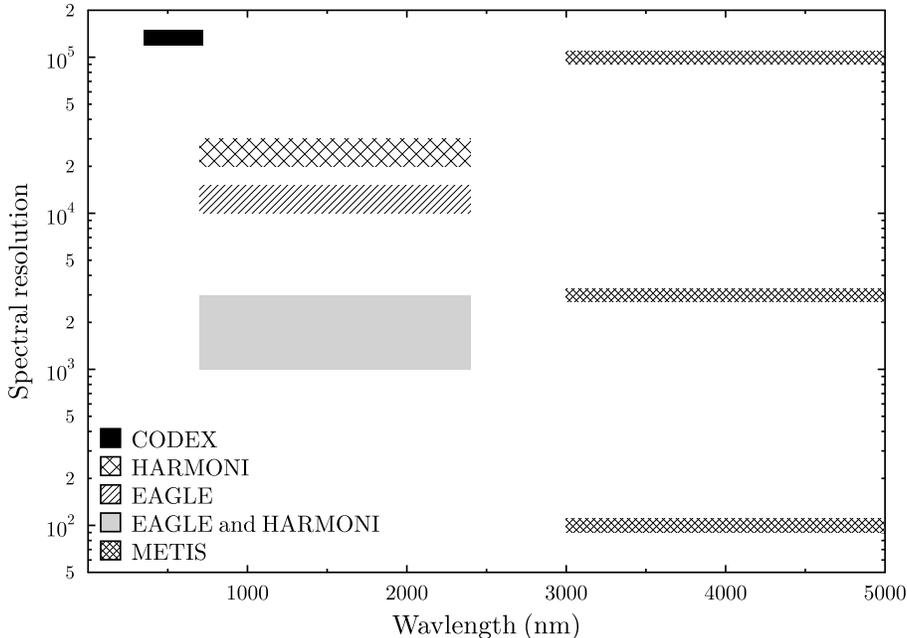
Figure 1. Parameter space covered by some of the projected E-ELT spectrographs. The numbers are preliminary since both wavelength range and spectral resolution will be optimized during the initial design.

2.2 Hollow cathode lamps

Gas discharge sources such as hollow cathode lamps (HCLs) have been used as sources for wavelength calibration of astronomical spectrographs for may decades. HCLs are mass produced for a commercial market and more than fifty elements are readily available from manufacturers. However, few have been studied for use in astronomy. The successful characterization of a Th-Ar HCL for CRIRES[1] (a joint ESO/NIST project) has improved the calibration of near-IR high-resolution spectrographs, while at lower resolution improved data for the noble gases[2–6] have made it possible to model and quantitatively predict the IR performance of the calibration system for X-shooter (see Kerber et al., these proceedings).

2.2.1 Selecting sources based on existing databases of laboratory measurements

Ideally, databases of atomic spectra would make it straightforward to select good calibration sources. The NIST Atomic Spectra Database (ASD)[7] is probably the most extensive database of experimental data, and NIST is continually expanding the data volume by adding critically compiled data from various sources. For the near-IR, the most recent comprehensive compilation of many elements dates back 30 years. Outred[8] compiled data for more than 50 elements for the wavelength range 1000 nm to 4000 nm giving a total of more than 5000 lines. However, 60 % of these lines are from only a dozen elements and many other elements are only represented by a few (< 30) lines. The scarcity of compiled data in the near-IR is illustrated by Figs. 2 and 3 which show the spectrum of titanium. Ti is a widely used element with many commercial applications. However, its near-IR spectrum is not well represented in ASD (Fig. 2 bottom panel) and is completely missing in the compilation by Outred. Many more lines of Ti I are available in the semi-empirical calculations of Kurucz (Fig. 2 middle panel). The spectrum of Ti II in the near-IR has not been studied in any detail. A very basic attempt with a simplistic calculation of the spectrum of Ti I and Ti II shows that many lines should be observable. For comparison, in Fig. 3 we show the spectrum of a Ti-Ne HCL recorded by the Fourier Transform (FT) spectrometer at ESO. All identified Ne lines have been removed, along with unknown lines also observed in the spectrum from the Zr-Ne HCL, most of which probably belonging to Ne.

In summary, it is currently not possible to select calibration sources in the near-IR based on the existing databases since these are not adequately populated with spectral data for many of the relevant elements. Even
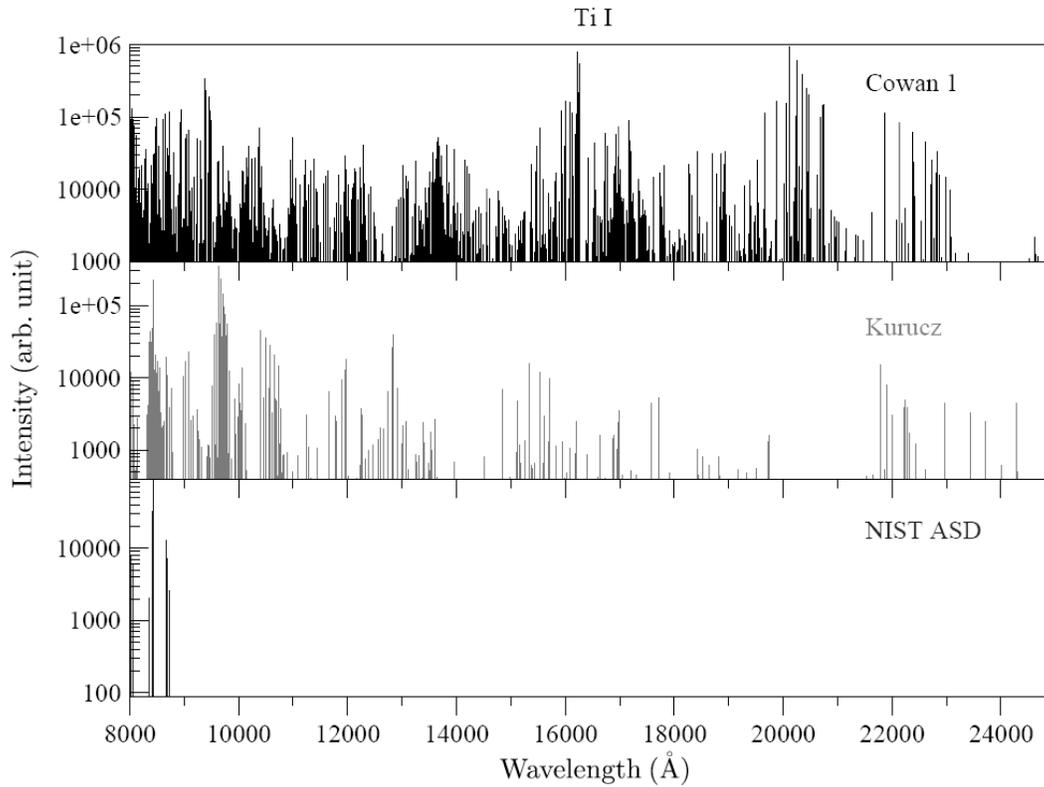
Figure 2. Spectrum of Ti I based on available information. Top panel: Calculation using the Cowan code.[9] Middle panel: Data available from Kurucz.[10] Bottom panel: Experimental data available in NIST ASD.[7]
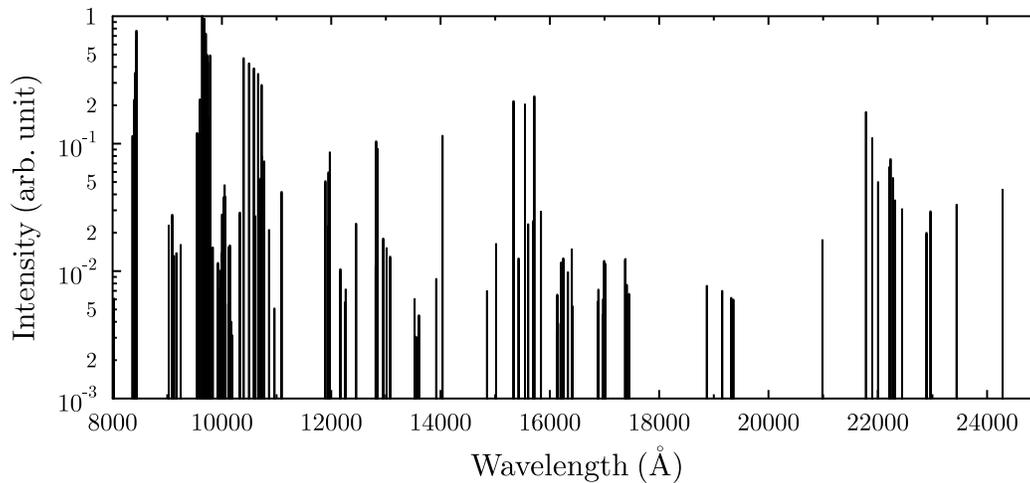

Figure 3. Observed spectral lines from the Ti-Ne lamp. Compare with calculations and available data in Fig. 2. All identified Ne lines have been removed along with unknown lines also observed in the spectrum from the Zr-Ne lamp, most probably belonging to Ne.

Table 1. Data for the HCLs acquired so far. Work function and first ionization potential of the metals are stated, together with recommended operating parameters.

Metal	Atomic number	Work function (eV)	1st ionization pot. (eV)	Fill gas	Op. current (mA)	Max current (mA)
Al	13	4.28	5.99	Ne	7–12	12
Ti	22	4.33	6.29	Ne	7–10	15
Cr	24	4.5	6.77	Ne	5–10	15
Fe	26	4.7	7.90	Ne	7–15	15
Zr	40	4.05	6.84	Ne	7–15	15
Hf	72	3.9	6.65	Ar	5–10	15
Ce	58	2.84	5.54	Ne	6–10	15
Ce	58	2.84	5.54	Ar	6–10	15
Dy	66		5.94	Ne	5–10	15
Tm	69		6.18	Ne	6–10	15

where spectral data in the near-IR are available, they are of limited relevance in predicting the spectra of commercial HCLs. Most of these data are based on spectra emitted by high-current HCLs, and these spectra are very different from the spectra emitted by commercial HCLs. These high-current lamps are not suitable for use at an astronomical telescope. Our project to observe several elements with a small commercial FT spectrometer is a pathfinder to a more detailed investigation to fill some of the large gaps in the knowledge of near-IR spectra.

2.2.2 Selecting elements based on first principles

Since HCLs are commercially available for more than 50 elements, it would be very convenient if their spectra could be predicted with some accuracy based on first principles. Unfortunately, reasonable accuracy can only be achieved with very considerable effort. We have used the freely available code by R.D. Cowan[9] that calculates atomic energy levels, transition rates and spectra. The single-configuration Hartree-Fock approximation is used to determine the radial wavefunctions that are then used to generate an energy matrix with account of configuration interaction. The electric dipole spectra, including wavelengths and radiative transition probabilities, are derived using the eigenvalues and eigenvectors of the energy matrix.

While the Cowan code can produce good results for many atomic systems, especially light elements, the calculation of spectra for heavier species is greatly exacerbated by strong correlation effects resulting from a large number of overlapping low-excited configurations. Such correlations are especially important for atoms with open *d*- and *f*-shells that have rich near-IR spectra of importance to the present work. A proper *ab initio* account of correlation effects would have to include an exceedingly large number of configurations and thus is hardly practical.

The process of calculating the spectra is greatly facilitated whenever a reasonable number of relevant spectral lines are known from laboratory work to guide the calculation. Moreover, the derived experimental energy levels can be directly used to improve the description of atomic structure parameters within the Cowan code. Unfortunately, as described in section 2.2.1 such support from laboratory measurements is very limited. Figure 2 (top panel) shows the result of some simplistic ad-hoc attempts to use the Cowan code to calculate spectra for Ti. Comparison with the few compiled measured line data is not very impressive. Some transitions can certainly be identified, albeit at shifted wavelengths.

In summary, the quality of spectral calculations (Fig. 2) could be improved but only with very substantial effort. Any attempt to survey 20 or more elements in this manner would incur long-term computational efforts, and hence such an approach is impractical for our project.

2.2.3 Practical considerations

In the absence of good line data or reliable calculations we restricted ourselves to using some very basic and practical considerations to guide our selection of elements for procuring HCLs for laboratory measurements.

In the process of choosing suitable lamps the properties of different metals have been considered in terms of e.g. availability, possible line structure, and possibility to produce a number of observable spectral lines in the wavelength region of interest. For calibration of high-resolution spectrographs, we have chosen elements dominated by even isotopes, as hyperfine structure in odd isotopes may produce asymmetric spectral lines. For the calibration of low-resolution spectrographs the line strengths are more important and any line structure will be negligible compared to instrument profiles. Theoretical calculations have also been made, see Fig. 2, in order to estimate the possible number of spectral lines. At the present time, ten different lamps with nine different metals have been selected (see Table 1).

Considerable uncertainty remains as to whether a given element or cathode material/fill gas combination will be usable. For example, both Ce-Ne and Ce-Ar HCLs were measured in order to study the HCL performance for different fill gases. Contrary to expectations the Ce-Ne HCL gave a much better spectrum than the Ce-Ar. No Ce lines were clearly identified in the Ce-Ar HCL. Given that most Ce lines are also faint in the Ce-Ne it is possible that they are too weak in the Ce-Ar HCL to be recordable by our equipment.

3. EXPERIMENTAL METHOD

Spectra of the commercial HCLs are being recorded with the commercial FT spectrometer at ESO. This is a Nicolet 5700 manufactured by Thermo Electron Corporation[*]. This type of spectrometer is mainly used for industrial applications using absorption spectroscopy, but it also provides a port for external sources. In order to duplicate the optical path used for internal sources the light from the external source is collimated using an elliptical and a parabolic mirror (see Kerber et al., these proceedings).

Spectra are recorded using an InGaAs detector and a CaF_2 beamsplitter in the spectral range between $3000\,\mathrm{cm}^{-1}$ and $14000\,\mathrm{cm}^{-1}$ ($3.3\,\mu\mathrm{m}$ to $0.7\,\mu\mathrm{m}$). Spectra of two lamps with different cathode materials and carrier gases are displayed in Figs. 4 and 5. Spectra from each lamp are recorded at six different operating currents (4, 6, 8, 10, 12 and $14\,\mathrm{mA}$) with a resolution of $0.125\,\mathrm{cm}^{-1}$. Between 128 and 1200 scans ($1\,\mathrm{h}$ to $10\,\mathrm{h}$) are co-added for each spectrum in order to increase the S/N of all lines. Spectra are also recorded with lower resolution (1, 4 and $8\,\mathrm{cm}^{-1}$), at an operating current of $10\,\mathrm{mA}$, in order to further investigate the spectral properties of the lamps. The highest operating current recommended by the lamp manufacturer varies between the different lamps (see Table 1), but $10\,\mathrm{mA}$ is allowed for all and this is therefore used as the standard operating current to which all comparisons are made.

4. ANALYSIS

The spectra are analyzed using a combination of software, including the tools provided by the manufacturer of the spectrometer and the FT spectrometry analysis program XGREMLIN.[11, 12]

The spectral lines are identified using available compilations,[8] databases,[7] individual publications, and comparisons to Ritz wavenumbers calculated using published energy level values. Gaussian profiles are fitted to all observable spectral lines and the integrated intensity is studied as a function of lamp operating current. For each spectral line the ratio of the intensity of the line to the intensity of the same line in the $10\,\mathrm{mA}$ spectrum is calculated. The ratios are then averaged for all lines of the corresponding species at each current, showing a distinct difference between the behaviors of the gas and the metal lines. The average behavior of line intensities as a function of current is displayed in Figs. 6 and 7 where only resolved lines present at all currents are included.

A qualitative explanation of this behavior is that the intensity of metal lines depends not only on the excitation rate, but also on the effect of sputtering which increases at higher currents. The sputtering of atoms from the cathode is caused by the impact of positive ions accelerated across the cathode fall. The electron density (and

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[*]Certain commercial equipment is identified in this article to adequately specify the experimental procedure. Such identification does not imply endorsement by the National Institute of Standards and Technology, nor does it imply that this equipment is the best available for the purpose.
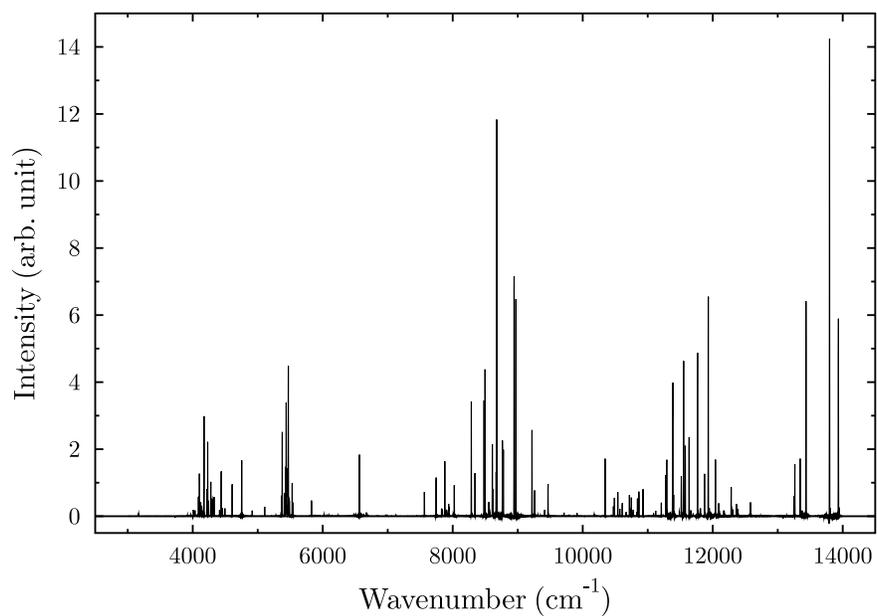
Figure 4. The observed spectrum of the Zr-Ne lamp at operating current $10\,\mathrm{mA}$ in the wavenumber range $3000\,\mathrm{cm}^{-1}$ to $14000\,\mathrm{cm}^{-1}$ ($3.3\,\mu\mathrm{m}$ to $0.7\,\mu\mathrm{m}$). The spectrum is dominated by lines from the carrier gas, but metal lines (Table 2) also contribute to the appearance.
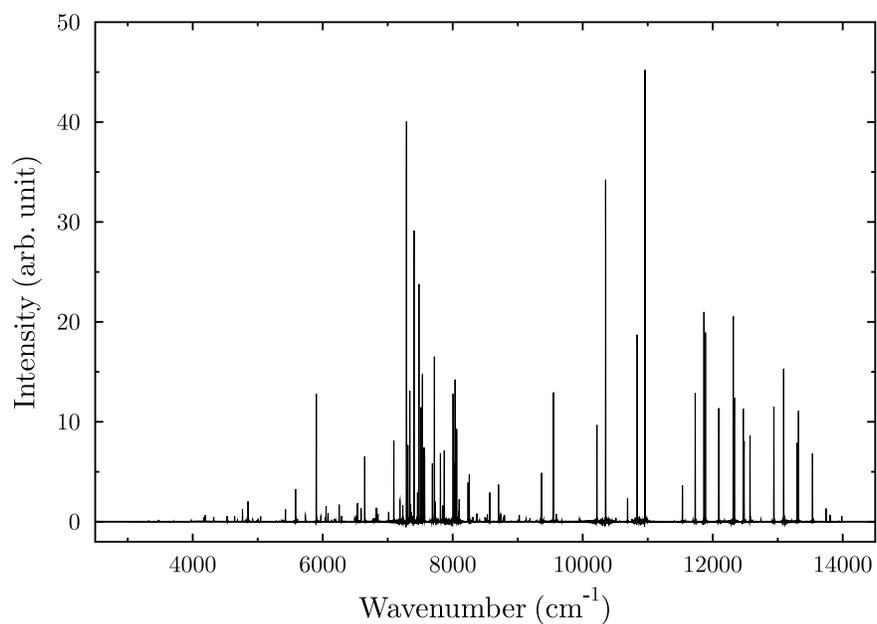

Figure 5. The observed spectrum of the Hf-Ar lamp at operating current $10\,\mathrm{mA}$ in the wavenumber range $3000\,\mathrm{cm}^{-1}$ to $14000\,\mathrm{cm}^{-1}$ ($3.3\,\mu\mathrm{m}$ to $0.7\,\mu\mathrm{m}$). The spectrum is dominated by lines from the carrier gas, but metal lines (Table 2) also contribute to the appearance.
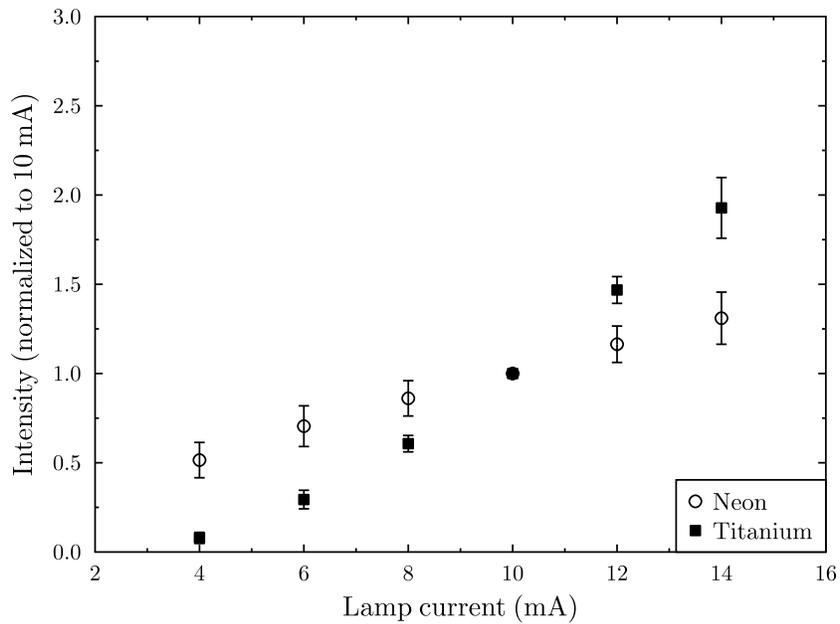
Figure 6. Line intensities as a function of operating current in the Ti-Ne HCL. The intensities are normalized to the intensity at 10 mA and average values are calculated for identified lines from the carrier gas and the metal respectively. The error bars represent one standard deviation. Only resolved lines present at all currents are included, resulting in about 240 Ne lines and 40 Ti lines.
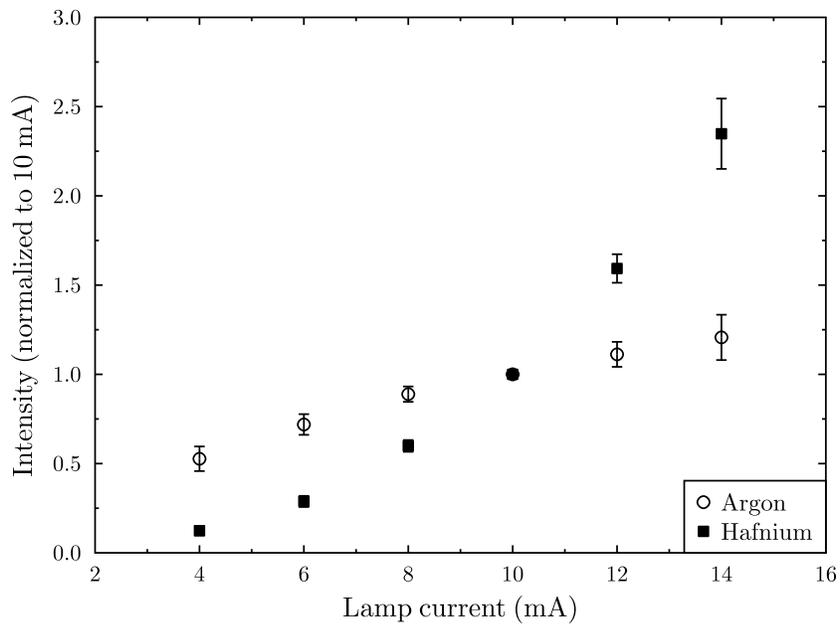

Figure 7. Line intensities as a function of operating current in the Hf-Ar HCL. The intensities are normalized to the intensity at 10 mA and average values are calculated for identified lines from the carrier gas and the metal respectively. The error bars represent one standard deviation. Only resolved lines present at all currents are included, resulting in about 190 Ar lines and 30 Hf lines.
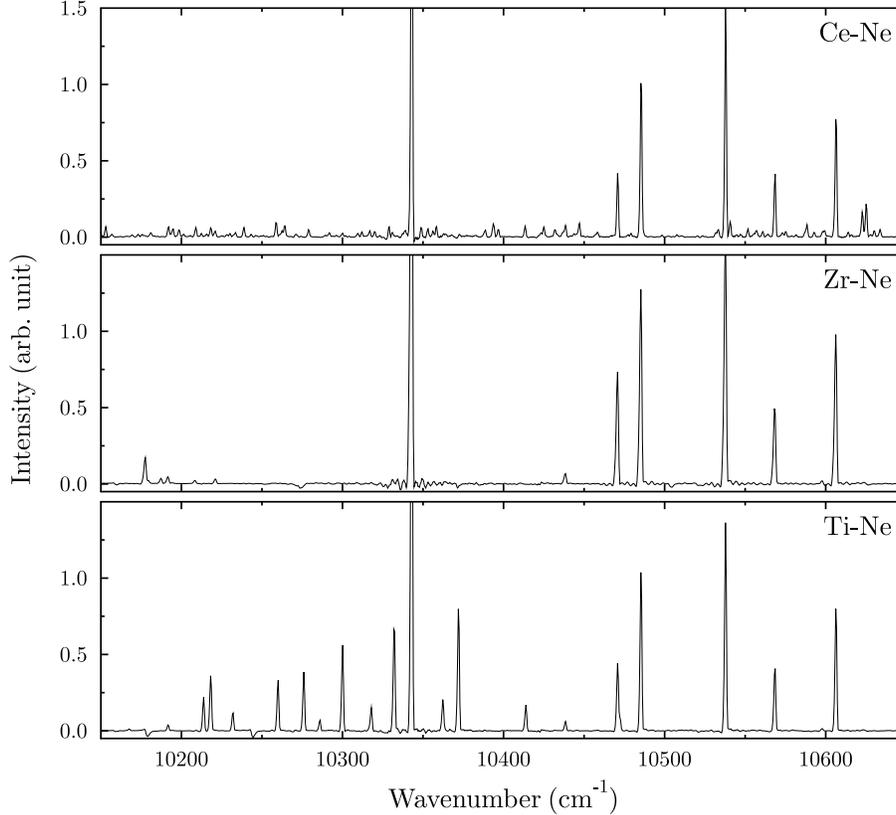
Figure 8. Observed spectra of the Ce-Ne, Zr-Ne and Ti-Ne lamps at operating current $10\,\text{mA}$ in the wavenumber range $10150\,\text{cm}^{-1}$ to $10650\,\text{cm}^{-1}$ ($0.99\,\mu\text{m}$ to $0.94\,\mu\text{m}$). The spectra are dominated by lines from Ne (the lines common to all spectra), but in the region between $10200\,\text{cm}^{-1}$ and $10400\,\text{cm}^{-1}$ there is an obvious difference with more Ti lines than Zr lines. For the Ce-Ne lamp almost the entire region is covered with a large number of weak Ce lines.

corresponding ion density) in the discharge is approximately proportional to lamp current. At higher lamp current more ions are available in the plasma and there is a corresponding increase in sputtering. Similar analyses have previously been carried out for Th-Ar[13] and Pt/Cr-Ne[14] lamps.

This distinctive behavior provides a useful tool in distinguishing between gas and metal lines when trying to identify the presently unidentified lines in the spectra. It has been shown that this method, used on a Th-Ar lamp, allows Th and Ar lines to be distinguished with a high degree ($> 90\%$) of confidence.[13] In addition to line identification, the results of the investigations of current dependence should also provide important information on how to optimize the operation of the calibration lamp. For example, the lamp could be run at higher currents for observations at wavelengths where the intensity and spectral density of lines is intrinsically lower.

5. RESULTS

Analysis and experimental work are still ongoing. Three lamps have to date been thoroughly analyzed resulting in knowledge about the behavior of line intensities as a function of lamp current. In general, the spectra are dominated by lines from the carrier gas, but metal lines also contribute to the characteristics. A small spectral region for the Ce-Ne, Zr-Ne and Ti-Ne lamps is displayed in Fig. 8. The three lamps have the same carrier gas and the spectra are therefore similar, but in certain regions the difference is apparent. Different metals produce lines in different spectral regions and lamps can be used in combination in order to optimize their utility.

The preliminary number of observed spectral lines from the analyzed lamps is shown in Table 2. Note that the number of unidentified lines will decrease as the process of line identification is ongoing. All lines have

Table 2. Preliminary number of lines in the spectra of the analyzed commercial HCLs observed at the operating current $10\,\mathrm{mA}$ in the spectral range $3000\,\mathrm{cm}^{-1}$ to $14000\,\mathrm{cm}^{-1}$ ($3.3\,\mu\mathrm{m}$ to $0.7\,\mu\mathrm{m}$).

Lamp elements (Metal / Gas)	No. lines (Total)	No. lines (Gas)	No. lines (Metal)	No. lines (Unidentified)
Ti / Ne	451	283	65	103
Zr / Ne	433	264	113	56
Hf / Ar	388	222	81	85

preliminary, uncalibrated wavenumbers and wavelengths. The lamps which are analyzed so far do not show a distinct difference in the total number of observed lines, but a preliminary analysis of the Ce-Ne lamp shows a very large number (> 700) of weak spectral lines distributed over the entire observed spectral range, see Fig. 8. This is an expected characteristic of the rare earth elements, which have an open 4f-shell and several close lying configurations resulting in many possible transitions in the IR and near-IR.

6. SUMMARY

The most recent dedicated compilation of near-IR spectra of elements is 30 years old. The current databases of atomic spectra contain only limited information, so it is not possible to select the most promising elements based on the information available. Laboratory work to this end is time consuming and only a few laboratories are equipped to deliver the required quality that is needed to produce wavelength standards. The wealth of information for UV and visible wavelengths is the result of about 100 years of effort. Hence this situation cannot be expected to change for the near-IR in the near-term. Unfortunately, it is not possible to predict the spectra of calibration lamps accurately based on first principles.

Our laboratory project to conduct a preliminary survey of about 20 elements with a small commercial FT spectrometer will form the basis for developing a more robust understanding of the near-IR spectra of elements suitable as wavelength calibration sources. We focus our effort on the needs of currently planned spectrographs for the E-ELT, which will require good calibration sources for various resolutions across the near-IR range. The results of our work will directly support the initial studies of ELT instruments currently underway. In a second phase we plan to establish the best qualified elements as wavelength standards by conducting dedicated laboratory measurements with high-precision FT spectrometers at qualified atomic spectroscopy laboratories.

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