WAVELENGTH STANDARDS FOR IR SPECTROGRAPHS AT ESO

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ABSTRACT

We report on our efforts to provide high accuracy wavelength calibration for scientific observations with the Cryogenic High-Resolution IR Echelle Spectrograph (CRIRES), ESO's new high resolution (R≈100,000) infrared (IR) spectrograph at the VLT. In order to provide reliable and accurate wavelength standards for CRIRES the European Southern Observatory (ESO), in collaboration with the National Institute of Standards and Technology (NIST) and the Space Telescope European Coordinating Facility (ST-ECF), embarked on a project to establish Th-Ar wavelength standards in the 900 nm - 5000 nm operating range of CRIRES. These calibration reference data are being used by a physical instrument model designed for the wavelength calibration in the science data reduction pipeline. With the availability of a reliable and well characterized source, wavelength calibration in the near IR will be very similar to the UV-visible region, and it will become possible to support high accuracy absolute wavelength calibration without having to rely on atmospheric features. In order to facilitate the use of Th-Ar lamps at other facilities we will make all relevant information available in a form compliant with Virtual Observatory standards. This will be one of the first comprehensive data sets resulting from laboratory atomic physics that is made accessible to the astronomical community in this manner.

Key words: Instruments: spectrographs; Standards; Technique: spectroscopic; Virtual Observatory.

1. NEAR-INFRARED WAVELENGTH CALIBRATION AND CRIRES

Traditionally, astronomical spectroscopy in the near infra-red (IR) has relied on atmospheric features of the night sky for wavelength calibration (Rousselot et al., 2000). The lines from rotational-vibrational levels of the hydroxyl radical OH (Meinel bands), which account for the night time OH airglow emission, are routinely used since they are very numerous, cover a wide wavelength range, and have been studied in detail at high resolution in the laboratory (Abrams et al., 1994).

Originally, the concept for CRIRES wavelength calibration was also based on the use of features provided by the night sky. During commissioning of the instrument we found that at the high resolution of CRIRES (≈100,000) only a few features are evident in most wavelength regions. These were obviously not appropriate to support high accuracy calibration. Based on considerations of scientific potential, practicability and availability we had previously selected Th-Ar hollow cathode lamps (HCLs) and N_2O gas cells as prime candidates for external standard sources on CRIRES. Good calibration reference data exist for N_2O because it is a primary calibration molecule from heterodyne frequency measurements at NIST (Maki & Wells (1998)). Hence wavelengths for a large number of lines of its fundamental mode have been established covering the range $523\,\mathrm{cm^{-1}}$–$2845\,\mathrm{cm^{-1}}$ (1912 nm–3515 nm). Here we will focus on the results of the work on Th-Ar HCLs.

2. BACKGROUND ON HOLLOW CATHODE LAMPS

The hollow cathode discharge was introduced as a light source for spectroscopy by Paschen (1916). Ever since it has been widely used in applications that require very sharp lines such as studies of hyperfine structure. The development of commercial hollow cathode lamps was driven by the requirements of the analytic technique of atomic absorption (AA) spectroscopy. Developed by A. Walsh in the 1950s (Walsh, 1955), AA is now a routine tool in chemical analysis using HCLs as a standard light source. Hence low current HCLs are mass produced in great diversity. Astronomy has benefited from this industrial development and has adopted the use of HCLs for its own needs.

3. BASIC FACTS ABOUT HOLLOW CATHODE LAMPS

Modern commercial hollow cathode lamps are sealed-off glass tubes that contain a metal cathode, a metal anode and a noble fill gas at a defined pressure. The light exits the lamp through a window made of a material that is transparent in the wavelength region of interest. Lamps with a great variety of cathode materials are commercially available.

The lamp is operated by applying a voltage of a few hundred volts between 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. They bombard the surface of the cathode at high velocity. Since their kinetic energy is considerably higher than the electronic work function of the cathode metal (few eV), atoms are released from the cathode's surface (sputtering). The sputtering rate depends on the mass of the incoming particle and on the cathode material. The sputtered material usually exits the cathode surface as neutral atoms in the ground state at high velocity (Walsh, 1973). Their energy is quickly dissipated in collisions with the fill gas. These collisions give rise to unstable excited states of the metal atoms which then decay to the ground state emitting radiation in the process. 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. We refer the interested reader to the dedicated discussion of HCLs and their operation provided by Kerber et al. (2007), which covers many technical aspects (design, operation, aging, lifetimes) that are usually not available in the astronomical literature.

4. CRIRES

CRIRES is a cryogenic, infrared Echelle spectrograph designed to provide a resolving power $\lambda/\Delta\lambda$ of 100,000 between about 950 nm and 5000 nm. The instrument was installed at the Nasmyth focus A of the 8 m VLT unit telescope #1 (Antu) in June 2006. A ZnSe prism is used as pre-disperser. A multiple applications curvature adaptive optics (MACAO) feed is employed to minimize slit losses and to provide diffraction limited spatial resolution along the slit. An Echelle grating with a blaze angle of 63.5 degrees and a groove density of 31.6 lines/mm provides dispersion in the main spectrograph. CRIRES is equipped with a detector system that consists of a mosaic of 4 Aladdin III 1k $\times$ 1k InSb-arrays[1]. This provides an effective $\sim$4000 $\times$ 500 pixel focal plane array, in order to maximize the free spectral range covered in each exposure. CRIRES (http://www.eso.org/instruments/crires/) is designed for stability and high throughput; it has been available to the community since April 2007. A detailed description of the instrument is given by Käufl et al. (2004).

[1]Certain commercial equipment is identified in this article to adequately specify the experimental procedure. Such identification does not imply endorsement by the NIST, nor does it imply that this equipment is the best available for the purpose.

5. TH-AR HOLLOW CATHODES LAMPS FOR ASTRONOMICAL APPLICATIONS

The rich spectrum of Thorium was studied more than 20 years ago by Palmer & Engleman (1983) covering the range 278 nm to about 1000 nm at high resolution. In nature Th has only one isotope, ^{232}Th, which has zero nuclear spin. Its emission lines are very narrow, and the use of Th for calibration lines avoids complex and asymmetric line profiles attributable to isotopic or hyperfine structure. Th-Ar lamps have been used successfully on several spectrographs at ESO and at other astronomical observatories. In a very interesting recent development the High Accuracy Radial velocity Planet Searcher (HARPS) at the ESO's 3.6 m telescope has been used to measure wavelengths for a few thousand additional Th lines in the range 378.5 nm to 691.5 nm (Lovis & Pepe , 2007). Their work achieves very high internal precision but relies on Palmer & Engleman (1983) for absolute calibration.

In the near-IR the situation is quite different, and only limited operational experience with Th-Ar calibration sources exist. There are two valuable studies of the Th-Ar spectrum in the near IR but neither is directly applicable to the operation of CRIRES:

1. Hinkle et al. (2001) produced an atlas of the Th-Ar spectrum covering the range 1000 nm to 2500 nm. They measured wavelength standards using the McMath 1-m laboratory Fourier Transform Spectrometer (FTS) at the US National Solar Observatory at Kitt Peak. For technical reasons their list of about 500 lines contains significant gaps in wavelength coverage.
2. A fundamental analysis of the Th-Ar spectrum was provided by Engleman, Hinkle, & Wallace (2003). Their list contains more than 5000 lines derived from observations of a high current Th-Ar source with the McMath FTS. They used a water-cooled demountable hollow cathode lamp operated at 320 mA with a continuous flow of argon at a pressure of 290 Pa (2.2 Torr). Such a lamp is not well-suited for operation at an astronomical facility. It produces a very rich Th spectrum, which is rather different from low current commercially available lamps.

6. LABORATORY WORK AND RESULTS

Spectra (Fig. 1) of the Th-Ar lamps operated at 20 mA were recorded on the NIST 2-m FTS. The FTS (Nave et al., 1997) was fitted with a CaF_2 beam splitter, silver coated mirrors, and InSb detectors. The optimum alignment of the spectrometer depends slightly on wavelength,

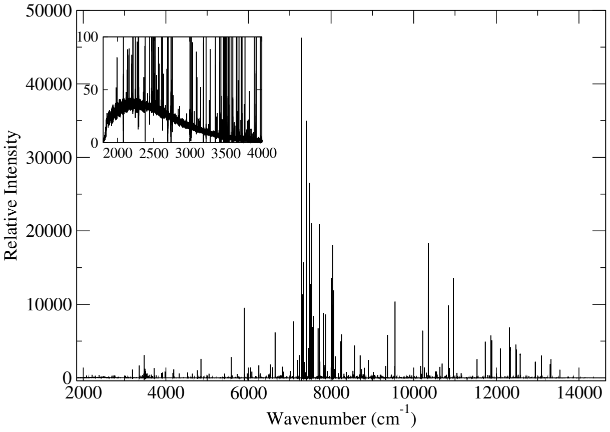

Figure 1. Overview spectrum of a Th-Ar lamp. Wavelength range is 715 nm to 5000 nm (14000 cm^{-1} to 2000 cm^{-1}). The line intensity is given in arbitrary units. The inset shows that longwards of 2500 nm (<4000 cm^{-1}), thermal emission from the hot cathode produces a continuum that underlies the pure emission line spectrum.

hence interferograms for two different wavelength regions were recorded – the first optimized for wavelengths between 800 nm and 2000 nm and the second for wavelengths greater than 2000 nm. A resolution of 0.01 cm^{-1} was used for the short wavelength region and a resolution of 0.005 cm^{-1} for the long wavelength region.

To obtain good signal-to-noise ratio many interferograms were co-added for each spectrum, corresponding to data acquisition times of up to 20 hours. For each hollow cathode spectrum a spectrum of a radiometrically-calibrated tungsten strip lamp was also recorded. This calibration spectrum was used to determine the instrumental response function for the foreoptics/FTS/detector combination. The response function was used to place the line intensities on a consistent scale.

Wavelength calibration of the spectra was derived by using laser measurements of seven Th lines (DeGraffenreid & Sansonetti (2002)) as internal standards. The relative uncertainty of the calibration (one standard deviation) is 1.4×10^{-8} × wavelength. For a detailed description of the experimental procedures and the results we refer to Kerber et al. (2007).

Our results for Th lines are in excellent agreement with Engleman, Hinkle, & Wallace (2003) (Fig.2). The weighted mean offset in wavenumber is $(4.4 \pm 1.5) \times 10^{-5}$. For Ar lines a much larger scatter is evident, which is attributable to differences in the operating conditions of the source. Since the list of Engleman, Hinkle, & Wallace (2003) contains many more spectral lines than ours (see 5.2), this comparison gives confidence that our list can be supplemented with additional Th lines from their list for calibration of CRIRES.

About 2500 lines in the range 900 nm to 4800 nm have been established as wavelength standards with an uncertainty of about 0.001 cm^{-1}, and are available for CRIRES wavelength calibration. The Th-Ar hollow cathode lamps have been successfully tested during commissioning and are now available for routine use on CRIRES.

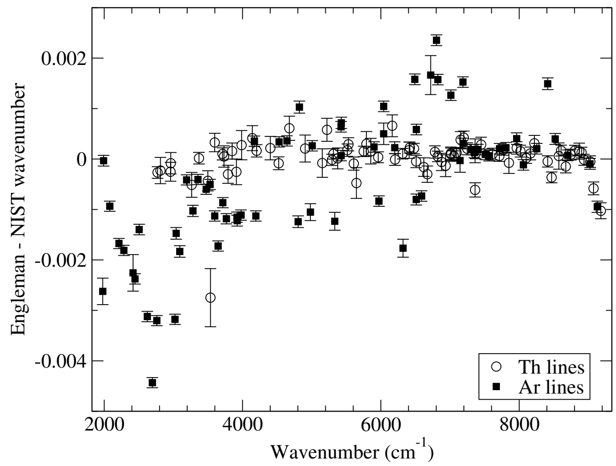

Figure 2. Comparison of our results with Engleman, Hinkle, & Wallace (2003). The Th I lines agree well, but the Ar I lines show increasing scatter at longer wavelengths that is dependent on the excitation of the upper level.

7. LABORATORY DATA IN THE VIRTUAL OBSERVATORY (VO)

Atomic physics and astrophysics have a long tradition of collaboration, but the usefulness of laboratory atomic physics data in astrophysical applications is often limited by lack of sufficient information about the experimental conditions under which the laboratory data were acquired. The availability of meta-data, that is data that describes how scientific data were created, is often essential for the data to be used correctly. Currently, many interesting data sets are of limited value because they lack proper meta-data. The reasons for this are manifold but a structural problem is that there are no well documented standards for publishing laboratory data which would ensure their usability for various purposes by users not familiar with the original laboratory work.

The efforts of the Virtual Observatory (VO) are centered around establishing the required infrastructure and tools to facilitate the exchange of fully documented data and their use across databases. One example of a database that strives to provide proper meta-data for many of its holdings is the NIST atomic spectra database (http://physics.nist.gov/asd3) (Ralchenko et al., 2007). This database offers critically evaluated data on astrophysically relevant parameters such as atomic energy levels, wavelengths, and transition probabilities.

The international Virtual Observatory Alliance (IVOA) is a global effort to establish standards that ensure interoperability between databases and VO services. Created by expert working groups these standards are eventually endorsed by the Virtual Observatory Working Group of Commission 5 (Astronomical Data) of the International Astronomical Union. In the context of the Th-Ar wavelength standards two IVOA standards are of particular relevance: the Spectrum Data Model (McDowell et al., 2007) and the Simple Spectral Access Protocol (Tody et al., 2007). In the case of laboratory data, meta-data are best created at the time when the actual laboratory work is done and by the people involved in the measurements. Our ESO/NIST collaboration plans to publish the data of the Th-Ar wavelength standards in a fully VO-compliant form in the near future. In this manner our results can be used as calibration reference data for CRIRES and other instruments. We consider the VO as one good way to enhance the exchange of information and foster communication between the atomic physics and astrophysics communities.

8. OUTLOOK

A number of steps are planned to further improve CRIRES wavelength calibration. We are carefully selecting additional Th-Ar lines from the literature to add them to our list for use in wavelength calibration. At wavelengths where the Th-Ar spectrum is sparse we are using a N_2O gas cell. For use on CRIRES the spectrum of the gas cell as a function of temperature and fill gas pressure still needs to be properly characterized. Additional fill gases such as carbonylsulfide (OCS) will also be studied.

Based on current findings we conclude that Th-Ar hollow cathode lamps hold the promise of becoming a standard source for wavelength calibration for near IR astronomy, providing a high density of sharp well-characterized emission lines with the ease and efficiency of operation of a commercial discharge lamp. The relevant calibration reference data will be made available in VO-compliant form.

With this development, wavelength calibration in the near IR will become very similar to the UV-visible region. This approach supports high accuracy absolute wavelength calibration without having to rely on atmospheric features. This is an essential step towards supporting the fundamental studies planned for the next generation of extremely large telescopes.

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