

THE SPECTRUM OF Th-Ar HOLLOW CATHODE LAMPS IN THE 691–5804 nm REGION: ESTABLISHING WAVELENGTH STANDARDS FOR THE CALIBRATION OF INFRARED SPECTROGRAPHS

F. KERBER^{1,2}

ESO, Karl-Schwarzschild-Strasse 2, 85748 Garching, Germany; fkerber@eso.org

AND

G. NAVE AND C. J. SANSONETTI

National Institute of Standards and Technology, Gaithersburg, MD 20899; gillian.nave@nist.gov, craig.sansonetti@nist.gov

Received 2008 February 5; accepted 2008 May 5

ABSTRACT

We report new observations of the infrared (IR) spectrum of low-current Th-Ar hollow cathode lamps with the 2 m Fourier transform spectrometer (FTS) at the National Institute of Standards and Technology. These observations establish more than 2400 lines that are suitable for use as wavelength standards in the range 900–4500 nm. The line list is used as input for a physical instrument model that provides the wavelength calibration for the Cryogenic High-Resolution IR Echelle Spectrometer (CRIRES), the European Southern Observatory’s new high-resolution ($R \sim 100,000$) IR spectrograph at the Very Large Telescope. We have also observed the variation of the spectrum of Th-Ar lamps as a function of operating current. The results allow us to optimize the spectral output in terms of relative intensity and line density for operation on the telescope. Our results should be generally useful for wavelength calibration in 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.

Subject headings: atomic data — catalogs — instrumentation: spectrographs — methods: laboratory — standards — techniques: spectroscopic

Online material: color figure, machine-readable table

1. INTRODUCTION

Traditionally, astronomical spectroscopy in the near-infrared (IR) has relied on atmospheric features of the night sky for wavelength calibration (Osterbrock et al. 1996, 1997; Rousselot et al. 2000). In particular the lines from rotational-vibrational levels of the hydroxyl radical OH (Meinel bands), which account for the nighttime 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 (Abrams et al. 1994). The main advantage of this approach is that the night-sky lines are imprinted on any spectrum of an astronomical target; hence, the need for dedicated calibration exposures is greatly reduced. The main limitation of the method is in the number and accuracy of lines available in a given wavelength range at a given resolution. Absorption features of the night sky are few below 2500 nm, but at longer wavelengths they become important. Beyond ≈ 3000 nm, calibration using these telluric features is possible. Of fundamental concern is the fact that the intensity of atmospheric features is site-dependent and varies on several different timescales (daily/nightly, seasonal, long term). Moreover, if a spectral stability of ≤ 25 m s⁻¹ is required, one can no longer ignore bulk atmospheric motions (e.g., high-altitude winds) along the line of sight.

The use of external calibration sources in the near-IR, such as lamps or gas cells (Marcy & Butler 1992; Mickelson et al. 2001), has been limited by the lack of suitable wavelength standards. Emission spectra of Ne (Sansonetti et al. 2002, 2004) and Kr (Sansonetti & Greene 2007) have been studied in detail recently, but the line density and distribution of Ne and Kr lamps are

inadequate for high-resolution spectroscopy using IR echelle spectrographs. Thus, the situation in the near-IR is in pronounced contrast to the ultraviolet (UV) and visible regions, where wavelength calibration is usually made using spectra provided by one of a variety of available standard lamps and where the study of the night-sky lines is left to dedicated observations (Hanuschik 2003).

Experience during commissioning of the new Cryogenic High-Resolution IR Echelle Spectrometer (CRIRES; Käufel et al. 2004) at the Very Large Telescope (VLT) immediately showed that the number and distribution of emission lines provided by the night sky are inadequate for calibration of a high-resolution spectrograph in the near-IR. At resolution $\approx 100,000$ few lines achieve good signal-to-noise ratio in a standard science exposure time (Fig. 1). Hence, the traditional approach of using night-sky features for calibration would fail for most CRIRES wavelength settings below 3000 nm. Above 3000 nm about 85% of CRIRES settings can be wavelength calibrated using telluric absorption features.

Limitations in the performance and understanding of calibration sources can introduce severe systematic uncertainties in the scientific results. A case in point are studies of the absorption lines in quasi-stellar object (QSO) spectra that have been used to test for space-time variation of the fine-structure constant α . The many-multiplet technique (Webb et al. 1999) measures the wavelength separation of selected spectral lines at different redshifts along the line of sight to a QSO. If α had a different value in high-redshift objects, the relative wavelengths of these lines would be different from those measured on earth. Since any possible variation in α must have been very small, the difference in wavelengths would also be very small ($< 1:10^6$), requiring both accurate laboratory wavelengths and an accurate calibration of the astronomical spectra. Although recent laboratory experiments (Peik et al. 2005) have not found any evidence for time dependence of

¹ Guest Researcher, NIST.

² formerly with the Space Telescope European Coordinating Facility, Garching, Germany.

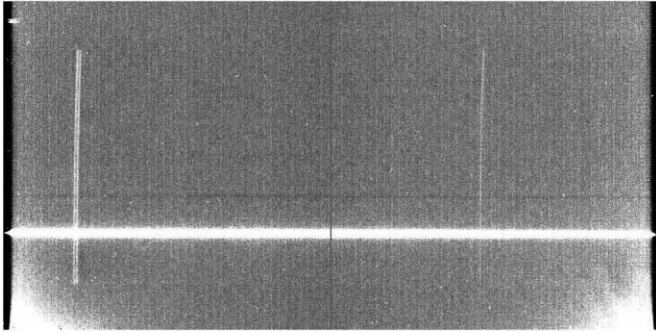


FIG. 1.—Example of a two-dimensional CRIFES spectrum. Shown is one of the four detectors of the array. The wavelength is about 1504 nm. Apart from the bright continuum of a star, only three lines, two of which form the doublet on the left, from the night sky are recorded in this 30 s exposure. [See the electronic edition of the Supplement for a color version of this figure.]

α over the past few years, it is possible that α changed rapidly during the early universe and has since stabilized. Findings based on observations of astrophysical sources are discrepant; Murphy et al. (2003, 2004) obtained a value of $\Delta\alpha/\alpha = (-0.57 \pm 0.11) \times 10^{-5}$, whereas Chand et al. (2004, 2006) find no evidence of a change in α . Since these two studies used different instruments, it is possible that the different results are due to a difference in calibration. This has resulted in a recent paper describing an algorithm for selecting Th-Ar emission lines for wavelength calibration in the visible that incorporates the properties of both a new list of laboratory wavelengths and of the spectrograph of interest (Murphy et al. 2007). Extension to IR wavelengths would enable the measurement of α at even higher redshifts, provided that an accurate wavelength calibration for the spectra could be derived.

Near-IR emission-line sources are highly relevant in the context of the next generation of extremely large telescopes (ELTs). These facilities will be most powerful in the near-IR, because adaptive optics are far more effective at these wavelengths than in the visible. Many of the science cases envisaged for the ELTs require quantitative analysis, and calibration reference data traceable to laboratory standards will be essential to support such science.

The European Southern Observatory (ESO), in collaboration with the Space Telescope European Coordinating Facility (ST-ECF) and the National Institute of Standards and Technology (NIST), has thus embarked on a project to establish Th-Ar wavelength standards in the 950–5000 nm operating range of CRIFES.

1.1. Hollow Cathode Lamps as Calibration Sources for Astronomical Spectrographs

Th-Ar hollow cathode lamps (HCLs) provide a rich spectrum in the UV–visible region and have been used in high-resolution

spectroscopy at several observatories for many years. Current examples of instruments at ESO that make use of such lamps include the Fiber-fed Extended Range Optical Spectrograph (FEROS), the Fiber Large Array Multielement Spectrograph (FLAMES), the High Accuracy Radial Velocity Planet Searcher (HARPS), and the Ultraviolet Visual Echelle Spectrograph (UVES). Future spectrographs, such as X-shooter (D’Odorico et al. 2004), will also make use of Th-Ar lamps for calibration. In the case of HARPS, calibration using a Th-Ar exposure simultaneous with the science exposure is the backbone of the highly successful searches for extrasolar planets based on variations of the radial velocity of the host star (Mayor et al. 2003; Lovis & Pepe 2007). Similarly, HCLs (Pt/Cr-Ne) are the standard calibration source for space-based UV–visible spectrographs (Reader et al. 1990; Sansonetti et al. 2004). A comprehensive review by Kerber et al. (2007) contains a detailed description of many aspects of the design and operation of HCLs, including technical information usually not available in the astronomical literature.

1.2. Th-Ar Lamps for Wavelength Calibration

Previous work on Th-Ar HCLs is summarized in Table 1. The Th spectrum (278 nm to about 1350 nm) was studied at high resolution more than 20 years ago by Palmer & Engleman (1983). 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. As a result there is no isotope or hyperfine structure. Several astronomical observatories have published Th atlases using their high-resolution spectrographs (see D’Odorico et al. 1987 for an example). Most recently the number of lines available for calibration in the visible region has been doubled by Lovis & Pepe (2007). From their spectra, acquired using HARPS, they also attempted to improve the internal precision of the Palmer & Engleman line list.

Two valuable studies of the Th-Ar spectrum in the near-IR have recently been published. Hinkle et al. (2001) produced an atlas of the Th-Ar spectrum covering selected regions in the range 1000–2500 nm. They established wavelength standards using the McMath 1 m laboratory Fourier Transform Spectrometer (FTS) at the US National Solar Observatory at Kitt Peak. However, the density of lines in their FTS spectra was insufficient in many regions for deriving dispersion solutions. They augmented their atlas by using blocking filters to observe selected regions with the Phoenix grating spectrograph at Kitt Peak. As a result, their list of about 500 lines contains significant gaps in wavelength coverage.

More recently, an analysis of the IR spectrum of a Th-Ar lamp was provided by Engleman et al. (2003). Their list contains more than 5000 lines derived from observations with the McMath FTS. They used a water-cooled demountable HCL operated at 320 mA with a continuous flow of argon at a pressure of 290 Pa (2.2 torr). This lamp produced a very rich Th spectrum, but it is

TABLE 1
SUMMARY OF PREVIOUS WORK ON Th-Ar HCLs (HCLs)

Reference	Wavelength (nm)	Source	Current	Instrument	Calibration
Palmer & Engleman (1983).....	278–1350	Commercial Th-Ne HCL	75 mA	FTS	Ne 1 lines
Hinkle et al. (2001)	1000–2500	Commercial Th-Ne HCL	14 mA	FTS & Echelle	Th, Ne lines
	Selected regions				Various references
Engleman et al. (2003).....	1090–5560	Water-cooled Th-Ar HCL,	320 mA	FTS	Unpublished list of Whaling et al. (2002)
Lovis & Pepe (2007).....	378–692	Commercial Th-Ar HCL	9 mA	Echelle	Palmer & Engleman (1983)

not well-suited for operations at an astronomical facility. Because of the different excitation conditions, line intensities in the demountable lamp are very different from low-current commercially available lamps. Although the spectrum from the high current lamp is significantly different from commercial Th-Ar lamps, the line list can be used to identify lines in low-current spectra.

The intrinsic properties of the Th-Ar HCL and the experience already gained in previous studies encouraged us to undertake the work necessary to establish the commercial Th-Ar lamp as a calibration source for CRIRES.

2. CRIRES

CRIRES is a cryogenic, IR echelle spectrograph designed to provide a resolving power $\lambda/\Delta\lambda$ of 100,000 between 950 and 5000 nm. The instrument was installed at the Nasmyth focus B of the 8 m VLT unit telescope 1 (Antu) in 2006 June and has been available to the scientific community since 2007 April. A ZnSe prism is used as predisperser. A curvature-sensing adaptive optics system feed is employed to minimize slit losses and to provide spatial resolution along the slit that approaches the diffraction limit at 1 μm . An echelle grating with a blaze angle of 63.5° and a groove density of 31.6 lines mm^{-1} provides dispersion in the main spectrograph.

CRIRES is equipped with a detector system that consists of a mosaic of four Aladdin III 1k \times 1k InSb-arrays.³ This provides an effective focal plane array of about 5000 \times 500 pixels, in order to maximize the free spectral range covered in each exposure. CRIRES is designed for stability and high throughput. A detailed description of the instrument is given in Käufel et al. (2004).

It is interesting to note that with the addition of CRIRES it is possible for observers at ESO to study the spectrum of an astronomical target at a resolution of 100,000 all the way from 306 to 5000 nm using only two spectrographs, UVES and CRIRES. The establishment of Th-Ar wavelength standards in the near-IR makes it possible to perform the wavelength calibration for this entire spectral region with a single standard source.

The data reduction pipeline makes use of a physical instrument model to support wavelength calibration. We know from the design process that even sophisticated spectrographs can be accurately modeled (Ballester & Rosa 1997, 2004). For this purpose we have developed a model kernel that is a fast, simplified ray-trace code. The speed with which this streamlined model can be solved makes it suitable for iterative evaluation for many different wavelengths and slit positions. Most importantly, parameters describing the configuration of the optical components can be optimized using wavelength data for a well-understood calibration source with a rich spectrum. The optimization code invokes the model kernel repeatedly, adjusting the parameters until the known spectral features are placed in the same locations on the detector as measured in the calibration data. Details of this approach and results from its application to the Space Telescope Imaging Spectrograph (STIS) are described in Bristow et al. (2006) and Kerber et al. (2006).

3. LABORATORY WORK

Spectra of the Th-Ar lamps were recorded on the NIST 2 m FTS. The FTS (Nave et al. 1997) was fitted with a CaF₂ beamsplitter, silver coated mirrors, and InSb detectors. The optimum alignment of the spectrometer depends slightly on wavelength. Hence, two

interferograms optimized for different wavelength regions were recorded; the first for wavelengths between 800 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.

The Th-Ar HCL and a calibrated tungsten ribbon lamp that served as a radiometric standard were mounted on a foreoptics system that was purged with dry, CO₂-free air to avoid IR absorption. This foreoptics system incorporated a remotely actuated rotating mirror that was used to switch between the two light sources and a concave mirror that imaged either source to the entrance aperture of the FTS.

To obtain good signal-to-noise ratio, many interferograms were co-added for each spectrum, corresponding to data acquisition times of up to 20 hr. For each hollow cathode spectrum a spectrum of the radiometric standard 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.

Spectra of three types of Th-Ar lamps were recorded at NIST. The first lamp had a Th cathode with a closed end. Previous spectra of similar lamps recorded on the McMath FTS had a high continuum background in the region above 2500 nm. In order to test whether radiation from the hot back surface of the Th cathode was a significant source of this continuum radiation, a second lamp was observed that contained a see-through cathode, that is, a cathode with both ends open. These two lamps had quartz windows that absorbed radiation at wavelengths longer than 3500 nm. A third lamp with a closed-end cathode and a sapphire window was also observed. This lamp produced a good spectrum up to 5500 nm. The pressure in all three lamps was 500 Pa (3.75 torr). The lamps were run at a current of 20 mA. No significant improvement in signal-to-noise ratio was observed when the current was increased to 30 mA.

The interferograms were transformed with the program Xgremlin (Nave et al. 1997). Careful attention was paid to the phase correction of the spectra, particularly when the alignment of the instrument was optimized for wavelengths above 2 μm . Voigt profiles were fitted to all the lines in the resulting spectra to obtain wavelengths, intensities, and line widths.

4. WAVELENGTH CALIBRATION

To obtain absolute accuracy better than a few parts in 10⁶ from FT spectra, it is necessary to determine a multiplicative correction to the wavenumber scale from accurately known internal standard lines. This correction is often specified by a factor, k_{eff} , such that

$$\sigma_c = (1 + k_{\text{eff}})\sigma_u, \quad (1)$$

where σ_c is the calibrated wavenumber and σ_u is the uncalibrated wavenumber.

In planning this work we expected to use the spectrum of Ar II for the absolute calibration. IR lines of Ar II, reported with an uncertainty of 0.0002 cm^{-1} by Whaling et al. (1995), have been widely used as standards for spectra observed in high-current HCLs with Ar carrier gas. In the spectra of our low-current commercial lamps, however, lines of Ar II were too weak to be used as standards.

Instead we used seven Th I lines (DeGraffenreid & Sansonetti 2002) measured by optogalvanic laser spectroscopy in a low-current Th-Ne HCL. These lines, which lie between 13,360 and 14,400 cm^{-1} , have a reported uncertainty of 0.0002 cm^{-1} (1.4 parts in 10⁸). The calibration derived from these lines (Fig. 2)

³ Identification of commercial equipment does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the equipment identified is necessarily the best available for the purpose.

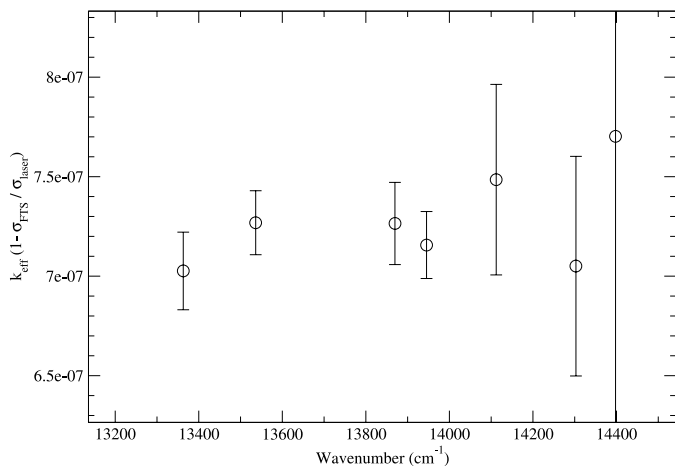


FIG. 2.—Value of the wavenumber correction factor k_{eff} obtained using laser measurements of seven Th lines (DeGraffenreid & Sansonetti 2002).

gives a k_{eff} value of $(7.20 \pm 0.14) \times 10^{-7}$. The error bars (one standard uncertainty) are dominated by the low signal-to-noise ratio in the FT spectrum at the extreme edge of the bandpass. Because the calibration lines are limited to a narrow region at the short-wavelength end of our spectra, it is desirable to have some check on the results in the long-wavelength region to ensure that the value of k_{eff} is actually constant across the region of interest as expected from the theory of FT spectroscopy. Comparison with results of Engleman et al. (2003) provides such a check, as shown by the comparison detailed in § 5. The spectrum optimized for wavelengths above 2000 nm was calibrated from the spectrum optimized for the region 800–2000 nm. The incremental contribution of this bootstrap procedure to the uncertainty in k_{eff} for the long-wavelength region is only 1.1×10^{-9} .

5. RESULTS

Figure 3 shows an overview of the spectrum obtained from the lamp with the sapphire window, covering the range 715–5000 nm ($14,000$ – 2000 cm^{-1}). Beyond 2500 nm, continuum emission from the hot cathode becomes noticeable (Fig. 3). Its intensity is strongly dependent on the operating current, but at all currents it is much weaker than the spectral lines, and thus, accurate wavenumbers for the lines could be measured. Although spectra recorded with the see-through cathode had a much lower continuum than those recorded with the other lamps, the overall intensity and signal-to-noise ratio in these spectra was much lower. Our best spectra were obtained with the lamp having a sapphire window and closed-end cathode. The results we report are based on the spectra from that lamp.

5.1. Wavelength Standards

Accurate wavelengths have been determined for about 2500 spectral lines of Th and Ar in the range 900–5408 nm. In general the density of lines drops significantly toward longer wavelengths. The region between 700 and 2500 nm has the highest density of lines, as can be seen from Figure 4. For CRIRES settings this distribution is more satisfactory than the figure might suggest, since the coverage for CRIRES orders increases significantly with wavelength, from about 13.5 nm wide at 1000 nm to ≈ 50 nm wide at 2600 nm and 130 nm at 5000 nm. For example, setting 56/0/n with a central wavelength of ≈ 1009.6 nm contains 56 lines in total, 47 lines net; that is accounting for the gaps in the detector mosaic. Very similar values are available at 1550 nm (setting 37/1/i): 50 (48 net). These numbers drop to 33 (26 net) at 1845 nm (31/1/n) and 11 net at 2570 nm (22/0/n).

Table 2 provides a sample of the line list covering a section of the spectrum between 1315 and 1330 nm. The full line list, containing over 2400 lines, is available in electronic form (see § 5.4).

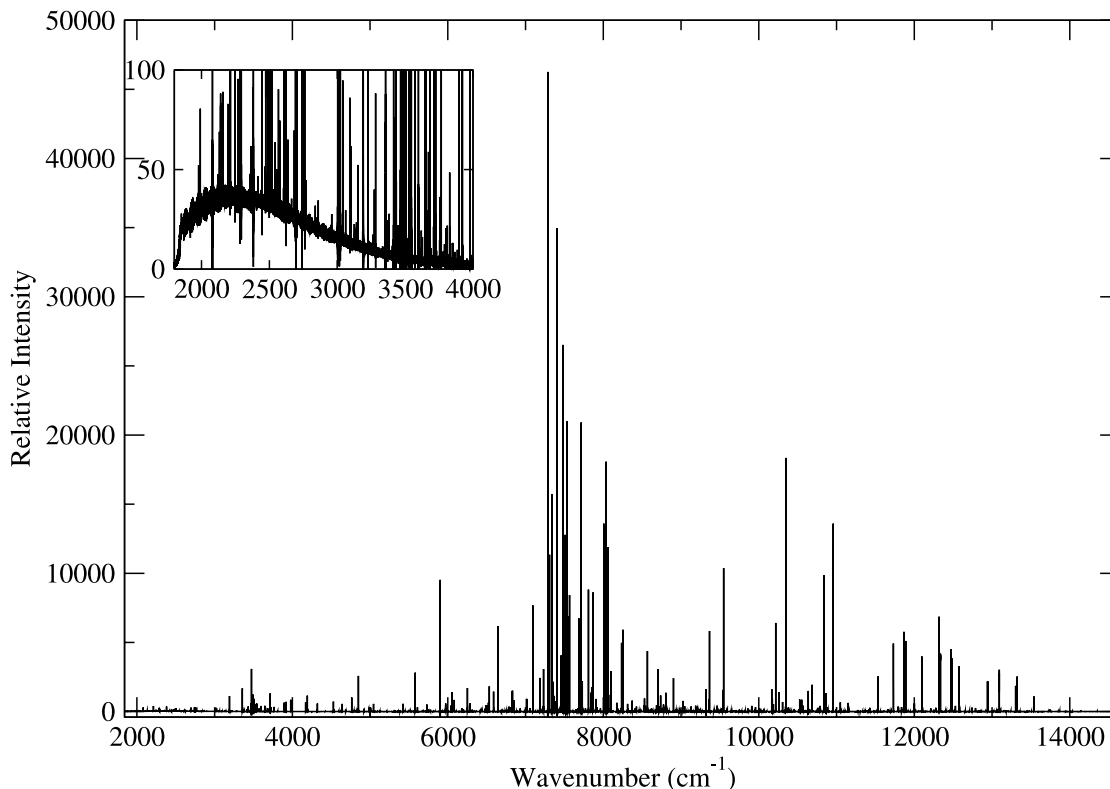


FIG. 3.—Overview spectrum of a Th-Ar lamp. Wavelength range is 715–5000 nm ($14,000$ – 2000 cm^{-1}). The line intensity is given in arbitrary units. Longward of 2500 nm ($<4000 \text{ cm}^{-1}$) thermal emission from the hot cathode introduces a continuum in the otherwise pure emission-lines spectrum.

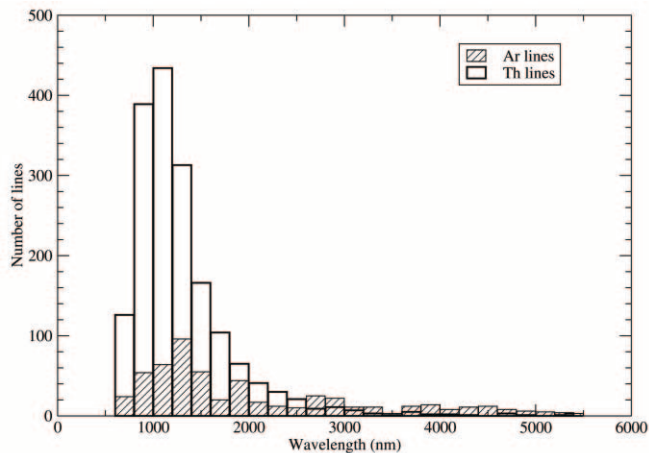


FIG. 4.—Histogram of the wavelength distribution of Th and Ar lines.

The wavenumber is given in column (1), with the corresponding vacuum wavelength in column (11). The wavenumbers and wavelengths are strictly valid only for a Th-Ar hollow cathode similar to the one used, operated at a current of 20 mA. However, wavelengths of Th I, Th II, and Ar II lines show little sensitivity to operating conditions, and our results can thus be reliably applied to lamps run at lower currents (see § 5.2). Low-excitation lines of Ar I are also reliable, but high-excitation lines (upper level higher than $115,000 \text{ cm}^{-1}$) may show large wavelength shifts when the pressure or current in the lamp is different from ours; these lines have an asterisk in column (13) of Table 2.

The signal-to-noise ratio is given in column (3) and the full width at half-maximum of the line in units of 10^{-3} cm^{-1} in column (4). The widths provide a verification of the identification of the lines, as Ar lines are roughly 2.6 times wider than Th lines. The signal-to-noise ratio and width for each line have been used to estimate a statistical uncertainty for the wavenumber and wavelength using the formula of Brault (1987). This statistical uncertainty has been combined in quadrature with the estimated calibration uncertainty of $2 \times 10^{-8} \times \text{wavenumber}$ to obtain the total wavenumber uncertainty (one standard deviation) in column (2) and corresponding wavelength uncertainty in column (12). The uncertainty of the strongest lines varies with wavelength from about $1 \times 10^{-4} \text{ nm}$ near 5000 nm to as low as $1.5 \times 10^{-5} \text{ nm}$ near 700 nm. Above 2500 nm, about 22% of the lines have uncertainties lower than 10^{-4} nm , but the percentage rises to 61% below 2500 nm. CRIRES provides a resolution between $4.5 \times 10^{-3} \text{ nm}$ (at 950 nm) and $25 \times 10^{-3} \text{ nm}$ (at 5000 nm) per pixel. The above uncertainties for the strong lines correspond to less than 1/100th of a CRIRES pixel at all wavelengths. Hence, the accuracy of the line list will ensure that quantitative science with CRIRES can be performed at maximum precision. Currently, the accuracy achieved is determined by repeatability of some of CRIRES's moveable components. Current modifications aim to optimize the performance of CRIRES in this respect (see § 5.3).

The integrated intensity of each line is given in column (5). It has been adjusted for the response of the spectrometer using the calibration spectra taken with the tungsten standard lamp. Since intensities are highly dependent on the running conditions of the lamp, they should be used with caution when comparing our results to those obtained under other operating conditions. The dynamic range is about 30,000, which can be accommodated in a standard CRIRES wavelength calibration exposure of about 2 minute duration (see § 5.3 for details). The identification of the line is in columns (6)–(10). Identifications of Ar lines were taken

from Whaling et al. (1995, 2002) and Th lines from Palmer & Engleman (1983) and Engleman et al. (2003). We identified some additional lines of Ar using spectra of electrodeless discharge lamps or HCLs taken from archival spectra in the National Solar Observatory Digital Library (2007). In addition, five impurity lines of Ca I were observed.

5.2. Comparison with Th and Ar Data from the Literature

Figure 5 shows a comparison of our measurements with those of Engleman et al. (2003). For Th I there is excellent agreement with a weighted mean relative deviation of $(6 \pm 2) \times 10^{-9}$. Given the significant difference in operating conditions (choice of fill gas, its pressure and operating current) it is important to note that the Th lines are very insensitive to the actual conditions in the discharge.

Ar I lines also show good agreement at larger wavenumbers, but poor agreement below about 5000 cm^{-1} . The reason for these discrepancies can be seen in Figure 6, where the relative deviation is plotted as a function of the energy of the upper level of the Ar I transition. The hollow cathode used by Engleman et al. (2003) runs at a lower pressure and much higher current than ours. High-excitation levels may be particularly subject to pressure- and field-induced shifts. Hence, although there is good agreement between our results and Engleman et al. (2003) for lines from low-excitation levels, there is a systematic difference between the two results for higher excitation lines. Lines with upper levels in the $5s$ configuration are an exception to this general rule. They are systematically shifted to lower wavenumbers by about 2×10^{-7} as compared to other lines having upper levels with similar energies.

Our data overlap the long-wavelength end of Palmer & Engleman (1983), and a comparison between our measurements and their atlas is given in Figure 7. The solid circles represent data where the uncertainty in the NIST measurements is less than 5 parts in 10^8 . The weighted mean is $(-2.75 \pm 0.10) \times 10^{-8}$, in good agreement with the difference of $(-2.4 \pm 0.4) \times 10^{-8}$ found from seven lines by DeGraffenreid & Sansonetti (2002).

Figure 8 shows a comparison of our Ar I lines with those of Whaling et al. (2002). The scatter is large for lines with highly excited upper levels, but the wavenumbers of low-excitation lines are systematically greater than ours over the entire spectral region by about $(1.07 \pm 0.04) \times 10^{-7}$, a difference of 2.6 standard deviations. Our results agree much better with an unpublished list from the same authors (W. Whaling 1997, private communication) that was distributed in the mid-1990s, differing by only 3×10^{-8} . The systematic offset between our results and Whaling et al. (2002) is particularly well defined in the short-wavelength region, where our calibration lines are concentrated; therefore, it seems unlikely that a calibration error in our work can be responsible for the discrepancy. We conclude that the unpublished Ar I list is more reliable than that in Whaling et al. (2002), despite the fact that the two lists of Ar I lines are based on the same spectra. This observation supports the results of Sansonetti (2007), who suggested that the wavenumbers of Whaling et al. (2002) should be corrected by a multiplicative factor of 0.999999933.

The Ar II measurements of Whaling et al. (1995) are based on the same spectra as the Ar I measurements of Whaling et al. (2002). Although Ar II lines are weak in our spectra, other spectra recorded in our laboratory indicate that the list in Whaling et al. (1995) is reliable.

5.3. Operational Aspects

In addition to the wavelength calibration measurements made at NIST, we made lower resolution observations of the Th-Ar

TABLE 2
SAMPLE OF THE LINE LIST DERIVED FROM THE Th-Ar SPECTRA

Wavenumber (cm ⁻¹) (1)	Uncertainty (0.001 cm ⁻¹) (2)	S/N (3)	FWHM (0.001 cm ⁻¹) (4)	Intensity (5)	Species (6)	Lower Level (7)	Lower J^a (8)	Upper Level (9)	Upper J^a (10)	Vacuum Wavelength (nm) (11)	Uncertainty (0.001 nm) (12)	Notes ^b (13)
5299.2082.....	0.3	19	6	208	Th I	16346	4	21645	4	1887.07439	0.09	
5303.3899.....	0.6	7	6	114	Th I	21077	5	26380	5	1885.5864	0.2	
5314.34080.....	0.11	232	7	2790	Th I	16783	4	22098	4	1881.70093	0.04	
5317.0165.....	0.6	8	8	111	Th I	16351	0	21668	1	1880.7540	0.2	
5325.4997.....	0.3	15	7	181	Th II	36583	7/2	41909	9/2	1877.75806	0.11	
5326.5979.....	1.0	7	17	300	Ar I	114862	0	120188	1	1877.3709	0.4	*
5328.0505.....	1.2	7	23	330	Ar I	117151	1	122479	1	1876.8591	0.4	*
5333.29983.....	0.16	59	19	1950	Ar I	111818	1	117151	1	1875.01178	0.06	*
5337.3434.....	0.6	8	6	90	Th I	10526	3	15863	2	1873.59128	0.20	
5354.9129.....	0.3	15	8	211	Th I	31271	5	36625	5	1867.44402	0.12	
5358.3935.....	0.5	8	6	103	Th I	22163	4	27521	4	1866.23100	0.19	
5359.96222.....	0.18	31	7	380	Th I	19039	2	24399	3	1865.68479	0.06	
5362.8603.....	1.6	6	32	460	Ar I	117151	1	122514	1	1864.6766	0.6	*
5365.56456.....	0.12	114	18	3910	Ar I	111818	1	117184	2	1863.73678	0.04	*
5373.582.....	2.6	4	38	260	Ar II	206397	[4]	211771	[5]	1860.9560	0.9	
5374.3424.....	1.1	4	7	69	Th I	2869	3	8243	2	1860.6928	0.4	
5376.0735.....	0.3	21	8	275	Th I	18614	1	23990	2	1860.09362	0.09	

NOTE.—Table 2 is published in its entirety in the electronic edition of the *Astrophysical Journal Supplement*. A portion is shown here for guidance regarding its form and content.

^a Value in square brackets refers to K in jK coupling.

^b An asterisk (*) denotes lines unsuitable as wavelength standards.

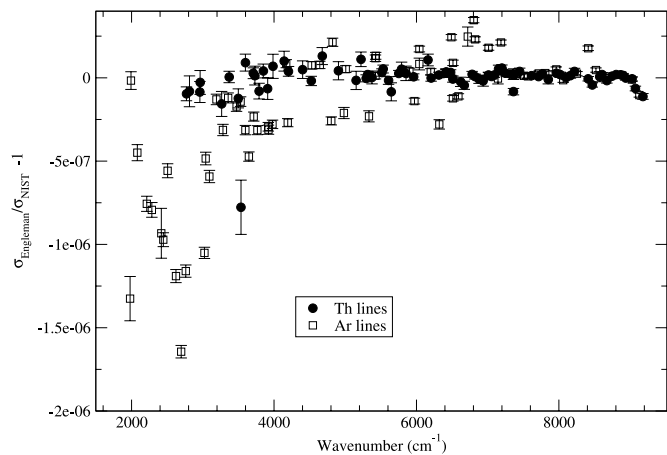


FIG. 5.—Comparison of this work with the values found by Engleman et al. (2003). The Th lines agree very well but the Ar lines show increasing scatter at lower wavenumbers. The error bars represent one standard uncertainty of our data.

HCL using a commercial FTS at ESO. The lamp was operated at nine different currents ranging from 4 to 20 mA. The intensity of the Th lines was found to be significantly enhanced at higher currents because of the increased sputtering efficiency. The distinctly different behavior of the metal and gas lines provides confirming evidence for the line identifications given in our line list. Details of the current dependent observations are reported in Kerber et al. (2007).

Based on these findings one can devise ways to optimize the use of a Th-Ar lamp for CRIRES calibration. Currently, the Th-Ar lamp is run at 10 mA and attenuated by a filter which has been chosen so that the strongest line at 1372.23 nm is not saturated with 1 s exposure time in order to protect the detector from persistence effects. ESO is currently working on a modified setup providing variable attenuation which will make it possible to optimize the output of the lamp for each wavelength setting individually. In addition, we plan to operate the lamp at somewhat higher currents (e.g., 15 mA) for observations in longer wavelength regions where the intensity and spectral density of Th lines are intrinsically lower. This may result in a reduced lifetime of the lamp, but this will be an acceptable drawback given the improved science performance. Results from observations of Th-Ar lamps in CRIRES operational tests will be reported elsewhere.

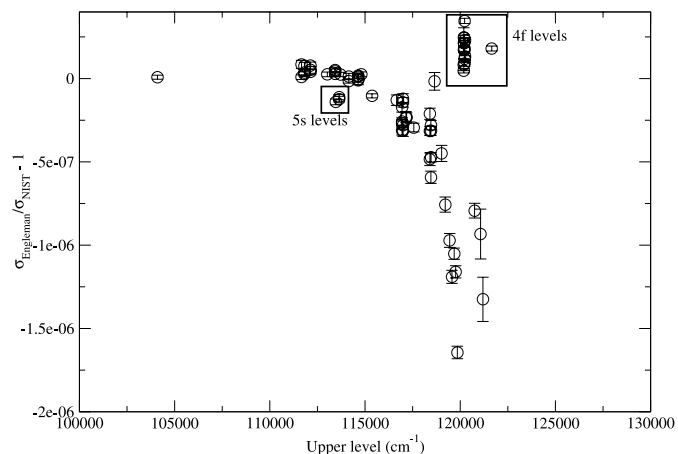


FIG. 6.—Comparison of this work with the values found by Engleman et al. (2003) as a function of the energy of the upper level of the Ar I transition. The error bars represent one standard uncertainty of our data. This analysis reveals that the offsets are dependent on the excitation of the upper level.

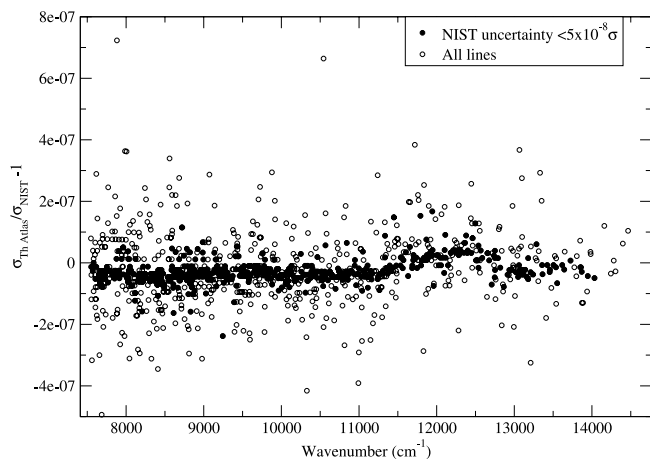


FIG. 7.—Comparison of this work with the Th lines in Palmer & Engleman (1983). Error bars have been omitted for clarity. The solid circles represent the best NIST data with relative uncertainties of less than 5×10^{-8} (0.0005 cm^{-1} at $10,000 \text{ cm}^{-1}$). The weighted mean of this smaller set is $(-2.75 \pm 0.10) \times 10^{-8}$.

5.4. Availability of the Data through the Virtual Observatory (VO)

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. Two IVOA standards are of particular relevance for Th-Ar wavelength standards: the Spectrum Data Model (McDowell et al. 2007) and the Simple Spectral Access Protocol (Tody et al. 2007). In the case of laboratory data, metadata are best created at the time when the actual laboratory work is done 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. The data will be made available through the NIST Physical Reference Data Web site⁴ and the ESO instrument page for CRIRES.⁵

⁴ Available online at <http://physics.nist.gov>.

⁵ See <http://www.eso.org/instruments/crides/>.

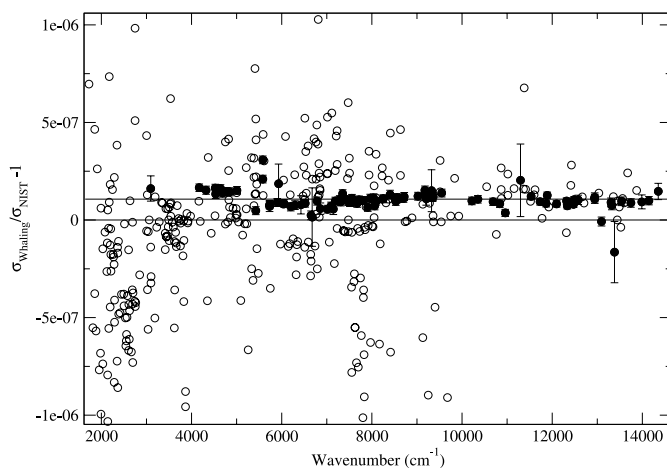


FIG. 8.—Comparison of our wavenumbers for Ar I with those of Whaling et al. (2002). The solid circles represent lines with an upper excitation of less than $115,000 \text{ cm}^{-1}$ that are not from the 5s configuration. The error bars represent one standard uncertainty of our data, but have been omitted from the full data set for clarity.

We also plan to make the Th-Ar spectrum available as an atlas in electronic form.

6. SUMMARY

We performed laboratory measurements using the NIST FTS to establish wavelengths for more than 2400 lines in the range 900–4500 nm in the spectrum of a commercial Th-Ar hollow cathode lamp. This line list serves as calibration reference data for the wavelength calibration of ESO's high-resolution IR spectrograph CRIRES by means of a physical model of CRIRES, which is included in the science data reduction pipeline.

Th-Ar HCLs hold the promise of becoming a generally applicable source of standards for wavelength calibration in near-IR (<2500 nm) astronomy, providing a high density of sharp well-characterized emission lines with the ease and efficiency of operation of a commercial discharge lamp. With this development, wavelength calibration for near-IR astronomy will no longer

be dependent on atmospheric features. The existence of a well-characterized calibration lamp will make it possible to use an external standards approach similar to the highly successful wavelength calibration procedures used in UV and visible astronomy. Only with such an approach can one support the quantitative science envisaged for the next generation of extremely large telescopes and their instruments.

We thank R. Engleman for providing his Th-Ar line lists in electronic form. We gratefully acknowledge financial support from the European Southern Observatory (ESO) and the European Space Agency (ESA). It is a pleasure to thank D. Macchetto (ESA, STScI) for his support. We also thank all members of the CRIRES team for the good collaboration. Special thanks go to Paul Bristow, Sandro D'Odorico, and B. Wolff (ESO).

REFERENCES

- Abrams, M. C., Davis, S. P., Rao, M. L. P., Engleman, Jr., R., & Brault, J. W. 1994, *ApJS*, 93, 351
- Ballester, P., & Rosa, M. R. 1997, *A&AS*, 126, 563
- . 2004, in *ASP Conf. Proc. 314, Astronomical Data Analysis Software and Systems (ADASS) XIII*, ed F. Ochsenbein, M. G. Allen, & D. Egret (San Francisco: ASP), 481
- Brault, J. W. 1987, *Mikrochim. Acta*, 3, 215
- Bristow, P., Kerber, F., & Rosa, M. R. 2006, in *HST Calibration Workshop*, ed. A. Koekemoer, P. Goudfrooij, & L. Dressel (Greenbelt: NASA), 299
- Chand, H., Srianand, R., Petitjean, P., & Aracil, B. 2004, *A&A*, 417, 853
- Chand, H., Srianand, R., Petitjean, P., Aracil, B., Quast, R., & Reimers, D. 2006, *A&A*, 451, 45
- DeGraffenreid, W., & Sansonetti, C. J. 2002, *J. Opt. Soc. Am. B*, 19, 1715
- D'Odorico, S., Ghigo, M., & Ponz, D. 1987, *ESO Scientific Report (Garching: ESO)*
- D'Odorico, S., et al. 2004, *Proc. SPIE*, 5492, 220
- Engleman, R., Jr., Hinkle, K. H., & Wallace, L. 2003, *J. Quant. Spectr. Rad. Trans.*, 78, 1
- Hanuschik, R. W. 2003, *A&A*, 407, 1157
- Hinkle, K. H., Joyce, R. R., Hedden, A., Wallace, L., & Engleman, R., Jr. 2001, *PASP*, 113, 548
- Käufel, H.-U., et al. 2004, *Proc. SPIE*, 5492, 1218
- Kerber, F., Bristow, P., & Rosa, M. R. 2006, in *HST Calibration Workshop*, ed. A. Koekemoer, P. Goudfrooij, & L. Dressel (Greenbelt: NASA), 309
- Kerber, F., Nave, G., Sansonetti, C. J., Bristow, P., & Rosa, M. R. 2007, in *ASP Conf. Ser. 364, The Future of Photometric, Spectrophotometric and Polarimetric Standardization*, ed. C. Sterken (San Francisco: ASP), 461
- Lovis, C. Pepe, F. 2007, *A&A*, 468, 1115
- Marcy, G. W., & Butler, R. P. 1992, *PASP*, 104, 270
- Mayor, M., et al. 2003, *Messenger*, 114, 20
- McDowell, J., et al. 2007, *Spectrum Data Model (Ver. 1.01, 15 May 2007)*, <http://www.ivoa.net/Documents/latest/SpectrumDM.html>
- Mickelson, M. E., Steyert, D. W., Sirota, J. M., & Reuter, D. C. 2001, *BAAS*, 33, 1141
- Murphy, M. T., Webb, J. K., & Flambaum, V. V. 2003, *MNRAS*, 345, 609
- Murphy, M. T., Flambaum, V. V., Webb, J. K., Dzuba, V. V., Prochaska, J. X., & Wolfe, A. M. 2004, *Lecture Notes Phys.*, 648, 131
- Murphy, M. T., Tzanavaris, P., Webb, J. K., & Lovis, C. 2007, *MNRAS*, 378, 221
- National Solar Observatory Digital Library (online). 2007, http://diglib.nso.edu/nso_user.html
- Nave, G., Sansonetti, C. J., & Griesmann, U. 1997, *Fourier Transform Spectroscopy: Methods and Applications (Washington: OSA)*
- Osterbrock, D. E., Fulbright, J. P., & Bida, T. A. 1997, *PASP*, 109, 614
- Osterbrock, D. E., Fulbright, J. P., Martel, A. R., Keane, M. J., Trager, S. C., & Basri, G. 1996, *PASP*, 108, 277
- Palmer, B. A., & Engleman, Jr., R. 1983, *Los Alamos National Laboratory Report, LA-9615*
- Peik, E., Lipphardt, B., Schnatz, H., Schneider, T., Tamm, C., & Karshenboim, S. G. 2005, *Laser Physics*, 15, 1028
- Reader, J., Acquista, N., Sansonetti, C. J., & Sansonetti, J. E. 1990, *ApJS*, 72, 831
- Rousselot, P., Lidman, C., Cuby, J.-G., Moreels, G., & Monnet, G. 2000, *A&A*, 354, 1134
- Sansonetti, C. J. 2007, *J. Res. Natl. Inst. Stand. Technol.* 112, 297
- Sansonetti, C. J., Blackwell, M. M., & Saloman, E. B. 2002, *Phys. Scr. T.*, 100, 120
- . 2004, *J. Res. NIST*, 109, 371
- Sansonetti, C. J., & Greene, M. B. 2007, *Phys. Scr.*, 75, 577
- Sansonetti, C. J., Kerber, F., Reader, J., & Rosa, M. R. 2004, *ApJS*, 153, 555
- Tody, D., et al. 2007, *Simple Spectral Access Protocol (Version 1.01, 29 May 2007)*, <http://www.ivoa.net/Documents/latest/SSA.html>
- Webb, J. K., Flambaum, V. V., Churchill, C. W., Drinkwater, M. J., & Barrow, J. D. 1999, *Phys. Rev. Lett.*, 82, 884
- Whaling, W., Anderson, W. H. C., Carle, M. T., Brault, J. W., & Zarem, H. A. 1995, *J. Quant. Spectrosc. Radiat. Transfer*, 53, 1
- Whaling, W., Anderson, W. H. C., Carle, M. T., Brault, J. W., & Zarem, H. A. 2002, *J. Res. NIST*, 107, 149